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Vision paper

Smoothed particle hydrodynamics (SPH) for free-surface flows: past, present and future

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ABSTRACT

This paper assesses some recent trends in the novel numerical meshless method smoothed particle hydrodynamics, with particular focus on its potential use in modelling free-surface flows. Due to its Lagrangian nature, smoothed particle hydrodynamics (SPH) appears to be effective in solving diverse fluid-dynamic problems with highly nonlinear deformation such as wave breaking and impact, multi-phase mixing processes, jet impact, sloshing, flooding and tsunami inundation, and fluid–structure interactions. The paper considers the key areas of rapid progress and development, including the numerical formulations, SPH operators, remedies to problems within the classical formulations, novel methodologies to improve the stability and robustness of the method, boundary conditions, multi-fluid approaches, particle adaptivity, and hardware acceleration. The key ongoing challenges in SPH that must be addressed by academic research and industrial users are identified and discussed. Finally, a roadmap is proposed for the future developments.

Keywords: Environmental fluid mechanics; free-surface flows; numerical methods; smoothed particle hydrodynamics; SPH

1 Introduction

Since its birth in 1977, smoothed particle hydrodynamics (SPH) has progressed tremendously due to intensive theoretical work and computational improvements, particularly since the 1990s. Currently it can be regarded as a numerical tool, although unlike most commonly used mesh-based methods it remains unconventional. Nevertheless, in spite of its present drawbacks SPH has become recognized as a predictive tool in a variety of industrial or environmental applications. In recent years, some SPH codes have become an inherent part of the numerical arsenal of industrial research and development laboratories and academic institutions. There are several reasons explaining this success: (1) the growing needs of industry and research for appropriate tools for complex hydrodynamics; (2) recent advancements in SPH theory that resolved a number of problems with this method; and (3) the emergence of general purpose graphic processing units (GPGPUs) that make it possible to use SPH codes to study complex 3-D flows at real-life scales, while keeping the computational times manageable.

Along with these improvements, SPH has been the topic of several review papers over the past two decades. The most famous of these is that of Monaghan (1992), who also published another review paper a decade ago (Monaghan, 2005). More recently, Gómez-Gesteira, Rogers, Dalrymple, and Crespo (2010) provided an overview focusing on hydrodynamics of free-surface flows. A few specialized SPH books have also been published, such as those by Liu and Liu (2003) and Violeau (2012). At a time when SPH is becoming increasingly well known, questions arise such as those related to the position of this method in the overall landscape of numerical tools of modern hydraulics, and the possible evolution of SPH in forthcoming years. This paper attempts to address these challenging questions and has two objectives: (1) to assess the current situation in SPH; and (2) to outline a vision and roadmap for SPH development in the foreseeable future, especially in relation to

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hydraulics of free-surface flows. In particular, an effort has been made to identify the areas where progress has been achieved and what are the grand challenges to address. The issues that require active collaboration between the academic and industrial communities are specifically highlighted. The paper is structured as follows. In section 2, the use of SPH in free-surface flows is discussed, giving examples of its application, validation and suitability. Then, the state-of-the-art of SPH is reviewed covering formulations, boundary conditions and applications in areas such as turbulence and shallow flows, before moving to advanced numerical features and hardware acceleration. Section 3 is devoted to the discussion of the future of SPH for free-surface flows, identifying the key challenges to be solved in the next 5–10 years, including the identification of rigorous standards for future developments and use in hydraulic and environmental engineering.

2 The current use of SPH in free-surface flows

2.1 *SPH in hydraulic research*

Origins of SPH

SPH was originally developed for astrophysics modelling, where the fluid density may vary in space and time over many orders of magnitude in the absence of physical boundaries. As often happens in science, two papers proposing the same original idea were published simultaneously (Gingold & Monaghan, 1977; Lucy, 1977), showing that the underlying idea of this method was gestating in the community of astrophysical modellers. The capability of SPH to deal with the issues of varying density and unbounded flows stemmed from its fully Lagrangian nature, since the central idea of this method is to follow moving fluid particles, free of any mesh/grid constraints. In the 1980s, while continuing its development in astrophysics and magnetohydrodynamics (see a recent review by Price, 2012), SPH was successfully applied to elasticity and fracturing processes (e.g. Campbell, Vignjevic, & Libersky, 2000). It is only in the mid-1990s that Monaghan (1994) made a first attempt of using SPH for “ordinary” fluids, i.e. applied it to free-surface hydraulics encountered in everyday life. For this purpose, he introduced two basic but useful recipes in order to solve the issues of (1) approximating constant density and (2) imposing rigid boundaries. Monaghan’s simple idea for enforcing a (nearly) incompressible condition was to use a state equation with a sufficiently large (numerical) speed of sound that did not prohibit simulations, a variant known today as WCSPH (weakly compressible SPH). Surprisingly enough, the treatment of the free surface did not require additional care in this initial attempt. This first success proved to be so impressive that the community of SPH modellers in hydraulics has grown rapidly since the mid-1990s, proposing new ideas and improvements to Monaghan’s original simple model.

Applications of SPH

One of the key features of SPH that frees it from the limitations of most mesh-based schemes is that it is a truly Lagrangian method where the motion of individual particles and their properties are predicted as they move through space and time with no requirement for any underlying mesh. This brings some key advantages and unique challenges to SPH which will now be briefly discussed.

The success of SPH in hydraulics is due to its extraordinary capability to simulate a large variety of complex flows, involving a wide spectrum of physical processes. The main interesting features it possesses are the ability to deal with:

- distorted and rapidly moving free surfaces without any restriction with respect to their topologies;
- highly nonlinear, inertia-dominated flows and impact processes;
- multi-fluid flows and multi-physics;
- fluid/structure interactions, including rigid body motion in a fluid and fluid/elasticity coupling
- ease of programming (at least for basics), either in 2-D or 3-D.

Other appealing features of SPH include its variational character, where it appears to live harmoniously with the basics of Lagrangian and Hamiltonian mechanics (at least for non-dissipative phenomena, see e.g. Price, 2012). The main drawbacks of SPH are described below.

Since its use in hydraulics, SPH has been applied to a diverse range of problems in fluid flow research and hydraulic engineering (summarized for example in the supplementary issue of the *Journal of Hydraulic Research* (2010, vol. 48); also Gómez-Gesteira, Rogers, Violeau, Grassa & Crespo, 2010). As it is not possible to draw an exhaustive list of all application fields here, below we highlight only problems that are among most extensively addressed in the SPH international community (see also examples in Fig. 1):

- water wave impacts on coastal and offshore structures (e.g. Altomare, Crespo et al., 2015; Lind et al., 2015; Ni, Feng, & Wu, 2014);
- flow over river waterworks, such as spillways and fish passes (e.g. Husain, Muhammed, Karunarathna, & Reeve, 2014; Lee, Violeau, Issa, & Ploix, 2010);
- sloshing of liquids in carriage tanks and nuclear vessels (e.g. Souto-Iglesias, Delorme, Pérez-Rojas, & Abril-Pérez, 2006);
- jet impact on hydraulic turbines (e.g. Koukouvinis, Anagnostopoulos, & Papantonis, 2013; Marongiu, Leboeuf, Caro, & Parkinson, 2010);
- flow around ships and ditching (e.g. Cartwright, Chhor, & Groenenboom, 2010; Marrone, Bouscasse, Colagrossi, & Antuono, 2012; Zhang, Cao, Ming, & Zhang, 2013);
- long waves, e.g. floods, tsunamis and landslide submersions (e.g. Ataie-Ashtiani & Shobeyri 2008, Capone et al., 2010,

Vacondio, Mignosa, & Pagani, 2013; Vacondio, Rogers, Stansby, & Mignosa, 2013; Wu, Zhang, Dalrymple, & Hérault, 2013);
- oil spill and floating boom dynamics (e.g. Violeau, Buvat, Abed-Meraïm, & de Nanteuil, 2007);
- groundwater flows and stability of levees (Bui & Fukagawa, 2013); and
- multi-phase flows for coastal and other hydraulic applications with air-water mixtures and sediment scouring (e.g. Fourtakas, Rogers, & Laurence, 2014; Manenti, Sibilla, Gallati, Agate, & Guandalini, 2012; Mokos, Rogers, & Stansby, 2015; Ulrich, Leonardi, & Rung, 2013).

The success of SPH in these fields is due to the relative ease with which SPH simulations have been able to produce results for cases involving complicated nonlinear and often multi-phase phenomena. With little modification of the basic methodology, SPH has been able to generate results in close agreement with reference solutions/data in validation tests, without highly sophisticated algorithms required in mesh-based schemes. Most of the aforementioned fields are deemed too difficult (not to say impossible) for other numerical methods. For these reasons, in complex free-surface flow modelling, SPH has challenged the dominance of volume-of-fluids (VOF), level set (LS) or other promising approaches dedicated to

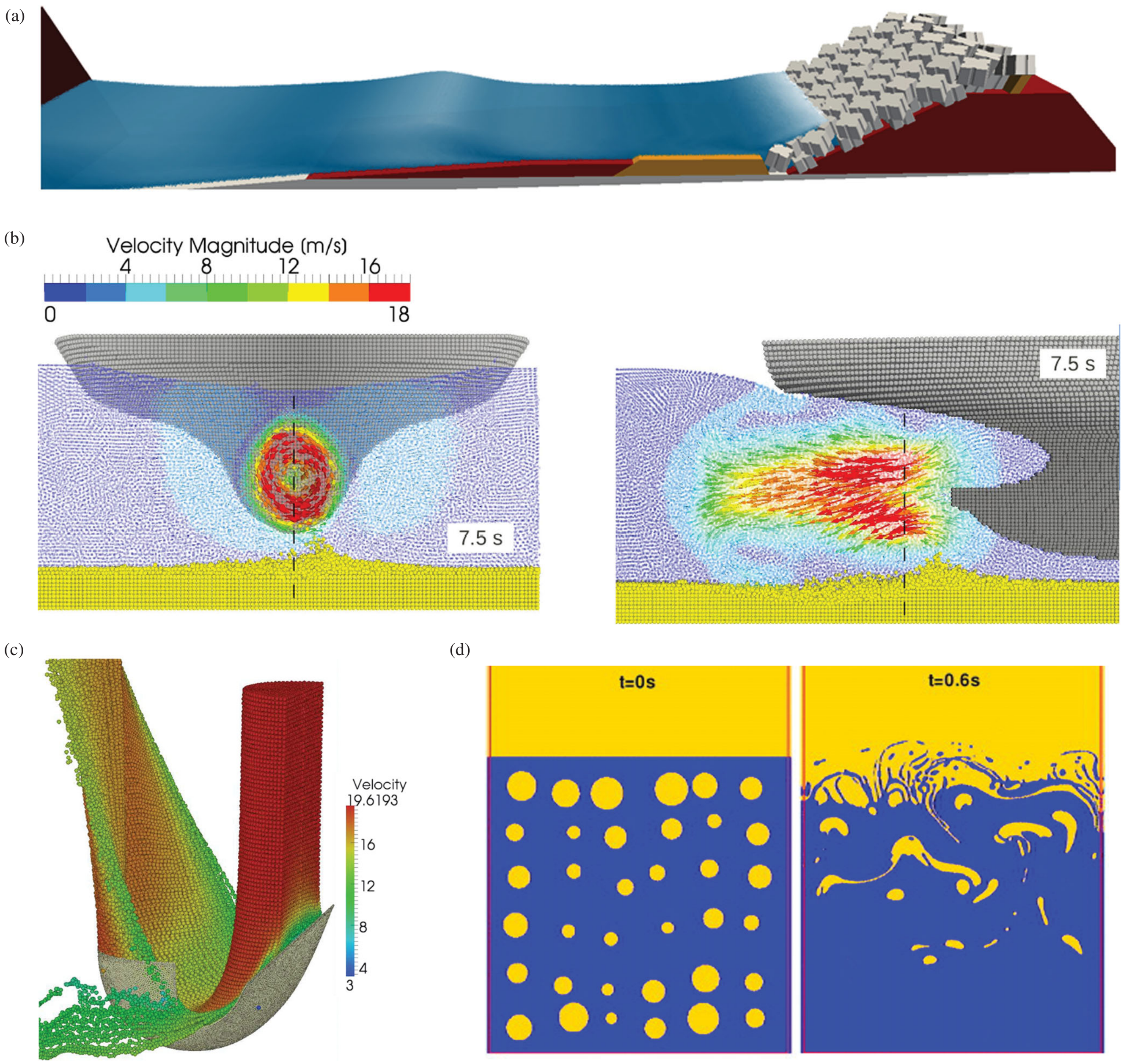
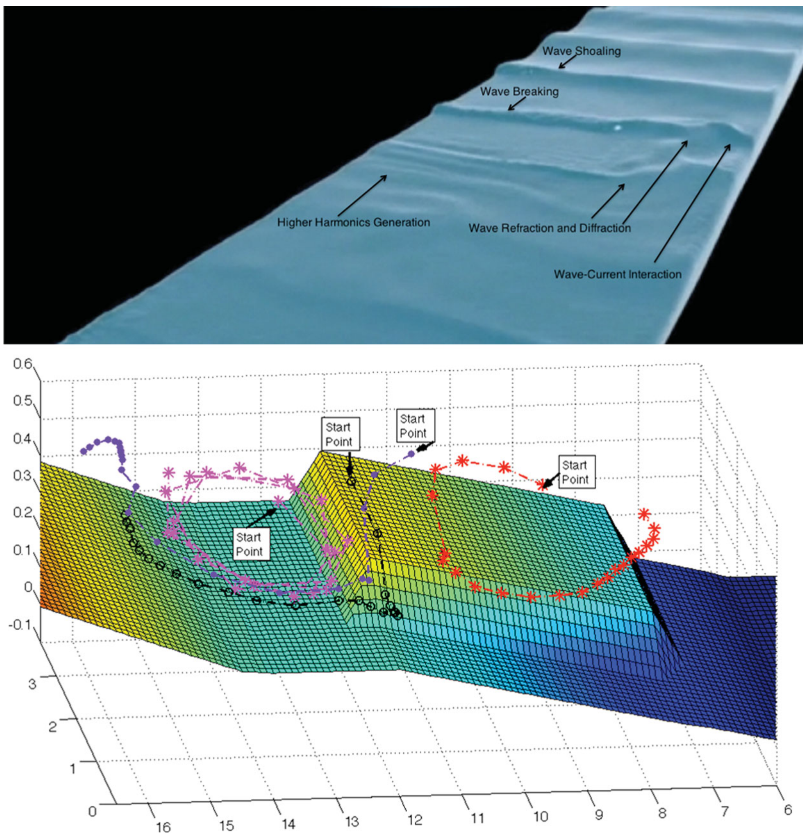


Figure 1 Example SPH applications: (a) wave interaction with a rubble mound breakwater (Altomare et al., 2014); (b) scour by a ship propeller (Ulrich 2013); (c) high velocity jet impinging Pelton turbine blade (Marongiu et al., 2010); (d) oil–water separator (Grenier, Le Touzé, Colagrossi, Antuono, & Colicchio, 2013); (e) 3-D nearshore circulations and trajectories under breaking waves (Farahani, Dalrymple, Hérault, & Bilotta, 2014); and (f) fluid–structure impact (Skillen et al., 2013)



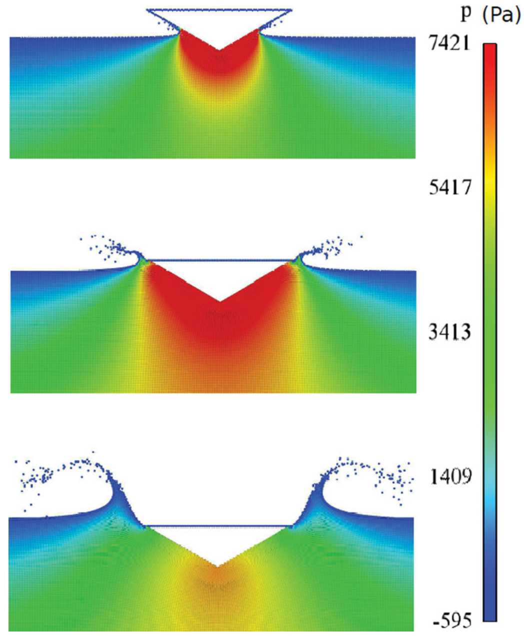


Figure 1 Continued.

these special kinds of flows. Moreover, recent progress in the numerical features of SPH has increased its credibility and made it increasingly attractive to mathematicians, so far exclusively concerned with more traditional, well-established techniques like the finite element method (FEM) and finite volume method (FVM).

Previous validation of SPH

A repeated criticism of SPH for free-surface flows relates to the lack of high-quality validation undertaken in published studies, with a tendency to produce snapshot images of flow quantities. Due to the drawbacks of the method (see below), SPH is still often considered by many as a promising but immature method. It is noteworthy, however, that convincing solutions have been proposed to fix these issues, as the reader will see in the next section. In many situations, SPH has recently proven to be just as efficient as FEM and FVM, even for confined, viscous-dominated flows (Lee et al., 2008). However, the SPH method is inappropriate for certain applications and is known to provide poor predictions for some phenomena, such as long-distance water wave propagation. Figure 2 shows example validation plots for SPH with benchmark test cases that are based either on an analytical solution or on reliable reference data. These cases are used to illustrate the high-quality validation using velocity and pressure profiles, error estimates, and convergence, i.e.:

- pressure coefficients for different wedge angles impacting a surface (Skillen, Lind, Stansby, & Rogers, 2013);
- lid-driven cavity flows (Leroy, Violeau, Ferrand, & Kassiotis, 2014, 2015) for which reference solutions are available as well as comparison with commercial computational fluid dynamics (CFD) solvers (Code_Saturne); and
- the non-hydrostatic pressure field under a propagating wave compared with a highly accurate stream function theory (Lind, Xu, Stansby, & Rogers, 2012).

Many more validation cases are now increasingly being used in SPH such as in the applications highlighted above. Hence, it is clear that greater mathematical and validation rigour is now used to demonstrate the potential applicability of SPH for applications. This is an essential recent development as SPH must not only demonstrate performance that is comparable to existing CFD methods, but also demonstrate capabilities beyond existing CFD methods. As will be discussed later in section 3, there are still significant challenges remaining and increasing academic rigour is a necessary and essential part of SPH.

Drawbacks of SPH

As a relatively young computational method, SPH has some disadvantages, including:

- large computational time, particularly in 3-D simulations;

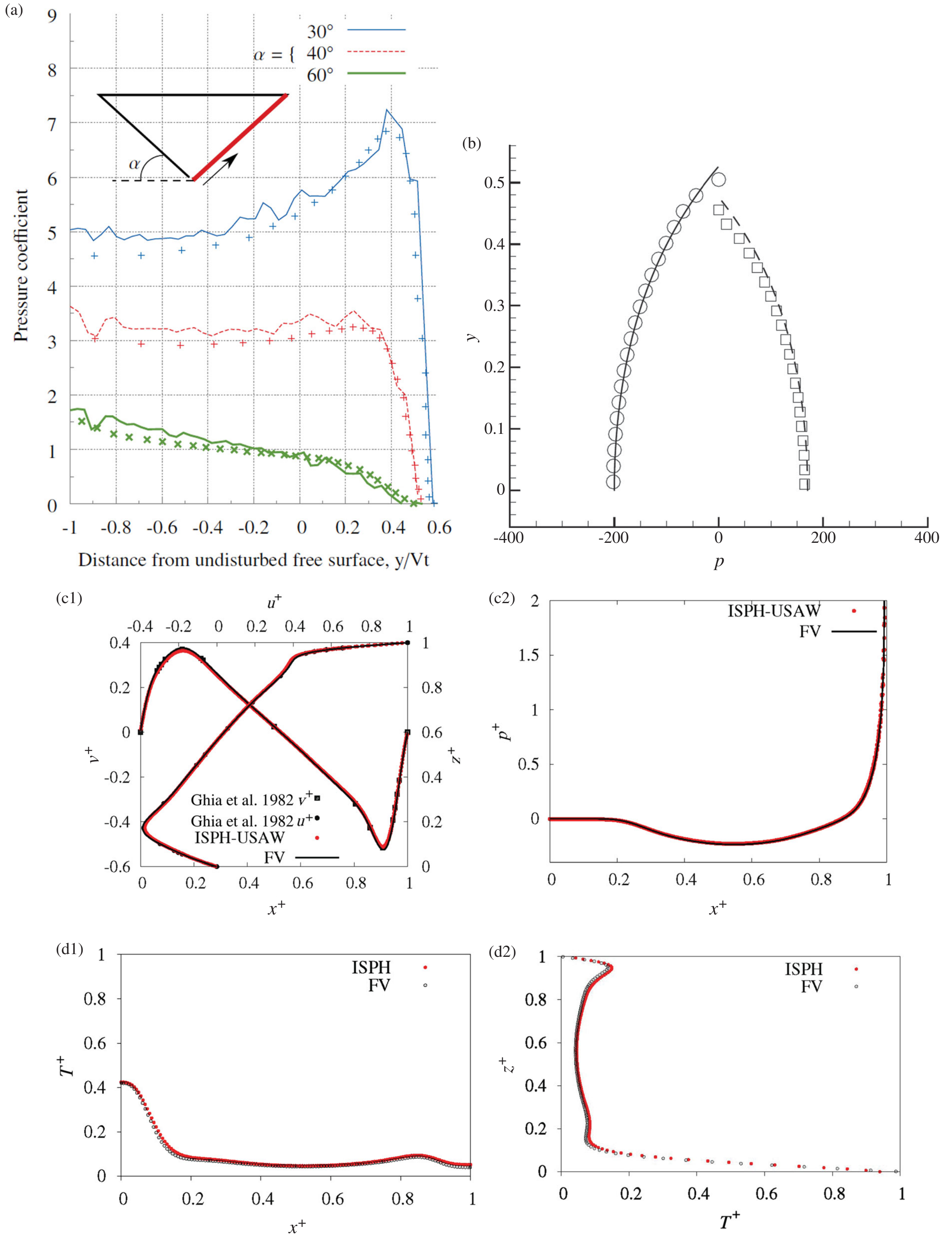


Figure 2 Validation examples of SPH. (a) Pressure coefficient for wedge impact compared with asymptotic data for different wedge angles (Skillen et al., 2013); (b) non-hydrostatic vertical distributions of pressure p under a crest and trough compared with stream function theory for propagating periodic regular wave (Lind et al., 2012); (c) lid-driven cavity, profiles of dimensionless velocities u^+ and v^+ (left) and pressure p^+ (right) on various sections as a function of horizontal and vertical dimensionless positions x^+ and z^+; the red lines are an ISPH model (Leroy et al., 2014), the black lines are a FV model (Code_Saturne, Archambeau et al., 2005) and the symbols are the reference results by Ghia et al. (1982); (d) horizontal and vertical profiles of dimensionless temperature T^+ in a heated lid-driven cavity; the red circles are the ISPH model with buoyancy by Leroy et al. (2015) and the black circles are from a FV model (Code_Saturne)

- difficulties in prescribing wall boundary conditions, and even greater problems at open (inflow/outflow) boundaries;
- lack of a consistent theory in relation to the mathematical foundation of the method (convergence, stability);
- inaccuracy of pressure prediction, at least for the original WCSPH variant described above; and
- difficulties in dealing with variable space resolution for (nearly) incompressible flows.

It is worth stressing that all pros and cons of SPH originate from its purely Lagrangian nature.

2.2 *SPH state-of-the art*

SPH tools

SPH interpolations As mentioned earlier, the idea of SPH is to follow particles in their motion. The particles (denoted by labels[1] a and b) can be viewed as material points carrying extensive (i.e. additive) quantities (e.g. mass m_a, volume V_a), as well as intensive quantities (e.g. velocity $\mathbf{v}_a$, pressure p_a, density $\rho_a = m_a/V_a$, specific internal energy e_a, turbulent kinetic energy (TKE) k_a). Since no computational mesh is used, interpolation is based on the particle position $\mathbf{r}_a$, using a weighting function or "kernel" w, being a differentiable, decreasing, compactly supported function of the particle distance $r_{ab} = |\mathbf{r}_{ab}| = |\mathbf{r}_a - \mathbf{r}_b|$ and the characteristic length, h, known as the smoothing length (Fig. 2). This is done in two steps: a continuous interpolation and a discrete approximation. For an arbitrary field $f(\mathbf{r})$, the first one reads:

$$f(\mathbf{r}_a) = \int_\Omega f(\mathbf{r}) w(|\mathbf{r}_a - \mathbf{r}|,\ h) \mathrm{d}\mathbf{r} + \mathrm{O}(h^2) \tag{1}$$

where Ω is the fluid domain. The smoothing length h is a measure of the kernel's support size and forms one of the discretization parameters of SPH, the other one being the initial distance between neighbouring particles, δr. The latter should remain approximately constant on average for an (almost) incompressible flow. The continuous approximation of Eq. (1) has second-order spatial accuracy in h provided the kernel is normalized, i.e. its integral is equal to 1 (Monaghan, 2005). Typical kernels are the B-splines (Monaghan, 1985) and the Wendland kernels (Wendland, 1995).

The discrete interpolation then consists of using weighted contributions of the surrounding particles to make an approximation of Eq. (1):

$$f(\mathbf{r}_a) \approx \sum_b V_b f_b w(|\mathbf{r}_a - \mathbf{r}_b|,\ h) \tag{2}$$

where the sum runs over the particles and f_b is equal to $f(\mathbf{r}_b)$. The ratio $h/\delta r$ determines the number of neighbouring particles contributing to the estimation of Eq. (2) of $f(\mathbf{r}_a)$ (Fig. 3). This number is typically *ca.* 30 in 2-D simulations and 250 in 3-D simulations. Estimating the error in making the discrete interpolation is not straightforward, since it depends on the particle distribution in space. For the generic case of a Cartesian grid, the error can be computed exactly (Violeau, 2012). Details about the effect of particle disorder can be found in Quinlan, Basa, and Lastiwka (2006) and Amicarelli, Marongiu, Leboeuf, Leduc, and Caro (2011).

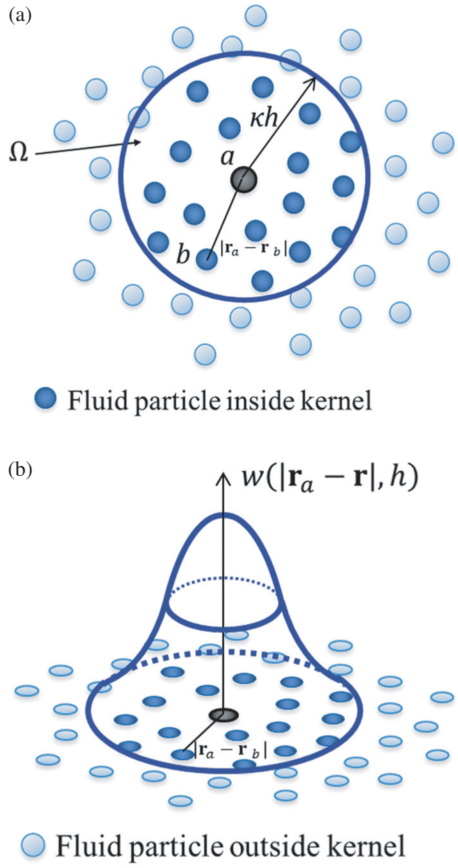


Figure 3 Example of a 2-D particle distribution surrounding particle a. The radius of influence of the kernel is expressed as a multiple, κ, of the smoothing length h

Applying Eq. (2) to define the density produces:

$$\rho_a \approx \sum_b m_b w_{ab} \tag{3}$$

where w_{ab} is a short notation for $w(|\mathbf{r}_a - \mathbf{r}_b|,\ h)$. In general for a given smoothing length, one can see that when particles are closer together with smaller inter-particle distances, the density is higher, in agreement with physical intuition. Equation (3) is sometimes used to compute the particle densities. Note that with a limited number of particles b being involved in SPH sums, computational efficiency requires building a neighbour particle list at every time step. An analysis of neighbour list creation algorithms is given by Dominguez, Crespo, and Gomez-Gesteira (2011).

SPH operators The next step is to approximate the derivatives in SPH. First considering the gradient operator, one could simply apply Eq. (1) to the vector function ∇f, but it proves better to derive alternative forms, for example, to apply it to $\nabla f = \rho\nabla(f/\rho) + (f/\rho)\nabla\rho$. After integrating by parts, one obtains:

$$\nabla f(\mathbf{r}_a) = \rho_a \int_\Omega \left[\frac{f_a}{\rho_a^2} + \frac{f(\mathbf{r})}{\rho(\mathbf{r})^2}\right] \nabla_a w(|\mathbf{r}_a - \mathbf{r}|, h)\rho(\mathbf{r})\mathrm{d}\mathbf{r} + \text{Boundary term} + \mathrm{O}(h^2) \quad (4)$$

where ∇_a stands for the gradient with respect to the coordinates of a. The boundary term will be explained later (see Boundary conditions). Considering a particle a remote from any boundary, this term vanishes and the discrete interpolation reads:

$$\nabla f(\mathbf{r}_a) \approx \rho_a \sum_b m_b \left(\frac{f_a}{\rho_a^2} + \frac{f_b}{\rho_b^2}\right) \nabla_a w_{ab} \quad (5)$$

where $\nabla_a w_{ab} = \nabla_a w(|\mathbf{r}_a - \mathbf{r}_b|, h)$. This is an SPH discrete gradient operator. It has been written in an antisymmetric form ($\nabla_a w_{ab} = -\nabla_b w_{ba}$ since the gradient of an even function is an odd function). More generally, SPH gradient operators can be expressed as a function of the particle properties, i.e.:

$$\boldsymbol{G}_a\{f_b\} = \rho_a \sum_b m_b Q^G(f_a, f_b, \rho_a, \rho_b)\nabla_a w_{ab} \approx \nabla f(\mathbf{r}_a) \quad (6)$$

where Q^G is a combination of $(f_a, f_b, \rho_a, \rho_b)$ which is symmetric or antisymmetric with respect to the a and b labels. As explained later, choosing one or the other of these properties has important consequences. Whatever the choice is, $\boldsymbol{G}_a$ is a linear operator transforming the discrete set $\{f_b\}$ into a set of approximations of ∇f at all particles a.

On similar grounds, one defines discrete divergence operators as:

$$D_a\{\mathbf{f}_b\} = -\frac{1}{\rho_a} \sum_b m_b \boldsymbol{Q}^D(\mathbf{f}_a, \mathbf{f}_b, \rho_a, \rho_b) \cdot \nabla_a w_{ab} \approx \nabla \cdot \mathbf{f}(\mathbf{r}_a) \quad (7)$$

for any discrete vector field $\{\mathbf{f}_b\}$. Again, $\boldsymbol{Q}^D$ is a combination of $(\mathbf{f}_a, \mathbf{f}_b, \rho_a, \rho_b)$ which may be symmetric or antisymmetric. The most commonly used form is given as $\boldsymbol{Q}^D = \mathbf{f}_a - \mathbf{f}_b$. It is generally useful to specify Q^G and $\boldsymbol{Q}^D$, in order to satisfy the property:

$$\langle\{f_a\}, \{D_a\{\mathbf{g}_b\}\}\rangle = -\langle\{\boldsymbol{G}_a\{f_b\}\}, \{\mathbf{g}_a\}\rangle \quad (8)$$

where the following inner product has been used:

$$\langle\{f_a\}, \{g_a\}\rangle \equiv \sum_a V_a f_a g_a \approx \int_\Omega f(\mathbf{r})g(\mathbf{r})\mathrm{d}\mathbf{r} \quad (9)$$

In other words, the SPH operators of the gradient and divergence should be skew-adjoint. The main reason for that will be explained in SPH governing equations and concerns the conservation of energy (Mayrhofer, Rogers, Violeau, & Ferrand, 2013). The condition of Eq. (8) is satisfied if $\sum_{a,b} f_a Q^D(g_a, g_b, \rho_a, \rho_b) = \sum_{a,b} \rho_a^2 Q^G(f_a, f_b, \rho_a, \rho_b) g_a$. When Q^G is given by Eq. (5), then $\boldsymbol{Q}^D = \mathbf{f}_a - \mathbf{f}_b$ as stated above.

Finally, discrete Laplacian (diffusion) operators read:

$$L_a\{K_b, \mathbf{f}_b\} = \sum_b V_b Q^L(K_a, K_b, \rho_a, \rho_b) \times \frac{\mathbf{f}_a - \mathbf{f}_b}{r_{ab}^2} \mathbf{r}_{ab} \cdot \nabla_a w_{ab} \approx (\nabla \cdot K\nabla \mathbf{f})(\mathbf{r}_a) \quad (10)$$

where K is a diffusion coefficient, which can vary in space and time. For viscous diffusion Morris, Fox, and Zhu (1997) proposed $Q^L = K_a + K_b$. This model was further extended to the scalar diffusion (e.g. Violeau & Issa, 2006). Monaghan and Gingold (1983) proposed an alternative model, which is often used as an artificial viscous term for stabilizing computations.

SPH governing equations

Weakly compressible SPH The WCSPH model as proposed by Monaghan (1994) solves the conservation of momentum and mass in Lagrangian form:

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla(\mu\nabla\mathbf{v}) + \mathbf{g} \quad (11a)$$

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{v} \quad (11b)$$

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\nabla \cdot \mathbf{v} \quad (11c)$$

$$p = f\left(\frac{\rho}{\rho_0}, p_B, c_0\right) \quad (11d)$$

As can be seen, these are the Navier–Stokes equations written in a Lagrangian form, for a weakly compressible flow. Recall that $\mathbf{v}$, $\mathbf{r}$, p, ρ, μ and $\mathbf{g}$ are the velocity, position, pressure, density, dynamic viscosity, and gravity, respectively. Density variations do not appear in the momentum Eq. (11a), but rather in the continuity Eq. (11c) and in the equation of state (Eq. (11d)) where ρ_0 is a reference density, p_B is background pressure and c_0 a numerical speed of sound. Using the governing equations expressed with primitive variables (that is $\mathbf{v}$, $\mathbf{r}$, ρ, p), assuming constant particle masses, and employing the SPH operators defined in Eqs (6), (7) and (10), the governing equations for each particle a read as:

$$\frac{\mathrm{d}\mathbf{v}_a}{\mathrm{d}t} = -\frac{1}{\rho_a}\boldsymbol{G}_a\{p_b\} + \frac{1}{\rho_a}L_a\{\mu_b, \mathbf{v}_b\} + \mathbf{g} \quad (12a)$$

$$\frac{\mathrm{d}\mathbf{r}_a}{\mathrm{d}t} = \mathbf{v}_a \quad (12b)$$

$$\frac{\mathrm{d}\rho_a}{\mathrm{d}t} = -\rho_a D_a\{\mathbf{v}_b\} \quad (12c)$$

$$p_a = f\left(\frac{\rho_a}{\rho_0}, p_B, c_0\right) \quad (12d)$$

Note that, as mentioned above, some researchers prefer using Eq. (3) to compute ρ_a instead of the continuity equation. An analysis of the compressible Navier–Stokes equations show that the maximum relative density fluctuations scale with the squared Mach number M^2. Thus, the numerical speed of sound c_0 in WCSPH is generally set to 10 times the maximum velocity in the flow, so that density fluctuations remain less than $\mathrm{M}^2 = 0.01$ or 1%, while the spacing between particles remains approximately constant. The state function f is chosen such that the pressure increases drastically while the density varies from its reference value, i.e.:

$$f\left(\frac{\rho_a}{\rho_0}, p_{\mathrm{B}}, \mathrm{c}_0\right) = \frac{\rho_0 c_0^2}{\gamma}\left[\left(\frac{\rho_a}{\rho_0}\right)^{\gamma} - 1\right] + p_B \tag{13}$$

where $\gamma = 7$ for water. This choice was recommended by Monaghan (1994) and proved to be efficient.

With the above considerations, a time integration scheme is further required to solve Eqs (12a) to (12c). Some authors use the symplectic Euler first-order schemes (e.g. Violeau & Issa, 2006) while other prefer higher-order schemes, such as fourth-order Runge–Kutta schemes (e.g. Antuono, Marrone, Colagrossi, & Bouscasse, 2015). A good balance between the algorithmic simplicity and numerical accuracy is the leapfrog (second-order) scheme (Monaghan, 2005):

$$\begin{aligned} \mathbf{v}_a^{n+1/2} &= \mathbf{v}_a^n + \mathbf{F}_a^n \frac{\Delta t}{2} \\ \mathbf{r}_a^{n+1} &= \mathbf{r}_a^n + \mathbf{v}_a^{n+1/2}\Delta t \\ \mathbf{v}_a^{n+1} &= \mathbf{v}_a^{n+1/2} + \mathbf{F}_a^{n+1}\frac{\Delta t}{2} \end{aligned} \tag{14}$$

In the above equations, the superscripts refer to the time iteration numbers while Δt is the time step (see Advanced numerical features) for the stability condition. The force $\mathbf{F}$ here refers to the right-hand side of the momentum equation. Irrespective of whether the density is computed through Eq. (3) or using the continuity equations, it is then updated using the new values of the particle positions and velocities.

As pointed out by Price (2012), using the antisymmetric form of the pressure gradient in Eq. (5) provides a better behaviour of particles in space. It is also obvious that such a discrete pressure force satisfies action-reaction, thus conservation of the total linear momentum. It can readily be checked that this choice also leads to angular momentum conservation, provided the kernel is invariant through rotations (Monaghan, 1994; Violeau, 2012). As already pointed out by many authors (e.g. Mayrhofer et al., 2013; Price, 2012), this behaviour of the SPH equations stems from a variational principle (Euler–Lagrange equations). As an example of the properties resulting from that, one should emphasize that the viscous forces in Eq. (11a) are the only dissipative forces, as required. As a proof, let us write the time derivative of the system Hamiltonian (energy) for an isentropic flow:

$$\begin{aligned} \frac{\mathrm{d}H}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\sum_a m_a\left(\frac{1}{2}\mathbf{v}_a^2 + e_a - \mathbf{g}\cdot\mathbf{r}_a\right) \\ &= \sum_a m_a\left(\mathbf{v}_{\boldsymbol{a}}\cdot\frac{\mathrm{d}\mathbf{v}_{\boldsymbol{a}}}{\mathrm{d}t} + \frac{\mathrm{d}e_a}{\mathrm{d}\rho_{\boldsymbol{a}}}\frac{\mathrm{d}\rho_{\boldsymbol{a}}}{\mathrm{d}t} - \mathbf{g}\cdot\frac{\mathrm{d}\mathbf{r}_{\boldsymbol{a}}}{\mathrm{d}t}\right) \\ &= \sum_a m_a\left[\mathbf{v}_{\boldsymbol{a}}\cdot\left(-\frac{1}{\rho_a}\mathbf{G}_{\boldsymbol{a}}\{p_b\} + L_a\{\upsilon_b, \mathbf{v}_b\}\right)\right. \\ &\quad \left. + \frac{p_a}{\rho_a^2}(-\rho_a D_a\{\mathbf{v}_b\})\right] \end{aligned} \tag{15}$$

where we have used the relation $\mathrm{d}e = (p/\rho^2)\mathrm{d}\rho$ and the first three lines of Eq. (12). Now, using the notation of Eq. (9) and accounting for Eq. (8), one can obtain:

$$\begin{aligned} \frac{\mathrm{d}H}{\mathrm{d}t} &= -\langle\{\boldsymbol{G}_a\{p_b\}\}, \{\mathbf{v}_a\}\rangle - \langle\{p_a\}, \{D_a\{\mathbf{v}_b\}\}\rangle + \text{dissipative term} \\ &= \text{dissipative term} \end{aligned} \tag{16}$$

thanks to the property of Eq. (8). Note that the first line in Eq. (15) is a discrete form of the following energy balance, which stems from the Navier–Stokes equations:

$$\begin{aligned} \frac{\mathrm{d}H}{\mathrm{d}t} &= -\int_{\Omega}(\nabla p\cdot\mathbf{v} + p\nabla\cdot\mathbf{v})\mathrm{d}\mathbf{r} + \text{dissipative term} \\ &= \int_{\partial\Omega} p\mathbf{v}\cdot\mathbf{n}\mathrm{d}S + \text{dissipative term} \end{aligned} \tag{17}$$

where $\mathbf{n}$ is the inward unit vector normal to the domain boundary Ω.

Problems with the basic SPH formulation Many of the modifications to the basic SPH formulation are motivated by one of the drawbacks of WCSPH: spurious pressure oscillations. These result from various sources including using a stiff equation of state which ignores thermodynamic effects (Eq. (12)), inaccuracies in the SPH interpolation procedure itself (Vaughan, Healy, Bryan, Sneyd, & Gorman, 2009), and, importantly, due to the collocation nature of the method where all quantities are estimated at the same computational points (Fatehi & Manzari, 2011a). In the early 2000s, the main technique to circumvent this issue in hydraulic applications was to use a posteriori numerical treatments. Early treatments for numerical stability included the X-SPH correction (Monaghan, 1994) which by definition introduces extra numerical diffusion into the results and is undesirable. The use of density filters is described in the next section (Colagrossi & Landrini, 2003; Gómez-Gesteira, Rogers, Dalrymple, et al., 2010). However, these do not address the root cause of the problem. In the past decade, three alternative solutions were proposed to address this issue: (1) density diffusion; (2) Godunov-type schemes using shock-capturing methods with Riemann solvers; and (3) incompressible SPH (ISPH). These approaches are presented in the following sections.

A posteriori numerical treatment: density filtering Using the artificial equation of state, Eq. (13), with a polytropic index of $\gamma = 7$ can lead to pressure fluctuations within the fluid domain. With pressure being evaluated as a function of density, a common technique to address the problem of the noisy pressure fields is to apply a density filter for each particle performing a renormalized SPH density summation every 20–50 time steps according to:

$$\rho_a^{\text{new}} = \sum_b \rho_b \tilde{w}_{ab} \frac{m_b}{\rho_b} \tag{18}$$

where $\tilde{w}_{ab}$ is a corrected kernel. Using either a zeroth-order (Shepard) or a first-order moving least squares (MLS) correction has proven sufficient for most applications (Colagrossi & Landrini, 2003; Dilts, 1999). However, such an a posteriori technique does not address the fundamental causes of the problem, leading to excessive dissipation which may be inappropriate in predictions of wave propagation (Khayyer & Gotoh, 2010; Rogers, Dalrymple, & Stansby, 2010).

Density diffusion Another technique for solving the issue of density fluctuations in SPH is to add a smoothing density term to the continuity equation. Ferrari, Dumbser, Toro, and Armanini (2009) proposed such an approach, with a similar technique by Molteni and Colagrossi (2009) to account for not modelling thermal variations in the equation of state. With this technique, Eq. (12c) now reads:

$$\frac{\mathrm{d}\rho_a}{\mathrm{d}t} = -\rho_a D_a\{\mathbf{v}_b\} + L_a\{K_b,\ \rho_b\} \tag{19}$$

where K is a numerical diffusion coefficient. Various forms of this corrective term have been proposed (Antuono, Colagrossi, & Marrone, 2012; Mayrhofer et al., 2013). The additional term in Eq. (19) is a discrete SPH form of $\nabla \cdot K\nabla\rho$. It is thus a diffusion term which tends to reduce spurious fluctuations of the density.

Riemann solvers In the fields of gas dynamics the accurate simulation of rapidly-varying flow properties such as those occurring in the propagation of shock waves was one of the greatest achievements of CFD in the twentieth century (Toro, 2009). Shock-capturing techniques in so-called Godunov-type methods have since been applied to many other fields to great effect, for example, shallow water flows (Rogers, Fujihara, & Borthwick, 2001). Its attraction for SPH was quickly realized in some early publications (Monaghan 1997), but it was not until the near simultaneous work of Inutsuka (2002), Cha and Whitworth (2003), Parshikov and Medin (2002), and Vila (1999) that a more formal development of shock-capturing techniques within SPH was achieved. These techniques require only minor changes to the SPH formulation, replacing the classical particle interactions with individual Riemann problems between each particle pair. With higher-order upwind reconstruction techniques, this produces pressure fields that are effectively noise free. There are two approaches to including the Riemann problem within SPH. First, the combined pressure in Eqs (5) and (12) can be replaced with the pressure in the so-called "star region" (the evolving region between the undisturbed left and right initial states in the solution to the Riemann problem) as recommended by Parshikov and Medin (2002) (see also Gomez-Gesteira et al., 2012). For example, the gradient and divergence operators:

$$\begin{aligned} -\frac{1}{\rho_a}\mathbf{G}_a\{p_b\} &= -\sum_b m_b\left(\frac{p_b}{\rho_b^2}+\frac{p_a}{\rho_a^2}\right)\nabla_a w_{ab} \\ D_a\{\mathbf{v}_b\} &= -\frac{1}{\rho_a}\sum_b m_b(\mathbf{v}_b-\mathbf{v}_a)\cdot\nabla_a w_{ab} \end{aligned} \tag{20}$$

become

$$\begin{aligned} -\frac{1}{\rho_a}\mathbf{G}_a\{p_b\} &= -\sum_b m_b 2p^*_{ab}\left(\frac{1}{\rho_b^2}+\frac{1}{\rho_a^2}\right)\nabla_a w_{ab} \\ D_a\{\mathbf{v}_b\} &= -\frac{2}{\rho_a}\sum_b m_b(\mathbf{v}^*_{ab}-\mathbf{v}_a)\cdot\nabla_a w_{ab} \end{aligned} \tag{21}$$

where p^* and $\mathbf{v}^*$ are solutions from the Riemann problem (approximate or otherwise). The process can be repeated with variationally consistent operators. Alternatively, Vila (1999) proposed an arbitrary Lagrange–Euler (ALE) formulation such that Eqs (11) are cast in terms of conserved variables (ρ, $\rho\mathbf{v}$, ...) and fluxes between particles.

Similar to mesh-based shock-capturing techniques, solving the Riemann problem is non-trivial with a robust option being the use of approximate Riemann solvers such as the Harten–Lax–van Leer contact (HLLC) solver (see Toro, 2009 for a full review). Combined with the shock-capturing behaviour of approximate Riemann solvers, this approach has clear advantages for simulating wave impact and fluid–structure impact problems. These techniques have been successfully applied to a variety of free-surface flows including objects impacting the surface (Oger, Doring, Alessandrini, & Ferrant, 2006), jets impacting turbines (Koukouvinis et al., 2013; Marongiu et al., 2010), wave impact on structures (Rogers et al., 2010), and wave propagation and fluid–structure impact for heaving wave energy devices (Omidvar, Stansby, & Rogers, 2012, 2013). It has since been applied to astrophysics which conventionally used artificial viscosity (Murante, Borgani, Brunino, & Cha, 2011). Well-known techniques for enhancing the performance including higher-order reconstruction and pre-conditioning have proven to be useful in reducing pressure oscillations (Leduc, Leboeuf, Lance, Parkinson, & Marongiu, 2010).

Incompressible SPH Cummins and Rudman (1999) were the first to propose an incompressible algorithm for SPH, today referred to as ISPH. The idea consists of applying to SPH the projection method developed by Chorin (1968) and Temam (1968). As explained by Cummins and Rudman (1999), this approach is justified in the framework of SPH because the discrete gradient and divergence operators in Eqs (6) and (7) are skew-adjoint (see Eq. (8)). The SPH form of this algorithm was originally written as:

$$\mathbf{r}_a^* = \mathbf{r}_a^n + \mathbf{u}_a^n \frac{\Delta t}{2} \tag{22a}$$

$$\mathbf{v}_a^* = \mathbf{v}_a^n + (L_a\{v_b^n,\ \mathbf{v}_b^n\} + \boldsymbol{g})\Delta t \tag{22b}$$

$$L_a\{1, \boldsymbol{p}_b^{n+1}\} = \frac{\rho}{\Delta t}\mathrm{D_a}\{\mathbf{v}_b^*\} \tag{22c}$$

$$\mathbf{v}_a^{n+1} = \mathbf{v}_a^* - \frac{1}{\rho}\mathbf{G}_a\{p_b^{n+1}\}\Delta t \tag{22d}$$

$$\mathbf{r}_a^{n+1} = \mathbf{r}_a^* + \mathbf{v}_a^{n+1}\frac{\Delta t}{2} \tag{22e}$$

where ρ is now constant. Equations (22b) to (22d) are SPH forms of the following projection scheme:

$$\mathbf{v}^* = \mathbf{v}^{\boldsymbol{n}} + (\nabla \cdot \nabla \mathbf{v} + \mathbf{g})^n \Delta t \tag{23a}$$

$$\nabla^2 p = \frac{\rho}{\Delta t}\nabla \cdot \mathbf{v}^* \tag{23b}$$

$$\mathbf{v}^{n+1} = \mathbf{v}^* - \frac{1}{\rho}\nabla p^{n+1}\Delta t \tag{23c}$$

It is thus a predictor-corrector scheme like the leapfrog Eq. (14), with the forces being split in two parts. The pressure is computed through the discrete Poisson Eq. (22c). Due to the definition of the SPH diffusion operator, Eq. (10), this is actually an asymmetric linear system with unknowns $\{p_b^{n+1}\}$, which can be solved using traditional methods like GMRES (Saad & Schultz, 1986) of Bi-CGSTAB (Van Der Vorst, 1992). ISPH was successfully compared to WCSPH by Lee et al. (2008), who proved its superiority in terms of pressure prediction and smoothness of velocity fields. The linear system to be solved does require further computational efforts, which are compensated by a larger time step (see Advanced numerical features). Variants of ISPH were proposed by Shao (2006) and Hu and Adams (2007), and applications to ocean engineering were published by Khayyer, Gotoh and Shah (2009) and Khayyer and Gotoh (2009).

Particle shifting An important consequence of improving the pressure fields, by using density diffusion techniques, Riemann solvers or ISPH, is that particles follow streamlines more accurately. This can create problems in the particle distribution which ultimately can lead to the simulation breakdown, when unphysical voids are created as particles converge on stagnation points making kernel supports no longer complete. A significant improvement was suggested by Xu, Stansby, and Laurence (2009), then extended by Lind et al. (2012) to free-surface flows, who introduced a particle shifting process in order to stabilize the particle motion and homogenize their distribution in space. At the end of each time step, each particle is shifted by a small distance $\delta\mathbf{r}_a$ given by:

$$\delta \boldsymbol{r}_a = -\mathcal{D}\left(\frac{\partial C}{\partial s}\boldsymbol{s} + \alpha\left(\frac{\partial C}{\partial n} - \beta\right)\boldsymbol{n}\right) \tag{24}$$

where $\mathcal{D}$ is a diffusion coefficient, C is a particle concentration, $\mathbf{s}$ and $\mathbf{n}$ are the tangential and normal vectors at the surface, α controls the diffusion normal to the surface, and β is a reference concentration gradient for non-violent flows. More recently, Szewc, Pozorski, and Tanière (2011) and Leroy, Violeau, Ferrand, and Joly (2015) extended ISPH to the treatment of temperature (or other scalars). An optimal algorithm for particle shifting is still to be formulated.

Boundary conditions

The treatment of boundary conditions in SPH is still an open question and is particularly important for free-surface flow. There is a large range of methods, in particular for rigid walls but less so for open boundaries. The next subsections will address the most common models in the SPH literature.

Free-surface conditions In traditional SPH, no kinematic boundary condition is required at the free surface, since the particles move according to their Lagrangian velocity. On the other hand, the surface position and shape are only resolved up to the particle size. As for the dynamic free surface condition, WCSPH manages to set the pressure as zero by itself, thanks to the state equation, Eq. (11d). This is because the density decreases near the free surface due to the lack of particles above, as can be seen from Eq. (3). In ISPH, however, with the pressure being computed from a linear system, the pressure of free-surface particles must be forced to zero (i.e. Dirichlet condition). This requires tracking the free-surface particles, which is sometimes ambiguous. Several criteria exist to do so (e.g. Nair & Tomar, 2014). For WCSPH, Colagrossi, Antuono, and Le Touzé (2009) have shown that, unless free-surface boundary conditions are not explicitly imposed at the surface, different operators are necessary to account for the incomplete kernel support, with consequences for convergence and conservation properties (e.g. Antuono, Colagrossi, Marrone, & Molteni, 2010, 2012).

Rigid walls For engineering applications, enforcing solid impermeable boundaries is essential. Since Monaghan's (1994) first SPH model of free-surface flow, there have been many proposals for boundary treatments. They can be grouped into three general approaches: (a) fictitious particles; (b) repulsive functions; and (c) boundary integrals. The first two approaches are pragmatic and have been very popular to enable simulations to be run without resolving flow details in the near-vicinity of the boundary. This general classification is depicted in Fig. 4.

The fictitious particles method (a) is widely used in many applications. There are three approaches that use fictitious particles: prescribed (or dummy) fluid particles, mirror (or ghost) particles, and image transpose particles.

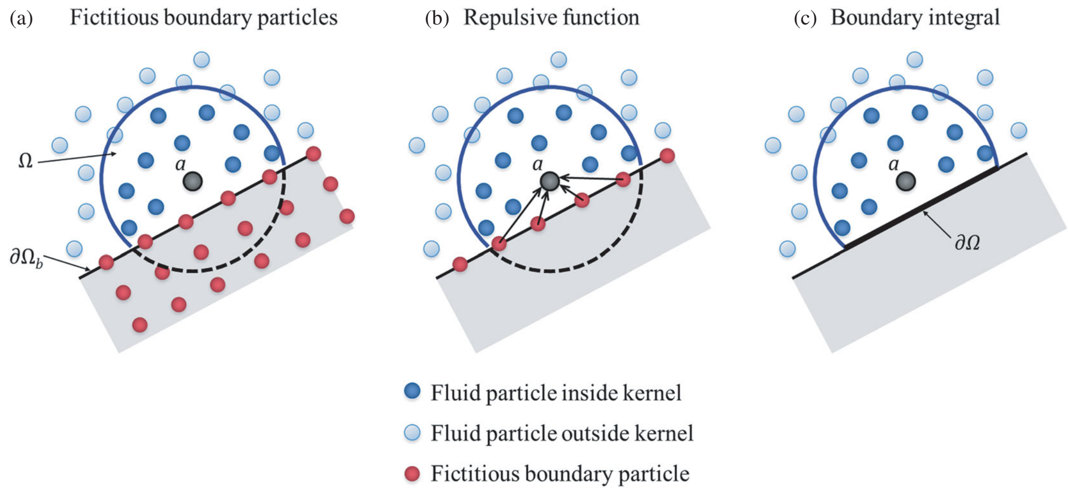


Figure 4 Generic SPH boundary treatments for rigid walls as particle a approaches the boundary $\partial\Omega_b$. The grey shaded area represents the solid boundary

The approach of prescribed (or dummy) fluid particles has many variants, with fluid particles placed inside the boundary area to complete the missing support of the kernel. The properties of the boundary particles can be specified in order to impose different boundary conditions (Issa, 2004), or they can vary to allow the density of the boundary particles to vary according to the continuity Eq. (12c), as used for example in the dynamic boundary condition of Crespo, Gómez-Gesteira, and Dalrymple (2007). Many of these techniques are very pragmatic but suffer from disadvantages such as not preventing particles penetrating the boundary and creating unphysical separation and boundary layers. In the context of imposing the shear stress in the vicinity of the wall, Maciá, Antuono, González, and Colagrossi (2011, 2012) assessed the errors in the Laplacian of the velocity and showed that a combination of the linear velocity profile and the technique of Takeda, Miyama, and Sekiya (1994) leads to the most accurate result. Adami, Hu, and Adams (2012) have further improved this technique by applying an additional velocity summation over the particles and a force balance to include the effect of body forces in the pressure assigned to the dummy particles. Mirror particles (sometimes referred to as ghost particles) are an intuitive approach to represent boundaries by generating a mirror image of the fluid particle arrangement. A fluid particle approaching a wall will interact with the mirror image particle of itself and therefore not penetrate a solid boundary since it cannot pass through itself. This approach is attractive since it works well for very simple geometries However, for complicated geometries, for example those that contain sharp vortex-forming corners, the use of a global mirror image is limited and becomes virtually prohibitively difficult (Børve, 2011). Other similar approaches have been suggested such as that of Bierbrauer, Bollada, and Phillips (2009). Ferrari et al. (2009) proposed a novel use of a local mirror image technique using virtual boundary particles (VBPs) where each individual fluid particle a, approaching a boundary, generates a single layer of mirror particles interacting only with particle a. Vacondio, Rogers, and Stansby (2011) showed that only generating a single layer of particles was not sufficiently accurate allowing particle penetration through the wall. The accuracy of the boundary condition in completing the kernel support was assessed by considering the zeroth-order moment of the kernel:

$$m_0(\mathbf{r}_a) = \int_\Omega w(|\mathbf{r}_a - \mathbf{r}|,\ h)\mathrm{d}\mathbf{r} \approx \sum_b V_b w_{ab} \tag{25}$$

which is a measure of the partition of unity (i.e.,1), an essential requirement for SPH kernels and their interpolation. Vacondio et al. (2011) proposed an improvement, the modified virtual boundary particle (MVBP) method, by adding one extra particle in a second layer and a treatment for corners where the method of Ferrari et al. (2009) only partially completes the kernel support. More recently, Fourtakas, Vacondio, and Rogers (2015) have addressed the accuracy of the local mirror approaches by proposing an extension to the MVBP method with an algorithm to complete the kernel support regardless of the geometrical complexity. The accuracy of the approach has been evaluated by examining numerical measures of accuracy appropriate for assessing the performance of derivatives (i.e. the ability of the SPH gradient and divergence to exactly reproduce constant or linear functions). Identifying measures of accuracy, such as the moments of the kernel, to compare different formulations should provide important uniformity of performance assessment of SPH (see section 3.3). The third type of solid boundary treatment that uses fictitious particles takes images of the particles in the fluid domain and transposes them from a Lagrangian to an Eulerian frame of reference (Marongiu, Leboeuf, & Parkinson, 2007; Narayanaswamy, 2009), then employs more conventional boundary treatments and transforms them back to the Lagrangian frame to impose the boundary condition. Combinations of the approaches based on prescribed (or dummy) fluid particles, mirror (or ghost) particles, and image transpose particles have also been proposed. These combined approaches use different elements such as the image transform approaches of Marrone, Colagrossi, Le Touzé, and Graziani (2010) where fluid properties are interpolated onto virtual particles in the fluid domain, which are then mirrored onto prescribed fictitious particles within the boundary.

The method of repulsive functions (b) is an alternative to using fictitious particles. In this method, fluid particles experience a repulsive force whose magnitude is a direct function of the distance between the particle and the boundary. Monaghan (1994) used a repulsive function based on the Lennard–Jones molecular potential to define a force which kept particles within the computational domain, but for a particle moving parallel to a boundary this does not produce a steady force. Later, in Monaghan and Kos (2000), this technique was modified to generate a constant force acting on a particle moving parallel to a wall. More recently, an alternative repulsive force boundary condition was suggested by Monaghan and Kajtar (2009) who used a Laplace summation to formulate the repulsion function. However, while all of the repulsive force-type boundary treatments prevent boundary penetration and perform adequately for macro-flows, none of them addresses the incomplete kernel support and therefore they are not as accurate as other techniques that properly address the lack of support in the kernel summation (Ferrand, Laurence, Rogers, Violeau, & Kassiotis, 2012).

More recently, alternative methods have been proposed to deal with complex wall boundary conditions in SPH, based on the boundary integrals of method (c). This idea was originated by Kulasegaram, Bonet, Lewis, and Profit (2004), followed by Feldman and Bonet (2007) and De Leffe, Le Touzé, and Alessandrini (2009). Ferrand et al. (2012) extended this approach to arbitrary wall boundary conditions, including the Neumann conditions for diffusion terms. This work was followed by Mayrhofer et al. (2013) and further simplifications were proposed by Amicarelli, Agate, and Guandalini (2013) and Cercos-Pita (2015). Recently, this technique has proved to be very efficient in predicting near-wall phenomena with ISPH (Leroy et al., 2014) and thermal processes (Leroy et al., 2015). At the heart of the boundary integral technique is the use of modified discrete SPH operators. For this purpose, one observes that when approaching a wall, the interpolation given by Eq. (1) should be renormalized in order to compensate the lack of neighbouring particles outside of the fluid domain (Fig. 4):

$$f(\mathbf{r}_a) = \frac{1}{\gamma_a} \int_\Omega f(\mathbf{r}) w(|\mathbf{r}_a - \mathbf{r}|,\ h) d\mathbf{r} + O(h^2) \qquad (26)$$

where γ_a is a renormalizing factor:

$$\gamma_a = \int_\Omega w(|\mathbf{r}_a - \mathbf{r}|,\ h) d\mathbf{r} \qquad (27)$$

(the integral is performed over the truncated circle of Fig. 4c). Numerically, this correction keeps the continuous interpolation accurate up to second order in h near the walls. The correcting factor γ_a is equal to 1 far from the boundaries, due to the kernel normalizing condition, while it is less than 1 near the walls. The continuous interpolation, Eq. (4), can then be modified as follows:

$$\nabla f(\mathbf{r}_a) \approx \frac{\rho_a}{\gamma_a} \int_\Omega \left[\frac{f_a}{\rho_a^2} + \frac{f(\mathbf{r})}{\rho(\mathbf{r})^2} \right] \nabla_a w(|\mathbf{r}_a - \mathbf{r}|,\ h) \rho(\mathbf{r}) d\mathbf{r} - \frac{\rho_a}{\gamma_a} \int_{\partial\Omega} \left[\frac{f_a}{\rho_a^2} + \frac{f(\mathbf{r})}{\rho(\mathbf{r})^2} \right] w(|\mathbf{r}_a - \mathbf{r}|,\ h) \mathbf{n}(\mathbf{r}) dS \qquad (28)$$

As pointed out by Ferrand et al. (Ferrand, Laurence, Rogers, & Violeau, 2010; Ferrand et al., 2012), the boundary integral may be discretized using boundary elements s (making a mesh of the boundary). The discrete gradient operator, Eq. (5), can then be rewritten as:

$$\mathbf{G}_a^\gamma\{f_b\} = \frac{\rho_a}{\gamma_a} \sum_b m_b \left(\frac{f_a}{\rho_a^2} + \frac{f_b}{\rho_b^2} \right) \nabla_a w_{ab} - \frac{\rho_a}{\gamma_a} \sum_s \rho_s \left(\frac{f_a}{\rho_a^2} + \frac{f_s}{\rho_s^2} \right) \nabla \gamma_{as} \qquad (29)$$

where $\nabla \gamma_{as}$ is the contribution of the boundary element s to the discretized boundary integral, i.e.:

$$\nabla \gamma_{as} = \int_s w(|\mathbf{r}_a - \mathbf{r}|,\ h) \mathbf{n}(\mathbf{r}) dS \qquad (30)$$

The final part of the process is to compute the values of the required quantities at the locations of the boundary elements (here f_s and ρ_s), which can be done by local interpolation, depending on the type of prescribed boundary condition (Mayrhofer et al., 2013). The SPH operators (Eqs (7) and (10)) of divergence and diffusion can be modified accordingly. The WCSPH Eqs (11) or ISPH Eqs (22) are then unchanged, the modified operators $\mathbf{G}_a^\gamma$ and others, being used in place of $\mathbf{G}_a$ and others.

Open boundaries Open boundaries are required as soon as one wants to simulate a large-scale flow, where the boundary conditions need to be prescribed either by a modeller or by a mesh-based code through coupling with SPH (see Advanced numerical features). However, such conditions are difficult to implement in SPH since an open boundary is Eulerian by nature. 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 (Vacondio, Rogers, Stansby & Mignosa, 2012). 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 problem (Mahmood, Kassiotis, Violeau, Rogers, & Ferrand, 2012), but treating a complex inlet where the flow is not parallel to the normal of the boundary remains a difficult issue. Similarly, a fluid particle leaving the domain through an outlet is first marked as a buffer particle, and some of its physical quantities are prescribed suddenly, generating shocks. More recently, Kassiotis, Ferrand, and Violeau (2013) proposed an alternative approach based on the boundary integrals technique described in Boundary conditions. Eulerian particles are placed on the open boundaries, with variable masses according to the desired inflow/outflow. The inflow Eulerian particles release fluid particles when their masses reach a threshold, while the masses of outgoing fluid particles are dispatched over the outflow Eulerian particles when they cross an outlet. This technique reduces spurious waves considerably and allows treatment of open boundaries in a unified way. Leroy (2014) proposed a similar technique for ISPH. However, despite these improvements, there is still no standard open boundary treatment in the SPH literature.

Overall, there has been steady progress in developing new boundary treatments in SPH with improved behaviour for flows in the vicinity of boundaries. However, it is clear that there is no consensus in the SPH community on the best approach and there are numerous phenomena which are not adequately captured by current formulations. Boundary conditions for SPH remain a challenge to be solved.

Advanced hydrodynamics with SPH

Turbulence In the early applications of SPH to hydraulic simulations, turbulence was generally ignored since SPH proved particularly appropriate for representing violent flows, where inertia, pressure and gravity play a major role. However, turbulence started to be addressed in SPH when it was also applied to confined flows.

As with many numerical methods, SPH has been used for modelling turbulent flows through direct numerical simulation (DNS), more precisely with very refined resolution. Most of these attempts have been conducted for 2-D simulations (e.g. Robinson, 2009; Robinson, Cleary, & Monaghan, 2008; Valizadeh & Monaghan, 2012), with a limited meaning and restricted field of application. A few attempts have been also made with 3-D simulations (Issa, 2004; Mayrhofer, Laurence, Rogers, & Violeau, 2015). For 3-D applications, large eddy simulation (LES) is obviously a more relevant approach, and it has been pointed out that the SPH interpolation in Eq. (1) is a kind of LES filter (e.g. Dalrymple & Rogers, 2006). However, though several successful simulations were performed for turbulence in a box with periodic conditions (Adami, Hu, & Adams, 2013; Shi, Ellero, & Adams, 2011), recent publications underline the difficulty of standard SPH to deal with wall boundary layers using the LES technique in SPH (Mayrhofer et al., 2015). It has also been pointed out by Monaghan (2002) that using the X-SPH variant mentioned in SPH governing equations amounts to modelling turbulence through the so-called α model (Holm, 1999). More details about the physical nature of this approach is provided by Violeau (2012). To date, the SPH turbulence models used for engineering applications have been based on RANS (Reynolds-averaged Navier–Stokes) approaches with first-order closure (eddy viscosity models), using mixing length (Violeau, Piccon, & Chabard, 2002) or k–ϵ models (Violeau, 2004). The latter was successfully applied e.g. by Shao (2006, wave overtopping, in association with ISPH) and De Padova, Mossa, Sibilla, and Torti (2013, 3-D hydraulic jump). Basically, a SPH k–ϵ model consists in writing the standard k–ϵ equations using the SPH discrete operators presented in SPH operators, i.e.:

$$\begin{aligned}\frac{\mathrm{d}k_a}{\mathrm{d}t} &= P_a + L_a\left\{\frac{\nu_{T,b}}{\sigma_k}, k_b\right\} - \varepsilon_a \\ \frac{\mathrm{d}\varepsilon_a}{\mathrm{d}t} &= C_{\varepsilon 1}\frac{\varepsilon_a}{k_a}P_a + L_a\left\{\frac{\nu_{T,b}}{\sigma_\varepsilon}, \varepsilon_b\right\} - C_{\varepsilon 2}\frac{\varepsilon_a^2}{k_a}\end{aligned} \tag{31}$$

The above equations are SPH approximations of:

$$\begin{aligned}\frac{\mathrm{d}k}{\mathrm{d}t} &= P + \nabla\cdot\frac{\nu_T}{\sigma_k}\nabla k - \varepsilon \\ \frac{\mathrm{d}\varepsilon}{\mathrm{d}t} &= C_{\varepsilon 1}\frac{\varepsilon}{k}P + \nabla\cdot\frac{\nu_T}{\sigma_\varepsilon}\nabla\varepsilon - C_{\varepsilon 2}\frac{\varepsilon^2}{k}\end{aligned} \tag{32}$$

The eddy viscosity $\nu_{T,a} = C_\mu k_a^2/\varepsilon_a$ is then used in the SPH momentum equation. The model constants σ_k, σ_ε, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$ and C_μ are set as in Launder and Spalding (1974). The turbulent kinetic energy production rate P_a is computed from the velocity gradient tensor using the SPH gradient operator. In the latest improvements, Ferrand et al. (2012) combined this SPH k–ϵ model with wall-renormalized operators (see Boundary conditions); Leroy et al. (2014) have mixed it with ISPH; Leroy et al. (2015) added buoyancy/turbulence coupling. Other RANS models in SPH (like the k–ω model and explicit algebraic Reynolds stress models; Wallin & Johansson, 2000) are suggested by Violeau (2012) and some of them were tested by Violeau and Issa (2006) and Issa, Violeau, Lee, and Flament (2010). Finally, one should mention that early attempts to use stochastic models based on the Langevin equations to deal with turbulence in SPH had limited success (Violeau et al., 2002; Welton & Pope, 1997).

Multi-fluid SPH One of the advantages of SPH is its ability to deal with multi-fluid flows, like air/water or water/oil mixtures, since the Lagrangian nature of this method makes it straightforward to capture the interface between various fluids. An application example with water and oil can be found in Violeau et al. (2007). However, as soon as large density variations are involved (like air/water), care should be given to the operators used in the spatial discretization. As pointed out by many authors (e.g. Colagrossi & Landrini, 2003; Hu & Adams, 2006), the squared density in the denominator of the discrete gradient, Eq. (5), leads to spurious voids at the fluids interface. Variants of the latter approximation were proposed to fix this issue, based on an alternative interpolation for density:

$$\rho_a \approx m_a \sum_b w_{ab} \tag{33}$$

This, in place of Eq. (3), allows working with particles of almost constant volumes, irrespective of their nature (air or water, for example). The resulting discrete gradient operator is:

$$\mathbf{G}_a\{f_b\} = \sigma_a \sum_b \left(\frac{f_a}{\sigma_a^2} + \frac{f_b}{\sigma_b^2} \right) \nabla_a w_{ab} \tag{34}$$

which is very similar to Eq. (5) with $\sigma_a \equiv \rho_a/m_a$ in place of ρ_a, and the mass m_b inside the sum removed. On similar grounds, Grenier, Antuono, Colagrossi, Le Touzé, and Alessandrini (2009) suggest:

$$\begin{aligned} \mathbf{G}_a\{f_b\} &= \sum_b V_a \left(\frac{f_a}{\Gamma_a} + \frac{f_b}{\Gamma_a} \right) \nabla_a w_{ab} \\ \Gamma_a &= \sum_b V_a w_{ab} \end{aligned} \tag{35}$$

where the sums run over all the neighbour particles b belonging to the same fluid (the one of particle a). Tartakovsky, Ferris, and Meakin (2009) present a very similar idea. Grenier et al.'s (2009) discrete divergence replaces Eq. (7), i.e.:

$$D_a\{\mathbf{f}_b\} = -\frac{1}{\Gamma_a} \sum_b V_b (\mathbf{f}_a - \mathbf{f}_b) \cdot \nabla_a w_{ab} \tag{36}$$

With this choice, the skew-adjointness property, Eq. (8), remains valid. Both models in Eqs (34) and (35) proved efficient, and the abovementioned papers (in particular Hu and Adams, 2006 and Grenier et al., 2009) also propose models to account for viscous forces and surface tension.

More recently, SPH has been applied to local (bed-load) sediment processes (e.g. Agate, Guandalini, Manenti, Sibilla, & Gallati, 2012, Leonardi & Rung, 2013; Manenti et al., 2012). The PhD theses of Ulrich (2013) and Fourtakas (2014) are probably the most advanced work done so far on SPH bed sediment motion with SPH. All these authors consider the sediment as a separate fluid phase with constant density and a more or less sophisticated rheology. None of these models use the above modified operators, considering that the sediment mixture has a density comparable to that of water. Validations were done on dam reservoir emptying, scour near waterworks, erosion due to ship blade motion, and others. Suspended sediment modelling has also been tried with SPH, but with an advection-diffusion approach that did not include pore water pressure (Zou, 2007).

Shallow water SPH One of the misunderstandings surrounding SPH is that the method only solves the Navier–Stokes equations. This is not correct; SPH is a methodology to perform a weighted interpolation of scattered data points to approximate operators (such as those given in SPH tools), which can then be used to solve ordinary or partial differential equations. A good example is the development of SPH to solve the (non-linear) shallow water equations (SWEs). The latter are a depth-averaged representation of the Navier–Stokes equations (depth averaging reduces the situation from 3-D to a 2-D problem) allowing simulations to be conducted at much larger horizontal scales. As hyperbolic partial differential equations, they are known to have specific methods of resolution (Riemann solvers with shock treatment) which make them particularly appealing. For solving the SWEs with SPH, some initial pioneering work has been conducted by Ata and Soulaïmani (2005) and then by Rodriguez-Paz and Bonet (2005). Using exactly the same technique as used for the Navier–Stokes equations, the shallow water equations are expressed in Lagrangian form as:

$$\begin{aligned} \frac{d\mathbf{v}}{dt} &= -\frac{\rho}{\rho_w} \nabla \rho + g(\nabla b + \mathbf{S}_f) \\ \frac{d\rho}{dt} &= -\rho \nabla . \mathbf{v} \end{aligned} \tag{37}$$

where the density ρ has been redefined as the mass of fluid per unit area in a 2-D domain such that $\rho = \rho_w d$, where ρ_w is the constant (conventional) density and d is the water depth, b is the bed elevation in this instance, and $\mathbf{S}_f$ is the bed friction. By deriving the equations from a variational principle, equations that can be used to simulate the shallow water can be solved using SPH (Rodriguez-Paz & Bonet, 2005). The final discrete equations are similar to Eq. (37) but use the SPH discrete operators as presented in SPH tools. Solving the SWEs with SPH has some distinct advantages including eliminating sources of numerical diffusion, simple and efficient set up, no need for any meshing that can be important during wetting and drying, and possibilities to include more physics which are beyond the limitations of mesh-based approaches.

The SPH particles now essentially become moving columns of water. This creates issues of accuracy when the columns of water move from deep water into shallower areas since the particles effectively change from being "tall and thin" with good accuracy to "short and fat" with severe deficiencies in terms of shallow flood waves (Vacondio, Rogers, & Stansby, 2012). This requires either re-meshing, which can be challenging numerically (Zhao, 2012), or variable resolution with particle splitting and coalescing (Vacondio, Rogers, Stansby, & Mignosa, 2013), which will be discussed in detail in Advanced numerical features. Multiple SPH codes for solving the shallow water equations now exist (e.g. De Leffe, Le Touzé, & Alessandrini, 2010; Vacondio, Rogers, Stansby, & Mignosa, 2012a) which are free for use and application. The development of SPH for the SWEs has opened up a new area of research, taking advantage of the meshless nature to simulate problems that are inherently difficult in mesh-based SWEs solvers such as complicated debris transport in flooding.

Advanced numerical features

Numerical stability As with all numerical methods, SPH suffers from numerical instabilities if the time step is not carefully controlled. These instabilities are enhanced by the Lagrangian nature of the method, and deserve special care. There are two approaches in studying SPH stability. The first one consists of keeping the discrete nature of the method in the analysis, while the second one consists of approximating the discrete SPH interpolation with its continuous form based on the interpolating kernel (see Eqs (1) and (4)). The latter approach can be performed in an arbitrary number of dimensions, but as an approximation it cannot handle all the numerical properties of SPH. The discrete approach is closer to the SPH approach but can hardly be conducted in the space of arbitrary dimension and with arbitrary number and position of neighbouring particles. With this approach, the particles are usually assumed to be placed on a Cartesian grid and only the closest neighbours are considered. Swegle, Hicks, and Attaway (1995) conducted a linear stability analysis of SPH for solids in one dimension from this discrete point of view, and determined a stability criterion based on the sign of the stress and kernel second derivative. Morris (1996) extended this work to an arbitrary number of neighbour particles for fluid flow, including viscous effects (see also De Leffe, 2011). On the other hand, Balsara (1995) used the method of continuous operators to investigate stability of SPH for fluids in one dimension and studied the impact of the kernel features and viscosity (see also Randles & Libersky, 1996). The last two authors came to the conclusion that the Fourier transform of the kernel plays a major role in the stability properties of SPH, which was later confirmed by Robinson (2009). It is more difficult to identify the kind of instabilities occurring and to remedy them. Recently, Dehnen and Aly (2012) studied the so-called pairing instability process in 3-D simulations, which consists of particle clustering by pairs. They demonstrate that the Wendland kernels help to avoid this issue. This is confirmed by several numerical investigations by other authors (e.g. Ferrand et al., 2012). However, none of the abovementioned papers give an explicit criterion for the maximum time step allowed in SPH. The time step is usually set according to numerical experiments. For WCSPH, Morris et al. (1997) suggest:

$$\Delta t = \min\left(0.25\frac{h}{c_0},\ 0.125\frac{h^2}{\max\,\nu_a},\ 0.25\sqrt{\frac{h}{\max|\mathbf{F}_a|}}\right) \tag{38}$$

that accounts for advection, diffusion and forces. This relation has been widely used since then. The first of the criteria of Eq. (38) is the traditional Courant–Friedrichs–Lewy condition. Morris (1999) proposed an additional criterion for surface tension. Recently, Violeau and Leroy (2014) proposed a consistent approach to improve the criteria of Eq. (38) based on a rigorous theoretical analysis. They proved that the stability properties of SPH are closely related to the choice of the time integrator, and further extended this work to ISPH (Violeau & Leroy, 2015). Their theory is well validated against extensive numerical tests.

Variable resolution Even with improved numerical behaviour and simulations accelerated using appropriate hardware (see below), the large majority of current SPH schemes employ a uniform particle resolution. A uniform particle resolution generally refers to the initial particle spacing which is uniform over the computational domain and, as mentioned previously, remains approximately constant during a simulation for an incompressible fluid. Primarily used for reasons of convenience, with limiting resolution required to simulate flow features of interest, the big drawback is that in many simulations much computational effort is wasted using uniform particle sizes in flow regions where the flow features can be adequately captured with larger interparticle distances. Indeed, following early work in astrophysics (Gingold & Monaghan, 1982; Hernquist & Katz, 1989), mathematical frameworks for variable resolution in SPH have been proposed, requiring minor adjustments to the basic formulations to ensure conservation of fundamental properties. Applying these ideas to hydraulic applications has presented a different set of challenges. For many problems in hydrodynamics, instead of allowing the particle interdistance to vary gradually, the use of regions of nested resolutions predefined by the modeller has been found to be acceptable (Oger et al., 2006, Omidvar et al., 2012, 2013). However, with violent hydrodynamics that often occur in free-surface flows, the distribution of particles of different sizes can change rapidly during a simulation. This suggests needs for a more efficient and dynamic approach for particle adaptivity. Providing efficient simulations with variable resolution using adaptive mesh refinement has been commonplace in FVM and FEM models since the early 1990s, but until recently there were no equivalent developments in SPH. Early efforts to employ the variable particle resolutions in SPH were made by Kitsionas and Whitworth (2002), and later strengthened using a variationally-derived formulation by Feldman and Bonet (2007). More recent work has focused on identifying the optimal refinement patterns (Vacondio, Rogers, & Stansby, 2012; Vacondio, Rogers, Stansby, & Mignosa, forthcoming; Vacondio, Rogers, Stansby, Mignosa, & Feldman, 2013). However, although particle splitting evidently increases resolution in required areas of the flow domain, on its own it leads to an ever increasing number of particles, which is ultimately inefficient.

Recently, novel work has been initiated whereby particles are coalesced or merged when such a fine particle resolution is not necessary (Barcarolo, Le Touzé, Oger, & De Vuyst, 2014; Reyes López, Roose, & Recarey Morfa, 2013; Vacondio, Rogers, Stanley, & Mignosa, 2013; Vacondio, Rogers, Stanley, Mignosa, & Feldman, 2013; Vacondio et al. forthcoming), leading to significant computational accelerations of up to 1–2 orders of magnitude compared to SPH with constantly uniform particle size. Of particular value are formulations that are derived from a variational principle that conserve the fundamental quantities.

The initial progress in developing dynamic particle adaptivity has been promising, but there are still some key challenges that need to be addressed in order to make the methodology robust. These challenges include:

- ensuring a uniform error distribution throughout the entire simulation domain;
- ensuring numerical convergence and stability;
- identifying the most efficient approach for activating adaptivity: e.g. block-structured adaptivity regions such as suggested by Barcarolo et al. (2014), or criteria-based local refinement as enabled by Vacondio et al. (2013b, forthcoming); and
- accommodating the consequences of rapidly varying smoothing lengths for use on a range of heterogeneous computer architectures, bearing in mind the need to "future proof" the development of SPH codes.

Coupling As pointed out in section 2.1, as a Lagrangian method SPH has great potential but also many drawbacks. Despite the new developments in variable space resolution presented above, in many cases it appears easier to restrict the use of SPH to relatively small domains. When analytical open boundary conditions cannot be prescribed, a coupling strategy can be used to inject some information into an SPH model from another (larger) model, for example, this might be a grid-based simulation. Here we define coupling to be the connection of SPH to another numerical model so that the advantages of two different numerical models are exploited. So far however, very little work on this topic has been published. For example, for free-surface flows Narayanaswamy, Gómez-Gesteira, Crespo, and Dalrymple (2010), Kassiotis et al. (2011), and Altomare, Suzuki et al. (2015b) coupled SPH with depth-integrated models appropriate for simulating large-plan areas such as coasts and shallow-water bodies (e.g. rivers, lakes and reservoirs). The philosophy behind these approaches is to use SPH for the highly localized flows, such as wave breaking, but using a more efficient model to simulate flow at much larger scale. For confined flows, for example, Neuhauser and Marongiu (2014) proposed an SPH-FV (finite volume) coupling of two Navier–Stokes models to treat boundary layers near hydrofoils. In all of these cases, SPH was coupled with a mesh-based method which was more appropriate for other areas of the flow. However, the most common topic of coupling SPH and other numerical methods concerns fluid/structure interactions. While rigid bodies moving in a fluid domain can be treated using SPH for both fluid and rigid bodies (e.g. Violeau et al., 2007), recent publications prefer a coupling strategy where the fluid is modelled with SPH while the rigid bodies are simulated by specific numerical approaches such as the discrete element method (DEM). A similar approach was successfully used by Canelas, Ferreira, Domínguez, and Crespo (2014) and Bilotta, Vorobyev, Mayrhofer, Hérault, and Violeau (2014) for real-life applications in hydraulics. On the other hand, computing the stresses and strain inside the solid can also be done using SPH (as mentioned earlier), but coupling SPH for the fluid with FVM or FEM for the solid has recently been employed with success (e.g. Groenenboom & Cartwright, 2010; Nunez, Li, Marongiu, & Combescure, 2014; Oger et al., 2009). All these coupling techniques have proven promising; however they have not reached their maturity, mainly due to the lack of a consensus for implementing boundary conditions accurately. More work is needed in this field both to identify the appropriate boundary conditions within SPH and to develop appropriate coupling strategies.

High-performance computing and graphics processing units SPH has traditionally been an expensive computational method, mainly due to two factors. First and foremost, compared to many mesh-based schemes, the number of interactions with neighbouring particles for each particle can be up to 100 in 2-D simulations and 200–500 in 3-D simulations, which is far greater than the number of neighbouring cells for FVM and FEM stencils. Secondly, the main options for simulating (almost) incompressible fluids are using the WCSPH which has a very small time step (typically on the order of 10^{-6}–10^{-5} s) due to the use of explicit[2] time integrators, or ISPH which uses time steps an order of magnitude larger, but requires the solution of a pressure Poisson equation (not a trivial task for simulations with many millions of particles). Hence, the simulation of cases involving anything more than a few hundred thousand particles is a major undertaking.

Until recently, the only viable option was to use high-performance computing (HPC) using many thousands of cores with a standard message passing interface (MPI) to handle communication between processors on distributed memory systems (Maruzewski, Le Touzé, Oger, & Avellan, 2010). Multi-core processors have become more popular in recent years, where the central processing unit (CPU) on each processor can have up to 16 cores (at the time of writing) with shared memory requiring programming frameworks such as OpenMP. Obtaining the maximum performance from multiple nodes with multiple cores with a mixture of distributed and shared memory has required a combination of OpenMP-MPI approaches working across heterogeneous architectures (Moulinec, Issa, Marongiu, & Violeau, 2008). This is technically difficult, expensive in terms of hardware investment and maintenance, and highly restrictive in terms of code portability across other architectures – an important consideration for disseminating use throughout industry.

More recently, graphics processing units (GPUs) have been used to take the place of HPC clusters. Originating from computer games and the computer graphics industry, GPUs are highly portable devices designed for high throughput data processing. Importantly, the emergence of GPUs and their rapid uptake within the scientific computing communities has enabled huge advances to be made (see list of CUDA Research Centres[3]). With SPH ideally suited to the streaming multiprocessor parallel architecture of GPUs, several free open-source GPU codes have been recently developed, including

GPUSPH (Hérault, Bilotta, & Dalrymple, 2010), DualSPHysics (Crespo et al., 2015) and AQUAgpusph (Cercós-Pita, 2015). Simulations with many millions of particles can now be performed using laptop computers with runtimes of the order of hours rather than months that are required for expensive HPC systems.

More generally, GPUs are a disruptive technology for computing that have enabled SPH to be attractive and feasible for industrial companies, where applications requiring simulations with many millions of particles are now within reach with minimal investment, enabling repeated design runs in reasonable runtimes (Longshaw & Rogers, 2015). Since the emergence of GPUs, other architectures have appeared, such as Intel's Xeon Phi, which has 60 cores on a single processor, again without needing the supporting architecture of HPC clusters. The challenge that now faces the SPH community is to develop new validated formulations that can be implemented within the parallel heterogeneous architectures of emerging technologies such as GPUs and other devices.

To conclude this brief review of SPH for hydraulics, it is worth mentioning that the tools presented here are far from being exhaustive. Additional features and recipes have been omitted for the sake of simplicity, e.g. governing equations for internal energy (e.g. Yue, Pearce, Kruisbrink, & Morvan, 2015), or renormalizing kernel techniques that improve the accuracy and consistency of SPH operators (e.g. Bonet & Lok, 1999; Fatehi & Manzari, 2011b).

3 Future of SPH in hydraulics

3.1 *Key ongoing challenges*

It is clear that SPH offers some key advantages over conventional mesh-based solvers and that considerable progress has been made since the early 2000s to make the method both numerically stable and computationally feasible for use by hydraulic engineers and practitioners. However, before its use can become widespread, there are important developments to undertake and challenging barriers to overcome. The main efforts, therefore, should be directed primarily at addressing the issues that prevent industry investing in and using the method.

As discussed in Previous validation of SPH, key in this process is the need for development of high quality benchmark test cases that can be used not just for academic validation, but also to compare rival SPH formulations and convince industry of the suitability and power of SPH for their applications. To date, the Smoothed Particle Hydrodynamics European Research Interest Community (SPHERIC, http://spheric-sph.org/) has been instrumental in pushing the development of SPH and engaging with water, energy, and environmental hydraulics companies and agencies. SPHERIC was founded to bring together SPH researchers and users, provide a forum for interaction and to combine efforts to enhance SPH development and applications through a collaborative push. This has been partially achieved with standardized benchmark test cases, and annual international workshops for discussing new significant developments, emerging research and end-user requirements. A recent key development from SPHERIC has been the identification of the following SPH Grand Challenges which must be tackled to bring the method to maturity: (i) numerical stability; (ii) convergence; (iii) boundary conditions; and (iv) adaptivity.

The SPHERIC Grand Challenges have been useful to focus development attention, although some challenges appear to be more tractable than others. Proofs of convergence, for instance, remain elusive but works on higher-order convergence are beginning to appear (Lind & Stansby, 2015; Litvinov, Hu, & Adams, 2014). From the perspective of making the method attractive to industry, the main practical challenges require a different emphasis and focus on making the method more usable for a wider range of applications. The key tasks for the next five years can be identified as:

(1) Coupling – this requires robust and accurate boundary conditions at open boundaries.
(2) Turbulence – despite the efforts made over the past 10 years (see Advanced hydrodynamics with SPH), advanced turbulence models for SPH (in particular, a convincing LES approach for SPH) are still poorly developed, requiring huge computation time even with GPUs (Mayrhofer et al., 2015).
(3) Variable resolution – some initial progress has been made in recent years, but providing robust schemes that give the user control over how it is employed over the potentially large range of temporal and spatial scales poses a significant challenge.
(4) Multi-phase – numerous multi-phase algorithms have been proposed (in addition to the multi-fluid developments highlighted in Advanced hydrodynamics with SPH), but there are many applications which physics are beyond the reach of current models, and validations need to be more extensive.

3.2 *Future developments*

There is currently a proliferation of different formulations and approaches, but which will prevail is unknown. The community of researchers, developers and engineers should be aiming to eliminate poorly validated codes and formulations that are not generalizable. To tackle this issue, the following developments are necessary and can be considered within four broad groups, as outlined below.

(1) The SPH community needs to move away from using formulations requiring empirical parameters that control the performance of the codes. An over-dependence on the use of parameters damages the credibility of the method.

(2) Research should focus on optimized simulations with minimized uniform error distributions. The continual increase in computational power should enable this development.
(3) Integration of well-validated SPH codes into the design methodologies should be promoted to hydraulic, water, energy, and environmental hydraulics companies and agencies, e.g. the design of breakwaters or spillways (Altomare et al., 2014; Lee et al., 2010; Rogers et al., 2010). Some example work has been undertaken for some applications such as jet impingement on turbines (Marongiu, Leduc, & Shaller, 2011) and fuel-tank sloshing (Longshaw & Rogers, 2015), but there is considerable work still required. This necessitates a dialogue with industrial companies to identify their needs at the same time as educating potential users of the possibilities and limitations of the method.
(4) The identification of new applications of SPH is essential in helping to push the development of the method forward. New applications help developers to identify the shortcomings of the method, but also highlight new opportunities for its development. For example, will developments in multiphase and adaptive multi-resolution approaches allow SPH developers to tackle more difficult challenges?

3.3 *Standards*

Although SPH for engineering applications has witnessed a significant improvement in academic rigour since the formation of SPHERIC in 2005, with increasing interest and activity in method development, the SPH community needs to be rigorous in defining acceptable standards. In the 1980s and 1990s, the aerospace research community underwent a period of self-examination and as result one of the outcomes was the introduction of the requirement that numerical papers should include convergence studies by default. This led to the emergence of uniform reporting of measures of errors, such as the grid convergence indicator (GCI) of Roache (1994), which allows different numerical studies to be compared within a consistent approach. In a similar manner, for the future credibility of the methodology, the SPH community needs to define standards of acceptability for future research and publications. Here we propose the following standards:

(1) Validation benchmarks with analytical, or semi-analytical, solutions or converged reference numerical solutions from validated numerical codes should be used as a rule.
(2) Validation benchmarks with experimental or field data with high degrees of repeatability, and estimations of variability, e.g. Lobovský, Botia-Vera, Castellana, Mas-Soler, and Souto-Iglesias (2014) for dam breaks, should supplement analytical benchmarks.
(3) Where a reference solution exists, a numerical convergence study needs to be conducted to estimate error norms such L_2 and L_1 or L_∞ where appropriate for at least three different resolutions, preferably using a consistent measure of error such as the GCI (Lee et al., 2008 and Leroy et al., 2014 provide examples of such a study with SPH).
(4) The simulation papers should report plots of all relevant flow fields which highlight problematic issues for the SPH community to address. For example, noisy pressure fields have been a notoriously difficult problem for SPH, but publications tend not to show problematic issues unless they have proposed a remedy.
(5) Use numerical measures of accuracy that allow assessment of the performance of new SPH schemes for consistency and convergence, for example the zeroth- and first-order moments of the smoothing kernel and their gradients (e.g. Fourtakas et al., 2015).

3.4 *SPH in the long term*

In the long term, one may envisage that:

- SPH should become part of the overall CFD landscape for hydraulic, water, energy, and environmental companies and government agencies, used appropriately and with experience-based insight. SPH is already part of undergraduate and MSc courses being offered around the world (e.g. University of Manchester, UK; École Centrale de Nantes, France, among others), and SPHERIC has been instrumental in introducing short courses (continuing professional development or CPD) tailored specifically for industry. As mentioned earlier, SPH is not always an appropriate tool for a given application. As a community intimately connected to teaching and learning, it needs to prepare the engineers and scientists of tomorrow to use the new technology appropriately.
- Formulations such as the classical WCSPH have some key attractions compared to ISPH, particularly in terms of simplicity, stability and computational expense. However for hydraulics/hydrodynamics applications, WCSPH will need to be supplemented with more robust formulations to compete with the highly accurate pressure fields predicted by ISPH.
- Although mathematically fascinating, the standard SPH formulation has been problematic with development of robust and rigorous treatments of boundary conditions and turbulence, among other issues, which are good examples of recent and current challenges. Increasing computing power could remove the barrier to alternative particle and meshless/meshfree methods, e.g. the finite volume particle method (FVPM) being developed by Quinlan, Lobovský, and Nestor (2014), the pointset method of Vacondio and Mignosa (2009), and peridynamics where the formulation for the governing equations is expressed in integral form and remains valid in the presence of ruptures in the medium (Ganzenmüller et al., 2015). Introducing boundary conditions and variable resolution in these models is considerably easier than in SPH. With improved mesh-based schemes, particle tracking methods such as the particle-in-cell (PIC) are re-emerging with

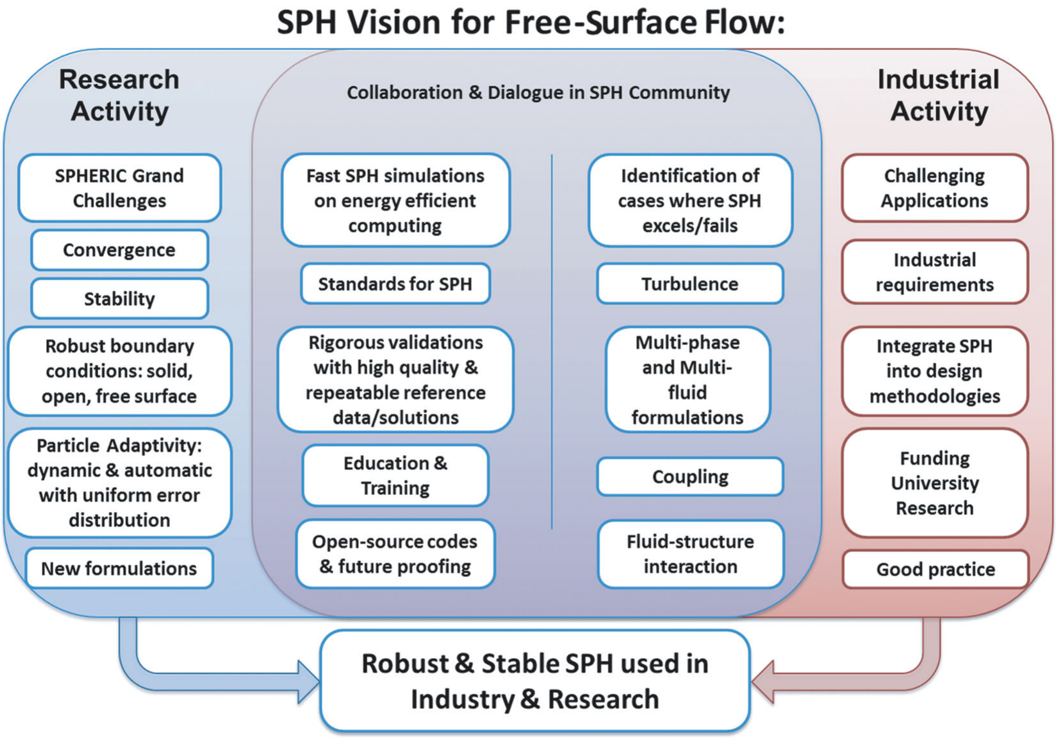


Figure 5 SPH vision for free-surface flow

new innovations (Kelly 2013); these methods are particularly attractive as they are several orders of magnitude faster than SPH. Similarly, the lattice-Boltzmann method (LBM) has made massive developments in the past 10 years, developing robust sharp interface multi-phase algorithms (Favier, Revell, & Pinelli, 2014). Many of these methods have their own advantages and disadvantages, and could be combined with SPH to create new numerical schemes and open new avenues in research and applications.

To conclude, SPH is at an exciting stage in its development. Its application to free-surface flows and in hydraulics in general continues to open new areas of activity. Our vision to focus activity in moving SPH forward is summarized in Fig. 5. The SPH community must strive to push the method forward in a rigorous and collaborative approach, liaising with industry and educating the users of tomorrow.

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Notes

1. There are several conventions about SPH notations in the literature (particles are often labelled as i and j). Here we follow the original notations of Monaghan (1992).
2. Using implicit time integration schemes in SPH have been poorly addressed in the literature. See e.g. Cueille (2005).
3. https://research.nvidia.com/content/cuda-research-centers

Notation

a, b = particle labels (–)
c_0 = speed of sound (ms^{-1})
C = particle concentration (–)
D_a = discrete divergence operator (m^{-1})
$\mathcal{D}$ = diffusion coefficient (–)
d = depth (m)
e = specific internal energy (m^2 s^{-2})
$\mathbf{F}$ = force (kg m s^{-2})
f, $\mathbf{f}$ = arbitrary scalar and vector functions (?)
f_a, $\mathbf{f}_a$ = function attached to particle a (?)
$\mathbf{G}_a$ = discrete gradient operator (m^{-1})
$\mathbf{g}$ = gravity (m s^{-2})
H = Hamiltonian (kg m^2 s^{-2})
h = smoothing length (m)
k = turbulent kinetic energy (m^2 s^{-2})
L_a = discrete Laplacian operator (m^{-2})
m = mass (kg)
n = space dimension
$\mathbf{n}$ = boundary inward, unit normal vector (–)
p = pressure (kg m^{-1} s^{-2})
$\mathbf{r}$ = position vector (m)
$\mathbf{r}_{ab}$ = vector linking two particles (m)
r_{ab} = particle distance (m)
$\mathbf{S}_f$ = bed friction (–)

$\mathbf{s}$ = tangential vector at free-surface (−)
V = volume (m^n)
$\mathbf{v}$ = velocity vector ($m\ s^{-1}$)
w = kernel (m^{-n})
α, β = shifting coefficients (−)
γ = boundary renormalization integral (−)
Δt = time step (s)
ϵ = energy dissipation rate ($m^2\ s^{-3}$)
ρ = density ($kg\ m^{-n}$)
ρ_0 = reference density ($kg\ m^{-n}$)
ρ_w = density of water ($kg\ m^{-n}$)
ν = kinematic molecular viscosity ($m^2\ s^{-1}$)
ν_T = kinematic eddy viscosity ($m^2\ s^{-1}$)
$*$ = property in the star region of a Riemann problem

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