An improved SPH method for multi-phase simulations

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ABSTRACT: In this work a new SPH model for simulating interface flows is presented. This new model is an extension of the formulation discussed in Colagrossi and Landrini (2003), and shows strong similarities with one proposed by Hu and Adams (2006) to study multiphase flow. The main difference between these two models is that the present formulation allows for simulating multiphase flows together with the presence of a free surface.

The new formulation is validated on test cases for which reference solutions are available in literature. A Rayleigh-Taylor instability is first studied. Then, the rise of an air bubble in a water column is investigated. Finally, the model capabilities are illustrated on the case of a drop of a heavy fluid entering a tank filled with water.

1 INTRODUCTION

Multiphase flows play a significant role in numerous engineering applications characterized by strong dynamics of the flow making the SPH scheme a valuable candidate as simulation method, e.g. flows involved in mixing/separation devices, engines, propellers with cavitation, etc. Even for free-surface water flows of strong dynamics (i.e. including jets, sprays, impacts, free-surface reconnections, etc.) usually simulated using one-phase SPH models, the air phase can have a large influence on the water flow evolution and on subsequent loads on structures.

Although the classical SPH formulation succeeds in correctly simulating one-phase flows, the presence of an interface and the physical conditions associated make a stable two-phase formulation more difficult to derive. The main issue is the estimation of the ratio between pressure gradient and density in the momentum equation in the region near the interface, where the density is discontinuous when crossing the interface. Actually, the SPH scheme relying on a smoothing, accuracy is lost when a particle has its compact support which intersects the interface, namely the density of the other phase spuriously influences the evaluation of acceleration of the concerned particle.

In the present work a new SPH model for simulating interface flows is presented. This new model is an extension of the formulation discussed in Colagrossi and Landrini (2003) and it is based on the variational approach introduced by Bonet and Lok (1999). The SPH formulation presented here shows strong similarities with one proposed by Hu and Adams (2006) to study multiphase flows. The main difference between these two models is that the present formulation allows for simulating multiphase flows together with the presence of a free surface (meaning here an interface without accounting for the (air) phase above it).

Further, in the present formulation a specific attention is paid to enhance the accuracy of the scheme, especially through the use of a Shepard kernel. This leads in particular to the derivation of an original variant of renormalization of the gradient of this kernel, which differs from the one usually associated in literature to this Shepard kernel.

The formulation is validated on test cases for which reference solutions are available in literature. After classical tests as the one of a droplet oscillating without gravity, more complex validation cases are simulated such as Rayleigh-Taylor instabilities, or an air bubble rising by gravity in a water column at rest. The last problem studied in the present work is the case of a droplet of a heavy fluid entering a tank filled with

water. The latter involves two different kinds of liquids and the free-surface dynamics, namely the droplet impact generates free-surface gravity waves which radiate far away.

2 PHYSICAL MODEL

In the present work we model the Navier-Stokes equations for a set of viscous newtonian fluids. The fluid domain Ω composed by different fluids $\mathcal{A}, \mathcal{B}, \ldots$. The boundaries of the domain Ω are constituted by a free-surface $\partial \Omega_F$ and by solid boundaries $\partial \Omega_B$.

The conservation of the momentum in Ω is written in lagrangian formalism as

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\frac{\nabla p}{\rho} + \mathbf{F}^{v} + \mathbf{f}$$
(1)

where \mathbf{u} , p and ρ are respectively, the velocity, the pressure and the density fields, while \mathbf{f}_V , and \mathbf{f} represent the viscous and the external body forces (here the force field $\rho \mathbf{f}$ is the gravity force $\rho \mathbf{g}$).

The spatial position of the generic material point **X**, at time t will be indicated through $\mathbf{x}(t)$, in other words

$$\mathbf{x}(t) = \phi(\mathbf{X}, t) \tag{2}$$

where ϕ is the map which link the lagrangian coordinates **X** with the physical ones **x**.

Weakly compressible fluids are considered. Under this assumption the pressure field can be directly linked to the density field neglecting the dependency on the specific entropy S. Therefore the state equation reduces to $p = f(\rho)$. Different choices are possible for the state equation (see Molteni *et al.* (2007)), here the Tait equation is considered

$$p = \frac{c_0^2 \rho_0}{\gamma} \left[\left(\frac{\rho}{\rho_0} \right)^{\gamma} - 1 \right] \tag{3}$$

where c_0 is the speed of sound in the condition $\rho = \rho_0$. From equation (3) derives that the speed of sound follows a polytropic law with a characteristic exponent γ .

Gaseous phases as well as liquid ones will be treated through the equation of state (3). As a consequence of the weakly compressible hypothesis the speed of sound c_0 is at least ten times greater than the maximum fluid velocity, therefore the inequality

$$c_0 > 10 \max(|\mathbf{u}|)_{\Omega} \tag{4}$$

is always satisfied. Condition (4) guarantees that the density variations are always smaller than $1\%\rho_0$. Nonetheless, for computational and numerical reasons it is not possible to adopt the real speed of sound of the treated liquid phases (see *e.g* Colagrossi (2005)). The condition (4) on the Mach number $M = |\mathbf{u}|/c < 0.1$ is thus satisfied by choosing a fictitious speed of sound (see Molteni *et al.* (2007)). The use of a state equation for the liquid phase allows to avoid the solution of the Poisson equation leading to a simple and efficient algorithm. The drawback of this model lies in the pressure field which can be affected by numerical errors and instabilities.

The continuity equation is written as

$$\frac{\mathrm{D}\log\mathcal{J}}{\mathrm{D}t} = \mathrm{div}(\mathbf{u}); \qquad \mathcal{J} = \frac{\rho_0(\mathbf{X})}{\rho(\mathbf{X},t)} = \frac{v(\mathbf{X},t)}{v_0(\mathbf{X})}$$
(5)

where the Jacobian determinant \mathcal{J} is linked to the map ϕ (see eq. 2) through

$$\mathcal{J} = det(\mathbf{F}) \qquad ; \qquad \mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$$

Therefore the continuity equation (5) prescribes that \mathcal{J} is equal to the ratio between the initial density $\rho_0(\mathbf{X})$ and the actual one $\rho(\mathbf{X}, t)$ of the generic material point \mathbf{X} at the time instant t. Obviously \mathcal{J} can be also read as the ratio between the specific volume $v(\mathbf{X}, t)$ and the initial one $v_0(\mathbf{X})$.

The continuity equation is written in term of \mathcal{J} instead of ρ for numerical reasons which will be explained further.

Summarizing, the governing equations used in this work for a set of different weakly compressible fluids $\mathcal{X} = (\mathcal{A}, \mathcal{B}, \ldots)$ are

$$\begin{cases}
\frac{D \log \mathcal{J}}{Dt} = \operatorname{div}(\mathbf{u}); v(\mathbf{X}) = \mathcal{J}(\mathbf{X}, t) v_0(\mathbf{X}); \rho(\mathbf{X}) = \frac{1}{v(\mathbf{X})} \\
p(\mathbf{X}) = \frac{c_{0\mathcal{X}}^2 \rho_{0\mathcal{X}}}{\gamma_{\mathcal{X}}} \left[\left(\frac{\rho(\mathbf{X})}{\rho_{0\mathcal{X}}} \right)^{\gamma_{\mathcal{X}}} - 1 \right]; \quad \forall \mathbf{X} \in \mathcal{X} \\
\frac{D \mathbf{u}}{Dt} = -\frac{1}{\rho} \nabla p + \mathbf{f}_V + \mathbf{f}(\mathbf{x}, t); \quad \frac{D \mathbf{x}}{Dt} = \mathbf{u}
\end{cases}$$
(6)

where \mathcal{X} indicates the generic fluid in the domain Ω composed by the fluids $\mathcal{A}, \mathcal{B}, \ldots$, therefore $\Omega = (\mathcal{A} \cup \mathcal{B} \cup \ldots)$.

3 NUMERICAL MODEL

3.1 Integral interpolation

In the SPH method, the fluid domain Ω is discretized in a finite number N of *particles* representing small volumes of fluid dV, each one with its own local mass m and other physical properties. In this context a generic field f is approximated at a generic position \vec{x} through the convolution sum

$$\langle f(\mathbf{x}) \rangle = \sum_{j} f_{j} W(\mathbf{x} - \mathbf{x}_{j}) dV_{j}$$
(7)

where f_j is the value of f associated to the generic particle j, dV_j is its volume and finally $W(\mathbf{x} - \mathbf{x}_j)$ is a kernel function. In practical SPH computations, the choice of the kernel function affects both the CPU requirements and the stability properties of the algorithm. In this work a renormalized Gaussian kernel is adopted

$$W(\mathbf{x} - \mathbf{x}_j) = W(r) = \frac{e^{-(r/h)^2} - e^{-(\delta/h)^2}}{2\pi \int_0^\delta r \left(e^{-(r/h)^2} - e^{-(\delta/h)^2}\right) dr}$$
(8)

where $r = \|\mathbf{x} - \mathbf{x}_j\|$ is the Euclidean distance between the particle j and the point \mathbf{x} . To make its support compact a cut-off radius δ is introduced, typically set equal to 3h as for the classical fifth-order B-spline support Monaghan (1992). h is called *smoothing length* and W becomes a delta Dirac function as h goes to zero.

The spatial derivatives of the field f evaluated at the particle positions can be estimated using the formula (7)

$$\langle \nabla f(\mathbf{x}) \rangle = \sum_{j} (\nabla f)_{j} W(\mathbf{x} - \mathbf{x}_{j}) dV_{j}.$$
(9)

After some manipulation (see e.g. Colagrossi (2005)) it is possible to move the gradient operator to the kernel and the previous formula can be approximated by

$$\langle \nabla f(\mathbf{x}) \rangle = -\sum_{j} f_{j} \nabla_{j} W(\mathbf{x} - \mathbf{x}_{j}) dV_{j} + f(\mathbf{x}) \sum_{j} \nabla_{j} W(\mathbf{x} - \mathbf{x}_{j}) dV_{j}$$
(10)

where ∇_j denotes the derivative with respect to \mathbf{x}_j . The second term of equation (10) is practically zero far from the free surface while it increases close to the free boundary; therefore this term acts as a boundary term. Equation (10) can be simply rearranged over the particle distribution as

$$\langle \nabla f(\mathbf{x}_i) \rangle = \sum_j (f_j - f_i) \nabla_i W(\mathbf{x}_i - \mathbf{x}_j) dV_j$$
(11)

where the antisymmetric property of the kernel $\nabla_j W(\mathbf{x}_i - \mathbf{x}_j) = -\nabla_i W(\mathbf{x}_i - \mathbf{x}_j)$ is used. Thanks to the difference $(f_j - f_i)$ this formula is null for a constant field for any particle distribution as prescribed by equation (9).

3.2 Present Formulation

In the present paper an SPH formulation based on the use of a Shepard kernel Belytschko *et al.* (1998) for the density evaluation is presented. The Shepard kernel has been used in Bonet and Rodriguez-Paz (2005) to evaluate the forces acting on the solid boundaries $\partial \Omega_B$ and to take into account the variation of the smoothing length, h, for problems characterized by strong compressibility. Here the solid boundaries are modelled through the ghost-particle technique, therefore there is no need for evaluating the boundary forces explicitly. Further, a constant smoothing length is used all over Ω since only weakly compressible effects are taken into account. The Shepard kernel is used here to model the presence of different fluids. The present SPH formulation shows similarities with the models derived in both Colagrossi and Landrini (2003) and Hu and Adams (2006).

The main idea of the present formulation is the following density evaluation

$$\langle \rho(\mathbf{x}) \rangle = \sum_{j \in \mathcal{X}} m_j W_j^S(\mathbf{x}); \quad W_j^S(\mathbf{x}) = \frac{W_j(\vec{x})}{c(\mathbf{x})}; \quad c(\mathbf{x}) = \sum_{k \in \mathcal{X}} W_k(\mathbf{x}) \, dV_k; \quad \forall \mathbf{x} \in \mathcal{X}$$
(12)

The Shepard kernel W^S is normalized by definition and therefore the identity

$$\sum_{j \in \mathcal{X}} W_j^S(\mathbf{x}) \, dV_j = 1 \qquad \forall \mathbf{x} \in \mathcal{X}$$
(13)

is always satisfied and does not depend on the number of particles.

The summation for calculating the term $c(\mathbf{x})$ is extended only to the particles belonging to the fluid containing the point \mathbf{x} . For this reason in (12) and in (13), the indices in the summation are restricted to the particles belonging to the generic fluid \mathcal{X} . In this way the discontinuities of the density field are treated explicitly.

Summarizing, in the present formulation it is necessary to time integrate the continuity equation to evaluate the particle volume distribution. Since the density is evaluated through the Shepard kernel the divergence of the velocity is

$$\langle \operatorname{div}(\mathbf{u}_i) \rangle = \frac{1}{d_i} \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla W_j(\mathbf{x}_i) dV_j \quad ; \quad d(\mathbf{x}) = \sum_k W_k(\mathbf{x}) dV_k \tag{14}$$

where the summation is extended to all the particle neighbourhood without taking into account the different phases. In this way the discontinuities of the velocity field at the interface will be *regularized* by the equation (14). Conversely, as already stressed, the density discontinuities are explicitly treated through equation (12).

Consistently, the new discrete formula for the smoothed pressure gradient is

$$\langle \nabla p_i \rangle = \sum_j \left(\frac{p_i}{d_i} + \frac{p_j}{d_j} \right) \nabla W_j(\mathbf{x}_i) \, dV_j \tag{15}$$

3.2.1 Introduction of the geometrical n - terms in the present formulation

As initial condition for all the simulations presented in this paper, particles are positioned on a regular lattice and, consequently, their volumes are identical. Since we are working with weakly compressible media, we assume that the volumes dV_j of the particles close to the generic particle *i* are almost identical to dV_i (*i.e.* spatial gradient of the volume distribution are negligible on length scale comparable to 3h). Under this hypothesis, it is possible to write that

$$\frac{W_j(\mathbf{x}_i) \, dV_j}{d(\mathbf{x})} = \frac{W_j(\mathbf{x}_i) \, dV_j}{\sum_k W_k(\mathbf{x}) \, dV_k} \simeq \frac{W_j(\mathbf{x}_i)}{\sum_k W_k(\mathbf{x})} = \frac{W_j(\mathbf{x}_i)}{n(\mathbf{x})}$$
(16)

Introducing this approximation into the divergence of the velocity (14) and into the pressure gradient (15) we get

$$\operatorname{div}(\mathbf{u}_i) = \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \frac{\nabla W_j(\mathbf{x}_i)}{n_i} \quad ; \quad \nabla p_i = \sum_j \left(\frac{p_i}{n_i} + \frac{p_j}{n_j}\right) \nabla W_j(\mathbf{x}_i) \tag{17}$$

In the previous equations, the influence of the particle volume is no more present and is replaced by the geometrical terms $n(\mathbf{x})$.

Similarly to the approximation made for the terms $d(\mathbf{x})$, a further simplification can be applied to $c(\mathbf{x})$

$$c_i = \sum_{k \in \mathcal{X}} W_k(\mathbf{x}_i) \, dV_k \simeq dV_i \sum_{k \in \mathcal{X}} W_k(\mathbf{x}_i) = dV_i \, l_i \tag{18}$$

As a consequence, the density equation (12) can be rewritten as

$$\rho(\mathbf{x}_i) = \frac{\sum_{j \in \mathcal{X}} m_j W_j(\mathbf{x}_i)}{l_i \, dV_i} = \frac{\mathcal{M}_i}{dV_i} \quad ; \quad \mathcal{M}_i = \frac{\sum_{j \in \mathcal{X}} m_j W_j(\mathbf{x}_i)}{\sum_{k \in \mathcal{X}} W_k(\mathbf{x}_i)} \tag{19}$$

This formula highlights that the density ρ_i and the volume dV_i are related through a *smoothed* distribution of mass \mathcal{M}_i (which does not coincide with the punctual mass m_i).

The geometrical terms $l(\mathbf{x})$ are used for the evaluation of \mathcal{M} , while the continuity equation (5) is integrated in time for the calculation of the volume distribution dV. Once the fields \mathcal{M} and dV are known it is possible to evaluate the density field ρ through equation (19) (and therefore the related pressure field).

Summarizing the formulation proposed in this work discretizes the continuum system of the governing equations (6) in the following way: at the generic time instant t positions, masses and volumes of the particles are known and, therefore, it is possible to evaluate the following quantities

$$\begin{cases} \mathcal{M}_{i} = \frac{\sum_{j \in \mathcal{X}} m_{j} W_{j}(\mathbf{x}_{i})}{l_{i}} ; \quad l_{i} = \sum_{\substack{k \in \mathcal{X} \\ \gamma_{\mathcal{X}}}} W_{k}(\mathbf{x}_{i}) \\ \rho_{i} = \frac{\mathcal{M}_{i}}{dV_{i}} \Rightarrow p(\mathbf{x}_{i}) = \frac{c_{0\mathcal{X}}^{2} \rho_{0\mathcal{X}}}{\gamma_{\mathcal{X}}} \left[\left(\frac{\rho(\mathbf{x}_{i})}{\rho_{0\mathcal{X}}} \right)^{\gamma_{\mathcal{X}}} - 1 \right]; \forall \mathbf{x}_{i} \in \mathcal{X} \end{cases}$$
(20)

Once the updated density and pressure distributions are known, the fundamental derivatives can be evaluated by

$$\begin{cases}
\frac{\mathbf{D}\mathbf{x}_{i}}{\mathbf{D}t} = \mathbf{u}_{i} ; \quad n_{i} = \sum_{k} W_{k}(\mathbf{x}_{i}) \\
\frac{\mathbf{D}\log\mathcal{J}_{i}}{\mathbf{D}t} = \sum_{j} (\mathbf{u}_{j} - \mathbf{u}_{i}) \cdot \frac{\nabla W_{j}(\mathbf{x}_{i})}{n_{i}}; \\
\frac{\mathbf{D}\mathbf{u}_{i}}{\mathbf{D}t} = -\frac{1}{\rho_{i}} \sum_{j} \left(\frac{p_{i}}{n_{i}} + \frac{p_{j}}{n_{j}}\right) \nabla W_{j}(\mathbf{x}_{i}) + \vec{f}(\mathbf{x}_{i}, t)
\end{cases}$$
(21)

Finally, using these derivatives it is possible to update volumes, velocities and positions of the particle set. Once again we underline that the present scheme allows to model both interfaces and free-surfaces. Note that if we consider only one fluid, it simply means that $l_i = n_i$.

3.2.2 Viscous forces

The viscous force $\mathbf{F}^{\mathbf{v}}$ acting on the generic particle *i* can be evaluated through the discrete formula

$$\mathbf{F}_{i}^{\mathbf{v}} = \sum_{j} \frac{2\mu_{i}\mu_{j}}{\mu_{i} + \mu_{j}} \left(\frac{1}{n_{i}} + \frac{1}{n_{j}}\right) \frac{(\mathbf{x}_{i} - \mathbf{x}_{j}) \cdot \nabla W_{j}(\mathbf{x}_{i})}{r_{ij}^{2}} (\mathbf{v}_{i} - \mathbf{v}_{j})$$
(22)

where μ is the viscosity coefficient related to the particle of the considered phase and r_{ij} is the distance between particles *i* and *j*. These formula resembles a mixing of the formulae adopted by Morris *et al.* (1997) and Monaghan (2005) with the presence of the new term $[1/n_i + 1/n_j]$.

3.2.3 Control of interface sharpness

For interface flow where surface tension effects are negligible, a numerical dispersion of the different phases can take place. To prevent this mixing a small repulsive force is introduced in the pressure gradient

$$\nabla p_i = \sum_j \left(\frac{p_i}{n_i} + \frac{p_j}{n_j}\right) \nabla W_j(\mathbf{x}_i) + \epsilon_I \sum_{j \in \mathcal{X}^C} \left(\left|\frac{p_i}{n_i}\right| + \left|\frac{p_j}{n_j}\right|\right) \nabla W_j(\mathbf{x}_i) \quad \forall i \in \mathcal{X}$$
(23)

where ϵ_I is of order $\mathcal{O}(0.01 \div 0.1)$, and the second summation is extended to all the particles which do not belong to the phase of the *i*-th particle; the latter set of particles is noted by \mathcal{X}^C .

4 VALIDATION RESULTS

4.1 Rayleigh-Taylor instabilities

We consider the problem of Rayleigh-Taylor instabilities where the interface between two different fluids needs to be accurately calculated Cummins and Rudman (1999). The computation domain is rectangular (twice as high as long) with particles distributed on a regular lattice. In the lower part of the domain, the fluid has a density equal to unity while the fluid above the interface located at $y = 1 - \sin(2\pi x)$ has got a density equal to 1.8 times the density of the lower fluid. The Reynolds number based on the half-height of the domain is equal to 420. The Froude number based on the same length scale is equal to unity. Surface tension is not taken into account. In the state equation $\gamma = 7$ for both fluids.

Numerically, 28800 particles are used in the simulation. The coefficient ϵ_I is equal to 0.02. Space resolution convergence has been checked.

Results are compared to a Level-Set Navier-Stokes model with 28800 elements, see figure 1. The



Figure 1: Rayleigh-Taylor instabilities. Comparaison at t = 5s versus a Level-Set model.

method shows a good ability to capture the strong roll-up of the interface.

Contour comparison at different space resolutions also shows a good agreement (45000 particles in the SPH simulation, 7200 and 28800 elements in the Level-Set one), see figure 2.

4.2 Air bubble rising in water

We consider an air bubble rising in water at rest in a closed domain. This case will exhibit tension surface effects and viscosity effects. Results are compared to Colagrossi and Landrini (2003).

The domain is 10 bubble radius high and 6 radius wide. The spatial resolution is h/R = 0.128. The gas has a density $\rho_{\chi} = 1kg.m^{-3}$, a viscosity $\nu_{\chi} = 2.10^{-5}kg.m^{-1}.s^{-1}$ and the sound speed is $c_{\chi} = 282.84m.s^{-1}$. The liquid has a density $\rho_{\mathcal{Y}} = 1000kg.m^{-3}$, a viscosity $\nu_{\mathcal{Y}} = 1.10^{-3}kg.m^{-1}.s^{-1}$ and the sound speed is $c_{\chi} = 20m.s^{-1}$. The surface tension between these two phases is $\sigma^{\chi\mathcal{Y}} = 0.073N.m^{-1}$.

Note that, as the classical SPH formulation, we do not capture some details of the Level-Set formulation such as small parts of fluid detaching the main bubble since $t\sqrt{g/R} = 4.8$. Nonetheless, the results are in good agreement with the Level-Set ones. And the results obtained with the standard SPH formulation are recovered with the present formulation which offers extended possibilities.

4.3 Drop impact

To illustrate the ability of the present model to simulate flows involving both multi-phases and a free surface, we consider the impact of a water drop on oil at rest. The water drop is initially placed in void at



Figure 2: Rayleigh-Taylor instabilities. Comparaison at different times versus a Level-Set code. Gray contour corresponds to the heavier fluid modelized by the present SPH model. Lines correspond to the interface of the Level-Set model on the coarse mesh (dashed line) and the fine mesh (solid line)



Figure 3: Air buble rising in water. Gray dots corresponds to the present SPH model, black dots to SPH model in Colagrossi and Landrini (2003), black diamonds to Level-Set solution in Sussman *et al.* (1994). Spatial coordinates are expressed in term of bubble radius

1.5 radius above the free surface. As shown in this first simulation, complex flows with multiphase and free surface fragmentations/reconnections are possible. Such a tentative simulation opens the door to a variety of applications where complex multi-phase flows interact with a free-surface.



Figure 4: Water drop impacting oil.

5 CONCLUSION

In this paper we present a new formulation of SPH dedicated to two-phase flows and based on Colagrossi and Landrini (2003) and Hu and Adams (2006). We show details of this formulation, its consistency and its implementation. Then validation results on well-known cases are presented: first one are the Rayleigh-Taylor instabilities and second one is an air bubble rising in water. These two cases present good agreement with other numerical formulations. A final test case run on a complex simulation with both multi-phase and free-surface shows the capability of this model to explore a new range of possibilities for SPH. In near future, the present model will be carefully validated regarding the surface tension effects and on complex situations.

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