Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Computational Physics 209 (2005) 541–558
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

Hamiltonian formulation of the variable-*h* SPH equations

Javier Bonet *, Miguel X. Rodríguez-Paz [1]

Civil and Computational Engineering Research Centre, School of Engineering, University of Wales, Swansea, Swansea SA2 8PP, United Kingdom

Received 9 June 2004; received in revised form 7 February 2005; accepted 7 March 2005
Available online 24 May 2005

Abstract

In this paper a variational formulation of smooth particle hydrodynamics for dynamic problems is presented. The resulting equations treat the continuum as a Hamiltonian system of particles where the constitutive equation of the material is represented via an internal energy term. In the case of fluids the internal energy term is a function of density. The new formulation introduces a variable smoothing length for the evaluation of density and incorporates a consistent approach for the treatment of rigid boundaries. The method overcomes some problems faced by standard SPH approaches that use constant smoothing lengths and provides a variational context for a variable smoothing length formulation. A numerical example shows the capabilities of this novel formulation.

Keywords: SPH; Variable smoothing-length; Variational formulation

1. Introduction

Twenty-five years have lapsed since the introduction of smooth particle hydrodynamics (SPH) as a powerful mesh free technique for the solution of non-axisymmetric phenomena in astrophysics [1,2]. It soon developed into a robust technique that could deal with complicated physics [3,4]. There have been many applications of the method in other fields including engineering, with applications such as metal forming [5] and the simulation of impact and mould filling casting processes. SPH has also been applied to free surface flows [6,7].

SPH is a Lagrangian particle method that does not require a grid to evaluate spatial derivatives. It is quite a simple but robust technique. However, there are certain problems that arise due to the nature of

* Corresponding author. Tel.: +52 222 3032084.
E-mail addresses: j.bonet@swan.ac.uk (J. Bonet), rodriguez.miguel@itesm.mx (M.X. Rodríguez-Paz).
[1] Present address: ITESM Campus Puebla, Via Atlixcayotl 2301, Puebla CP72800, Mexico.

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2005.03.030

the interpolation, e.g., tension instability [8–10]. Several of these problems have been studied by a number of researchers see for instance the papers by Monaghan [4,8], Benz [10], Randles and Libersky [11], Gray et al. [12]. The convergence of the SPH technique to the continuous model has been studied by Vila [19].

The standard SPH method uses a constant smoothing length (h) for the particles. However, the need for a variable smoothing length appears as a consequence of the physics of certain problems such as the expansion of a very compressible material. If such problems are treated with a constant h approach, after certain analysis time, very few neighbour particles will be found for a particle that at the beginning of the analysis was well covered. On the other hand, problems like contraction of a compressible material would result in a large number of neighbour particles, resulting in expensive computations. Algorithms to vary the smoothing length have been proposed in the past [10].

The aim of this paper is to introduce a novel formulation of the SPH method based on a variable smoothing length (*variable-h*) within a variational framework. In this way, the continuum is represented by a discrete set of particles each with a given mass and velocity. The constitutive representation of the material is achieved via an internal energy term, which for adiabatic reversible problems is simply a function of the particle positions. This leads to the continuum being modelled as a Hamiltonian system of particles where the equations of motion of each particle are given by the classical Lagrange equations. This procedure of deriving the governing equations bypasses the standard differential equations of equilibrium and, more importantly, ensures that the constants of motion such as linear and angular momentum are preserved. For fluids the internal energy term is derived from the traditional SPH equation for the density.

Fahrenthold and Koo [17] have presented a Hamiltonian particle hydrodynamics method, in which the physical system is modelled using a system of 'n' thermomechanically interacting physical particles. As the authors mention in their report, their method differs from SPH methods as there is no interpolation or weighted residual solution techniques involved and it relies exclusively on energy concepts.

2. Smooth particle hydrodynamics

In the SPH method, a function $f(\mathbf{x})$ and its gradient ∇f are approximated in terms of values of the function at a number of neighbouring particles and a kernel function $W(\mathbf{x}-\mathbf{x}_b) = W_b(\mathbf{x}, h_b)$ as [5],

$$f_h(\mathbf{x}) = \sum_{b=1}^{M} V_b f_b W_b(\mathbf{x}, h_b) \quad \text{and} \quad \nabla f_h(\mathbf{x}) = \sum_{b=1}^{M} f_b \mathbf{g}_b(\mathbf{x}), \tag{1}$$

where h is the smoothing length and determines the support of the kernel (see Fig. 1). V_b denotes a tributary volume associated to particle b. In the standard SPH method, the gradient vectors $\mathbf{g}$ are simply $\mathbf{g}_b = V_b \nabla W_b$.

In order to ensure linear consistency (i.e., the interpolation and gradients of constant and linear functions are exactly evaluated) some correction techniques have been introduced (see for instance [7]).

2.1. Density evaluation in standard SPH

In the standard SPH formulation, the mass of a particle is smoothed over a sub-domain of radius $2h$, where h the so-called smoothing length. In order to understand this, consider a system of particles with masses m_I distributed over a domain as shown in Fig. 1. The discrete system of particles has a density distribution of the form

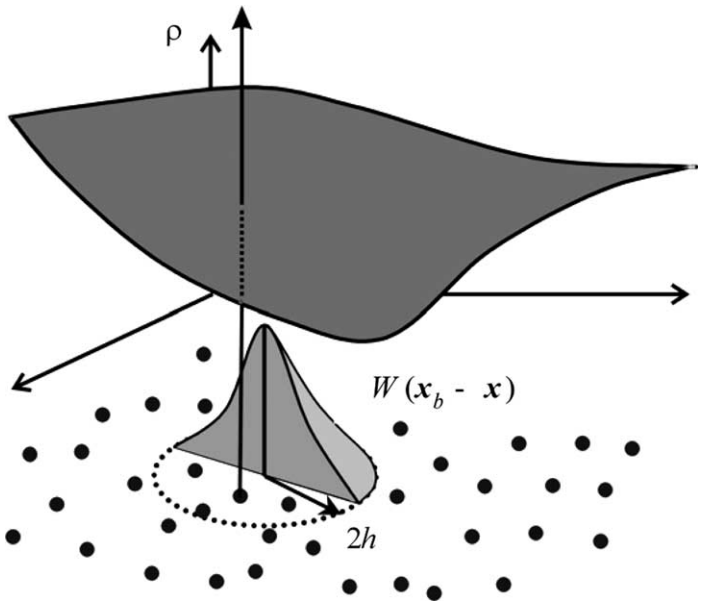

Fig. 1. SPH density interpolation.

$$\hat{\rho}(\mathbf{x}) = \sum_{I}^{N} m_I \delta(\mathbf{x} - \mathbf{x}_I), \tag{2}$$

where δ is the Dirac's delta and N is the number of particles in the system. In order to reconstruct a continuum density interpolation, the kernel smoothing concept can be applied to the discrete density (2) is smoothed or filtered using a convolution integral with a kernel function W as,

$$\rho(\mathbf{x}) = \frac{\int_\Omega \hat{\rho}(\mathbf{x}') W_x(\mathbf{x}')\, \mathrm{d}\mathbf{x}'}{\int_\Omega W_x(\mathbf{x}')\, \mathrm{d}\mathbf{x}'}, \tag{3}$$

where $W(\mathbf{x}, \mathbf{x}', h) = W_{x'}(\mathbf{x}, h)$ has a compact support of radius $2h$ and a continuous bell shape shown in Fig. 1 and Ω represents the entire domain. Substituting Eq. (2) into above expression and noting the Dirac's delta properties gives

$$\rho_I = \frac{\sum_J m_J W_I(\mathbf{x}_J, h_I)}{\int_\Omega W_I(\mathbf{x}_J, h_I)\, \mathrm{d}V}, \tag{4}$$

where J are the neighbour particles for particle I. The integral in the denominator in Eq. (4) has usually a value of 1 since the kernel function is scaled to yield a unit integral. However, this is not the case for particles close to a boundary, as explained in the following section.

3. Correction function γ_I

In the standard SPH formulation and in the absence of boundaries the denominator integral in Eq. (4) is assumed to be equal to one. This is no longer valid for particles that are within a distance to a rigid boundary that is less than $2h$ for that particle (see Fig. 2).

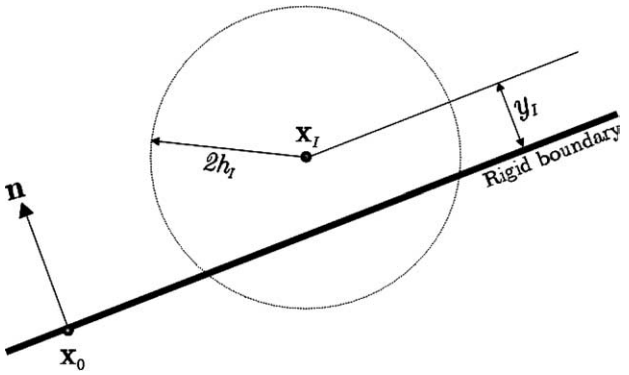

Fig. 2. Particle near a rigid boundary.

Defining a function gamma [13] as follows:

$$\gamma_I(\mathbf{x}_I, h_I) = \int_\Omega W_I(\mathbf{x}, h_I)\, \mathrm{d}V. \tag{5}$$

Then Eq. (4) becomes

$$\rho_I = \frac{1}{\gamma_I} \sum_J m_J W_I(\mathbf{x}_J, h_I). \tag{6}$$

For simple boundaries the function γ_I can be expressed in terms of the distance y_I to the rigid boundary, e.g., for a plane,

$$y_I = (\mathbf{x}_I - \mathbf{x}_0) \cdot \mathbf{n}, \tag{7}$$

where $\mathbf{n}$ is the unit vector normal to the boundary and $\mathbf{x}_0$ is any point on the boundary.

3.1. Density evaluation – variable-h

The evaluation of the density using a constant smoothing length is a normal practice in SPH, this can lead to resolution problems if the length scale of the problem changes considerably [10]. In the case of fluids with certain compressibility, for instance, a case of uniform expansion or contraction of the system of particles (see Fig. 3), the smoothing length needs to vary in order to get a realistically simulation of the problem.

In the case of an uniform expansion (Fig. 3(a)), the particle in the centre would eventually have no neighbours around it. And in the case of a contraction case (Fig. 3(b)), all the particles would eventually be within $2h$ for the particle in the centre and according to Benz [10], this would case the breakdown of the method.

Different approaches have been proposed in order to estimate the smoothing length from previous values of density or increasing it until a certain number of neighbours have been found. However, those approaches can lead to particle clumping [10].

Several attempts have been made by SPH practitioners to overcome these difficulties such as the use of symmetrised forms of the kernel functions and smoothing lengths [10].

In general, h must change in such a way that the number of particles contributing to the integrals remain constant, or

$$\rho h^{d_m} = \text{constant} = \rho_0 h_0^{d_m}. \tag{8}$$

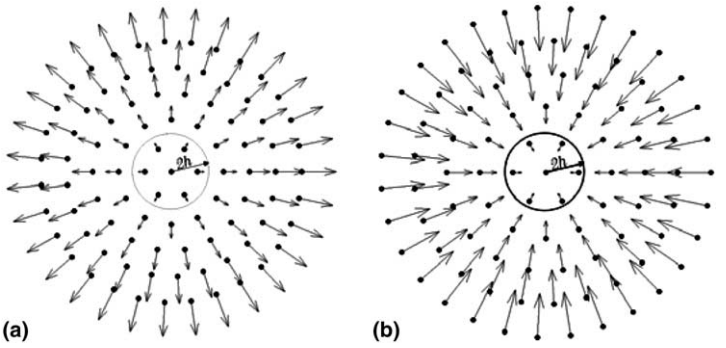

Fig. 3. Situations in which the use of constant h leads to poor results: (a) uniform expansion, (b) uniform contraction.

This gives an equation for the instantaneous smoothing length h as

$$h = \left(\frac{\rho_0}{\rho}\right)^{1/d_m} h_0, \tag{9}$$

where d_m is the number of space dimensions. It is important to note that if the above equation is enforced strictly, density and smoothing length are dependent on each other.

In this case the density equation (6) is an implicit non-linear equation for ρ_I due to the dependency of h_I on ρ_I. Furthermore, the value of γ_I will also be affected by changes in ρ_I. In order to solve this difficulty, Eq. (9) is typically enforced in a relaxed way by taking density at a previous time-step.

In the following sections a more consistent approach is presented in order to solve the system of non-linear equations defined by (6) and (9) and to obtain the associated variational consistent forces that emerge as a consequence of changes in h.

4. Rate of change of density with variable-h

In order to derive the variational consistent forces and to develop a simple algorithm for the solution of Eqs. (6)–(9), it is first convenient to obtain the variation of density that emerges from changes in particle positions. For this purpose, differentiating the density equation gives

$$\rho_I D\gamma_I[\delta\mathbf{v}] + \gamma_I D\rho_I[\delta\mathbf{v}] = \sum_J m_J \left(\frac{\mathrm{d}W_I}{\mathrm{d}r_{IJ}} Dr_{IJ}[\delta\mathbf{v}] + \frac{\mathrm{d}W_I}{\mathrm{d}h_I} Dh_I[\delta\mathbf{v}]\right). \tag{10}$$

In order to solve this equation for $D\rho_I[\delta\mathbf{v}]$ it is first necessary to evaluate the derivatives of the correction function γ_I and other derivatives such as: $\frac{\mathrm{d}W_I}{\mathrm{d}r_{IJ}}$, $Dh[\delta\mathbf{v}]$, $D\gamma_I[\delta\mathbf{v}]$ and $Dr_{IJ}[\delta\mathbf{v}]$.

The derivative of first term in Eq. (10) is found from Eq. (6) as

$$D\gamma_I[\delta\mathbf{v}] = \frac{\gamma_I'}{h_I}[\mathbf{n}\cdot\delta\mathbf{v}_I] + \frac{\gamma_I' y_I}{h_I \rho_I d_m} D\rho_I[\delta\mathbf{v}], \tag{11}$$

where $\gamma' = \frac{\mathrm{d}\gamma}{\mathrm{d}y}$. From Eq. (8), we obtain the following expressions for the derivative of the smoothing length,

$$h^{d_m} D\rho[\delta\mathbf{v}] + \rho d_m h^{d_m-1} Dh[\delta\mathbf{v}] = 0, \tag{12}$$

$$Dh[\delta\mathbf{v}] = -\frac{h}{d_m} D\rho[\delta\mathbf{v}]. \tag{13}$$

The kernel function is a function f of the non-dimensional distance between two particles and in general has the form

$$W_I(\mathbf{x}_J, h_I) = \frac{1}{h^{d_m}} f\left(\frac{r_{IJ}}{h_I}\right), \tag{14}$$

where r_{IJ} is the distance between particle I and its neighbour J, given by

$$r_{IJ^2} = (\mathbf{x}_J - \mathbf{x}_I)\cdot(\mathbf{x}_J - \mathbf{x}_I). \tag{15}$$

Hence, then the derivative of the kernel function is

$$\frac{\mathrm{d}W_I}{\mathrm{d}r_{IJ}} = \frac{1}{h_I^{d_m+2}} f'\left(\frac{r_{IJ}}{h_I}\right), \tag{16}$$

where $f' = \frac{\mathrm{d}f}{\mathrm{d}(r/h)}$ and differentiating using the chain rule, the derivative of the kernel function with respect to the smoothing length is

$$\frac{\mathrm{d}W}{\mathrm{d}h_I} = \frac{-d_m}{h_I^{d_m+1}} f\left(\frac{r_{IJ}}{h_I}\right) - \frac{r_{IJ}}{h_I^{d_m+2}} f'\left(\frac{r_{IJ}}{h_I}\right) = -\frac{1}{h_I}\left(d_m W_I(\mathbf{x}_J, h_I) + r_{IJ}\frac{\mathrm{d}W_1}{\mathrm{d}r_{IJ}}\right). \tag{17}$$

Finally, differentiating Eq. (15) gives

$$Dr_{IJ}[\delta\mathbf{v}] = \frac{1}{r_{IJ}}(\mathbf{x}_J - \mathbf{x}_I)\cdot(\delta\mathbf{v}_J - \delta\mathbf{v}_I). \tag{18}$$

Substituting Eqs. (13), (17) and (18) into Eq. (10) yields:

$$\begin{aligned}\rho_I D\gamma_I[\delta\mathbf{v}] + \gamma_I D\rho_I[\delta\mathbf{v}] = {} & \sum_J m_J\left(\frac{\mathrm{d}W_I}{\mathrm{d}r_{IJ}}(\mathbf{x}_J - \mathbf{x}_I)\cdot(\delta\mathbf{v}_J - \delta\mathbf{v}_I)\right) \\ & + \left[\sum_J m_J \frac{1}{h_I}\left(d_m W_I(\mathbf{x}_J, h_I) + r_{IJ}\frac{d_m W_I}{\mathrm{d}r_{IJ}}\right)\right]\frac{h_I}{\rho_I d_m} D\rho_I[\delta\mathbf{v}],\end{aligned} \tag{19}$$

$$\rho_I D\gamma_I[\delta\mathbf{v}] + \left(\frac{\alpha_I}{\rho_I d_m}\right) D\rho_I[\delta\mathbf{v}] = \sum_J m_J\left(\frac{\mathrm{d}W_I}{\mathrm{d}r_{IJ}}\frac{1}{r_{IJ}}(\mathbf{x}_J - \mathbf{x}_I)\cdot(\delta\mathbf{v}_J - \delta\mathbf{v}_I)\right), \tag{20}$$

where

$$\alpha_I = -\sum_J m_J r_{IJ}\frac{\mathrm{d}W_I}{\mathrm{d}r_{IJ}}. \tag{21}$$

Finally, substituting Eq. (11) into Eq. (20) yields after simple algebra

$$\left(\frac{\gamma_I' y_I}{h_I d_m} + \frac{\alpha_I}{\rho_I d_m}\right) D\rho_I[\delta\mathbf{v}] = \sum_J m_J\left(\frac{\mathrm{d}W_I}{\mathrm{d}r_{IJ}}\frac{1}{r_{IJ}}(\mathbf{x}_J - \mathbf{x}_I)\cdot(\delta\mathbf{v}_J - \delta\mathbf{v}_I)\right) - \frac{\rho_I\gamma_I'}{h_I}[\mathbf{n}\cdot\delta\mathbf{v}_I] \tag{22}$$

or

$$D\rho_I[\delta\mathbf{v}] = \beta_I\sum_J m_J\nabla W_I(\mathbf{x}_J, h_I)\cdot(\delta\mathbf{v}_J - \delta\mathbf{v}_I) - \frac{\beta_I\rho_I\gamma_I'}{h_I}[\mathbf{n}\cdot\delta\mathbf{v}_I], \tag{23}$$

where

$$\beta_I = \left(\frac{\gamma_I' y_I}{h_I d_m} + \frac{\alpha_I}{\rho_I d_m}\right)^{-1}. \tag{24}$$

Noting that taking $\delta \mathbf{v}_J = \mathbf{v}_J$ and $\delta v_I = \mathbf{v}_I$, then Eq. (24) gives the rate of density as:

$$\dot{\rho}_I = \rho_I \left[\frac{\beta_I}{\rho_I} \sum_J m_J \nabla W_I(\mathbf{x}_J, h_I) \cdot (\mathbf{v}_J - \mathbf{v}_I) - \frac{\beta_I \gamma'_I}{h_I} [\mathbf{n} \cdot \mathbf{v}_I] \right]. \tag{25}$$

Note that this equation is very similar to the standard SPH density rate equation except for the boundary term $\frac{\beta_I \gamma'_I}{h_I}[\mathbf{n} \cdot \mathbf{v}_I]$ and the correction term $\frac{\beta_I}{\rho_I}$ which is due to changes in h.

The equations derived above will now be used to obtain the equilibrium equations of a continuum represented by a system of SPH particles with variable resolution length.

5. Dynamic problems: governing equations

Consider a system of particles in space, with positions defined by the vector $\mathbf{x}_I$. Each particle carries a mass m_I, and has velocity $\mathbf{v}_I$ and an acceleration defined by $\mathbf{a}_I$ as shown in Fig. 4. In SPH, the position of the particles is followed in time and the particles are not considered discrete bodies but points of the continuum. In order to derive the equations of motion within a variational framework, it is first necessary to define the total potential energy and the total kinetic energy of the continuum.

Assuming a reversible process and using the Euler–Lagrange equation of motion [14], the equilibrium equation for the system of particles can be expressed as

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \mathbf{v}_I} - \frac{\partial L}{\partial \mathbf{x}_I} = 0, \quad I = 1, \ldots, N, \tag{26}$$

where $L = K - \pi$ is the kinetic potential or Lagrangian, K is the total kinetic energy and the total potential energy of the system of particles has gravitational and internal components π_{g} and π_{int}, respectively.

Noting that π is only a function of nodal positions, the equilibrium equation becomes

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial K}{\partial \mathbf{v}_I} - \frac{\partial K}{\partial \mathbf{x}_I} = \frac{\partial \pi_{\mathrm{g}}}{\partial \mathbf{x}_I} - \frac{\partial \pi_{\mathrm{int}}}{\partial \mathbf{x}_I}, \quad I = 1, \ldots, N. \tag{27}$$

5.1. Kinetic energy

Considering a system of SPH particles representing a continuum, the total kinetic energy K can be reasonably approximated as [15],

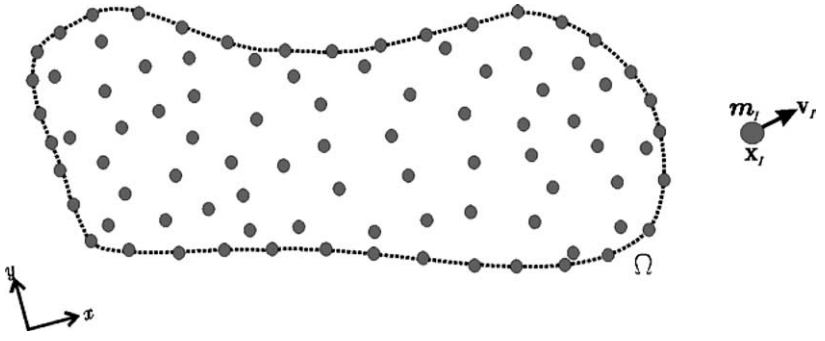

Fig. 4. Discretisation of the continuum as a system of particles.

$$K = \frac{1}{2}\sum_{I=1}^{N} m_I \mathbf{v}_I \cdot \mathbf{v}_I, \tag{28}$$

where m_I is the mass for particle I and $\mathbf{v}_I$ is the velocity vector for that particle.

5.2. Potential energy

If all external forces of the system are conservative, it is possible to define an external potential energy, for instance for the case of gravitational forces, as

$$\pi_{\mathrm{g}}(\mathbf{x}_I) = -\sum_{I=1}^{N} m_I(\mathbf{g}\cdot\mathbf{x}_I), \tag{29}$$

where $\mathbf{g}$ is the gravity acceleration vector and $\mathbf{x}_I$ is the position vector for particle I.

5.3. Internal energy potential

The internal potential energy represents the recoverable energy stored in the continuum. In general, it is possible to express this total internal energy, as particle contributions, as

$$\pi_{\mathrm{int}}(\mathbf{x}_I) = \sum_{I=1}^{N} m_I \pi(\rho_I), \tag{30}$$

where $\pi(\rho)$ represents the internal energy per unit mass of the material and is given by the equation of state. Relating $\pi(\rho)$ and $U(J)$, the energy stored per unit initial volume, via $J = \frac{\rho_0}{\rho}$, the internal energy can be expressed as

$$U = \rho_0 \pi(\rho). \tag{31}$$

The pressure p, which is taken as positive in compression, is given by

$$p = -\frac{\mathrm{d}U}{\mathrm{d}J} = -\rho_0 \frac{\mathrm{d}\pi}{\mathrm{d}J} = -\rho_0 \frac{\mathrm{d}\pi}{\mathrm{d}\rho}\frac{\mathrm{d}\rho}{\mathrm{d}J}, \tag{32}$$

therefore

$$p = \rho^2 \frac{\mathrm{d}\pi}{\mathrm{d}\rho} \tag{33}$$

which is the standard energy equation for a perfect fluid.

5.4. Equilibrium equations

Eq. (27) can also be expressed in the standard Newton's second law form as,

$$m_I \mathbf{a}_I = \mathbf{F}_I - \mathbf{T}_I, \tag{34}$$

where $\mathbf{F}_I$ are the external forces of the system and T_I the internal forces of the system of particles, defined as

$$\mathbf{F}_I = -\frac{\partial \pi_{\mathrm{g}}}{\partial \mathbf{x}_I}, \tag{35}$$

$$\mathbf{T}_I = \frac{\partial \pi_{\mathrm{int}}}{\partial \mathbf{x}_I}. \tag{36}$$

The evaluation of this last term (36) requires the constitutive definition of the material in question but provided that the internal forces are evaluated in accordance with the above equation, the resulting expression will be consistent with the preservation of linear and angular momentum [7].

5.5. External forces: non-dissipative case

The external forces $\mathbf{F}_I$ of the system are defined by the body forces acting on each particle. For the case of a gravitational field, the external forces can be evaluated as

$$\mathbf{F}_I = -\frac{\partial \pi_g}{\partial \mathbf{x}_I} = m_I \mathbf{g}. \tag{37}$$

As it is noted, the external forces are given exclusively by the self-weight of the particles and they do not take into account any losses due to boundary friction.

6. Internal forces

The internal forces should also consider the case in which the particle is close to a rigid boundary and the variable smoothing length.

In order to derive the variable-h SPH equations for the internal forces let us introduce the notation:

$$D\pi_{\text{int}}[\delta \mathbf{v}] = \sum_I \mathbf{T}_I \cdot \delta \mathbf{v}_I. \tag{38}$$

The left-hand side of this equation becomes

$$D\pi_{\text{int}}[\delta \mathbf{v}] = \sum_I m_I \frac{p_I}{\rho_I^2} D\rho_I[\delta \mathbf{v}]. \tag{39}$$

Substituting Eq. (23) into this last equation gives

$$D\pi_{\text{int}}[\delta \mathbf{v}] = \sum_I m_I \frac{\mathrm{d}\pi}{\mathrm{d}\rho_I} \left[\beta_I \sum_J m_J \nabla W_I(\mathbf{x}_J, h_I) \cdot (\delta \mathbf{v}_J - \delta \mathbf{v}_I) - \frac{\beta_I \rho_I \gamma_I'}{h_I} [\mathbf{n} \cdot \delta \mathbf{v}_I] \right]. \tag{40}$$

After simple algebra the internal forces emerge as:

$$\mathbf{T}_I = \sum_J m_I m_J \left(\frac{\beta_J p_J}{\rho_J^2} \nabla W_J(\mathbf{x}_I, h_J) - \frac{\beta_I p_I}{\rho_I^2} \nabla W_I(\mathbf{x}_J, h_I) \right) - \frac{m_I \beta_I p_I \gamma_I'}{h_I \rho_I} \mathbf{n}. \tag{41}$$

The previous equation gives the internal forces for each particle considering the case of variable smoothing length. This is particularly important if the flow is highly compressible.

The last term in Eq. (41) can be interpreted as the boundary contact force, $\mathbf{B}_I$:

$$\mathbf{B}_I = b_I \mathbf{n}, \quad b_I = \frac{m_I \beta_I p_I \gamma_I'}{h_I \rho_I} \tag{42}$$

which is responsible for preventing the penetration of particles into the rigid boundaries [13].

6.1. Viscosity

In the context of the proposed variational formulation, viscosity can be introduced with a new term in the equation of motion via a dissipative potential [15]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \mathbf{v}_I} - \frac{\partial L}{\partial \mathbf{x}_I} = -\frac{\partial \pi_{\mathrm{dis}}}{\partial \mathbf{v}_I}, \quad I = 1, \ldots, N. \tag{43}$$

This dissipative potential will be expressed as the sum of viscous potentials per unit mass ψ, which are functions of the rate of deformation tensor $\mathbf{d}$, as

$$\pi_{\mathrm{dis}} = \sum_I^N m_I \psi(\mathbf{d}), \quad 2\mathbf{d} = \nabla \mathbf{v} + \nabla \mathbf{v}^{\mathrm{T}}. \tag{44}$$

Let us consider the case of a Newtonian fluid with kinematic viscosity $v = \mu/\rho$, the viscous potential is then

$$\psi(\mathbf{d}) = v(\mathbf{d}' : \mathbf{d}'), \quad \mathbf{d}' = \mathbf{d} - \frac{1}{3}(\mathrm{tr}\,\mathbf{d})\mathbf{I} \tag{45}$$

the viscous stresses can be obtained by differentiation to give

$$\boldsymbol{\sigma}^{\mathrm{vis}} = \rho \frac{\partial \psi}{\partial \mathbf{d}} = 2\mu \mathbf{d}'. \tag{46}$$

For the evaluation of $\mathbf{d}'$, the gradient of velocity needs to be obtained using Eq. (1) as

$$\nabla \mathbf{v}_I = \sum_J \mathbf{v}_J \otimes \mathbf{g}_J(\mathbf{x}_I). \tag{47}$$

The internal forces due to viscous effects can be evaluated after simple algebra and included in the equation of motion (34). The internal viscous forces term is

$$\mathbf{T}_I^{\mathrm{vis}} = \frac{\partial \pi_{\mathrm{dis}}}{\partial \mathbf{v}_I} = \sum_J m_J \left(\frac{s_I^{\mathrm{vis}}}{\rho_I}\right) \mathbf{g}_I(\mathbf{x}_J). \tag{48}$$

The resulting equation of motion for the system of particles is now

$$m_I \mathbf{a}_I = \mathbf{F}_I - \mathbf{T}_I - \mathbf{T}_I^{\mathrm{vis}}. \tag{49}$$

The variable-h SPH method proposed in this paper can also be applied for cases in which the smoothing length h may not vary in space and time due to the nature of the flow, e.g., flow through a pipe or enclosed cavity. For such cases the method will converge much faster for each particle. However, the use of the variable-h approach allows for changes in such cavities to be captured in a better way. For instance, for the case of an increase in the diameter of a pipe, the h might need to be enlarged for some particles and decrease for the case of a reduction in diameter. Some simulations of die castings, using a constant h variational SPH, have been reported by Kulasegaram et al. [13] in which the treatment of solid walls is similar to the one presented in this paper. The method can be extended to simulations in three dimensions by defining an appropriate function γ_I.

7. Implementation of the method

7.1. Correction functions γ_I, γ_I'

In order to evaluate the contact forces and the density when there are rigid boundaries within the radius of the smoothing length for a particle, the gamma correction function and its derivative are not equal to zero and therefore they must be calculated. Kulasegaram et al. [13] have proposed a method based on a numerical approximation of the integral given in Eq. (4). Using spline curve fitting the expressions for γ_I, γ_I' are (for 2-D case):

$$\left.\begin{aligned}\gamma_I &= 1.0 + (0.0625 - 0.0531\varepsilon)(\varepsilon - 2.0)^3 \\ \gamma'_I &= (0.2937 - 0.2124\varepsilon)(\varepsilon - 2)^2\end{aligned}\right\} \quad \text{if } 0 \leqslant \varepsilon \leqslant 2.0, \qquad \gamma_I = 1.0, \quad \gamma'_I = 0.0 \quad \text{if } \varepsilon > 2.0, \tag{50}$$

where $\varepsilon = \frac{y}{h_I}$. Fig. 5 shows the plot of these functions.

7.2. Numerical evaluation of the density equation

Eq. (9) is highly non-linear in ρ_I, and in order to solve it, a Newton–Raphson solution procedure can be used. Let us define a residual $R(\rho_I)$ as:

$$R(\rho_I) = \gamma_I \rho_I - \sum_J m_J W_I(\mathbf{x}_J, h_I(\rho_I)) \cong 0 \tag{51}$$

and considering as well that h is a function of the density:

$$h_I(\rho_I) = h_I^{(0)} \left(\frac{\rho_I^{(0)}}{\rho_I} \right)^{1/d_m}, \tag{52}$$

where $h^{(0)}$ is the initial iterative value for h, $\rho_I^{(0)}$ the initial guess for ρ_I. In order to solve the density equation, a Newton–Raphson procedure can be used by the iteration of the following equation:

$$\rho_I^{(k+1)} = \rho_I^{(k)} - \frac{R_I^{(k)}}{\left(\frac{\mathrm{d}R}{\mathrm{d}\rho}\right)_I^k}, \tag{53}$$

where

$$\frac{\mathrm{d}R}{\mathrm{d}\rho} = \gamma_I + \rho_I \frac{\mathrm{d}\gamma_I}{\mathrm{d}h} \frac{\mathrm{d}h}{\mathrm{d}\rho} - \sum_J m_J \frac{\mathrm{d}W_I}{\mathrm{d}h} \frac{\mathrm{d}h}{\mathrm{d}\rho}. \tag{54}$$

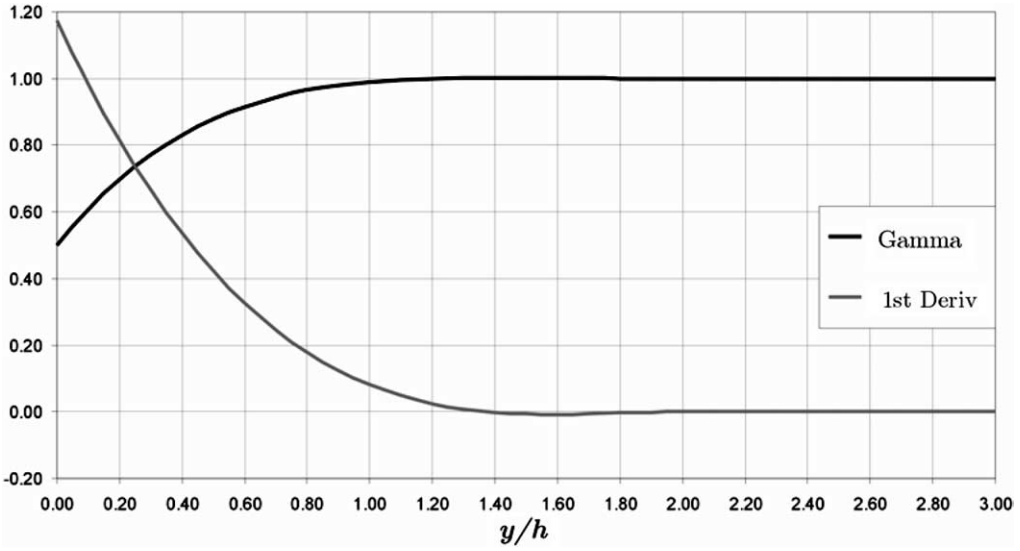

Fig. 5. Plots of the correction functions.

After substituting the expressions for the derivatives, Eq. (54) becomes:

$$\frac{\mathrm{d}R}{\mathrm{d}\rho} = \frac{\gamma_I' y_I}{h_I d_m} + \frac{\alpha_I}{\rho_I d_m} + \gamma_I - \frac{1}{\rho_I}\sum_J m_J W_I(\mathbf{x}_J, h_I(\rho_I)). \tag{55}$$

Hence the iterative procedure is defined by

$$\rho_I^{(k+1)} = \rho_I^{(k)}\left(1 - \frac{\beta_I^k R_I^k}{\beta_I^k R_I^k + \rho_I^k}\right). \tag{56}$$

As a first guess, Eq. (25) can be integrated in time giving:

$$\rho_{I,n+1}^{(0)} = \rho_{I,n} \mathrm{e}^{\Delta t(\dot{\rho}_I/\rho_I)}, \tag{57}$$

where Δt is the current time-step. In this way, for small timesteps this time integration should be very accurate and hence the number of Newton–Raphson iterations will be very small.

7.2.1. Convergence

In order to stop the Newton–Raphson iterative procedure, a tolerance that is within the machine precision must be defined. Convergence is achieved when

$$\frac{|R_I^{(k+1)}|}{\rho_I^{(k)}} \leqslant tol. \tag{58}$$

Typical values in a double precision machine are: $tol = 1\mathrm{E}-15$, which is usually achieved within a few iterations.

The use of this methodology has a higher computational cost than other non-iterative procedures for the evaluation of density. However, the improvements in the accuracy of the solution can make it cost-effective since fewer particles are needed and, in some cases, the solution obtained using standard SPH techniques is inaccurate, as it will be shown in the first example of next section.

7.3. Update of particle positions

The positions of the particles are updated by integrating Eq. (34) in time. For instance, using an explicit leap-frog scheme the new position of the particles is given by

$$\mathbf{v}_I^{(n+1/2)} = \mathbf{v}_I^{(n-1/2)} + \overline{\Delta t}\,\mathbf{a}_I^n, \tag{59}$$

$$\mathbf{x}_I^{n+1} = \mathbf{x}_I^n + \Delta t^{n+1}\mathbf{v}_I^{n+1/2}, \tag{60}$$

where

$$\overline{\Delta t} = \frac{1}{2}\left(\Delta t^n + \Delta t^{n+1}\right). \tag{61}$$

Due to the explicit nature of the scheme, the Courant–Friedrichs–Lewy (CFL) stability criteria must be satisfied. This implies that the time step size must be less than:

$$\Delta t = \mathrm{CFL}\frac{h_{\min}}{\max(c_I + \|\mathbf{v}_I\|)}, \quad 0 \leqslant \mathrm{CFL} \leqslant 1.0, \tag{62}$$

where c_I is the wave speed of propagation or speed of sound for particle I.

8. Numerical examples

In order to show the improvements of the method in comparison of constant h SPH approaches, three simple example showing the case in which a water dam breaks. The fluid is modelled using the Shallow Waters assumptions within a SPH approach, which leads to a two-dimensional model in which the density will change significantly due to the changes in h.

The two-dimensional density ρ (mass per unit projected horizontal are) and the height h_t of the column of water are related as

$$\rho = h_t \rho_w, \tag{63}$$

where ρ_w is the constant density of the fluid.

8.1. 1-D breaking dam

For the case of a infinite breaking-dam of initial height h_0, an analytical solution exists. A dam of certain depth and infinite transversal dimension brakes at time $t = 0$ s. This problem is clearly of interest in a number of real situations, ranging from the catastrophic flood following the collapse of a dam, to the operation of sluice gates in an irrigation channel.

An analytical solution exits for the problem and is presented in [18]. The results provided by the variable-h SPH method are compared to those obtained with the analytical solution for the position of the front, the depth at the initial gate and velocity at the front.

For the numerical simulation, only a strip of 1 m was considered, as shown in Fig. 6. On the right-hand side of the dam, at $x = 2$ m there is a gate that is instantaneously removed at time $t = 0.0$ s.

A total of 6601 particles were used, simulating the solid wall on the left with a symmetry condition in the fluid. According to the analytical solution, the depth of the water and the original position of the gate should remain constant and equal to $4/9\,h_0$ until the point where the wave that travels backwards reaches the solid wall at $x = 0.0$ m. This occurs approximately at $t = 0.65$ s. In this case, the depth of the fluid should be $h = 0.444$ m, until $t = 0.64$ s. The results are shown in Fig. 7, compared to the value predicted by the analytical solution. In the same manner, the velocity of the fluid at the point of the gate ($x = 2.0$) should remain constant and equal to $2/3\,c_0$, where $c_0 = \sqrt{gh_0} = 3.1314\ \mathrm{m\,s^{-1}}$ (see Fig. 8). Fig. 9 shows the comparison of the profile of the dam at $t = 0.6$ s compared to the analytical solution. As we can observe from these figures, the variable-h SPH shows good agreement with analytical solutions for an infinite breaking dam.

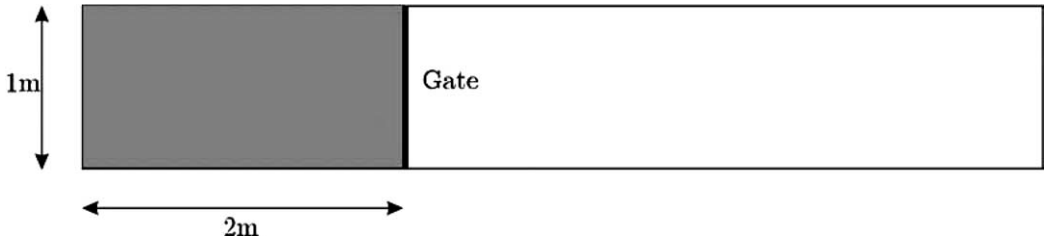

Fig. 6. Dimensions of the channel and the dam.

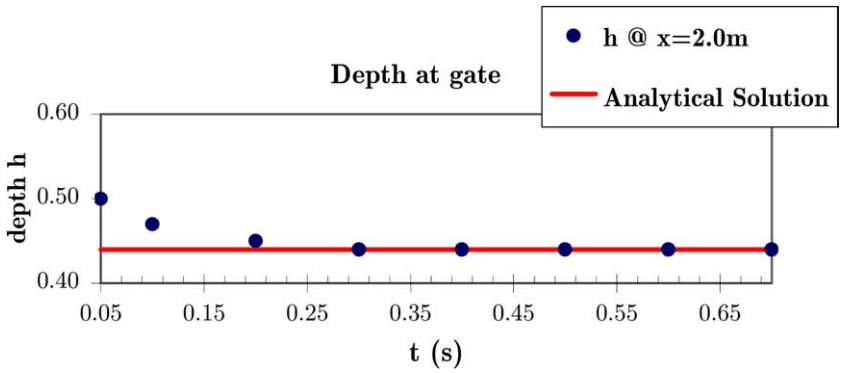

Fig. 7. Variable-*h* SPH results vs. analytical solution for depth at $x = 2.0$ m.

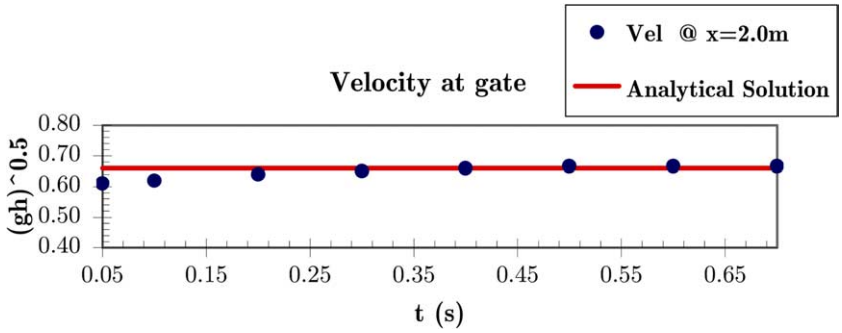

Fig. 8. Velocities at $x = 2.0$ m.

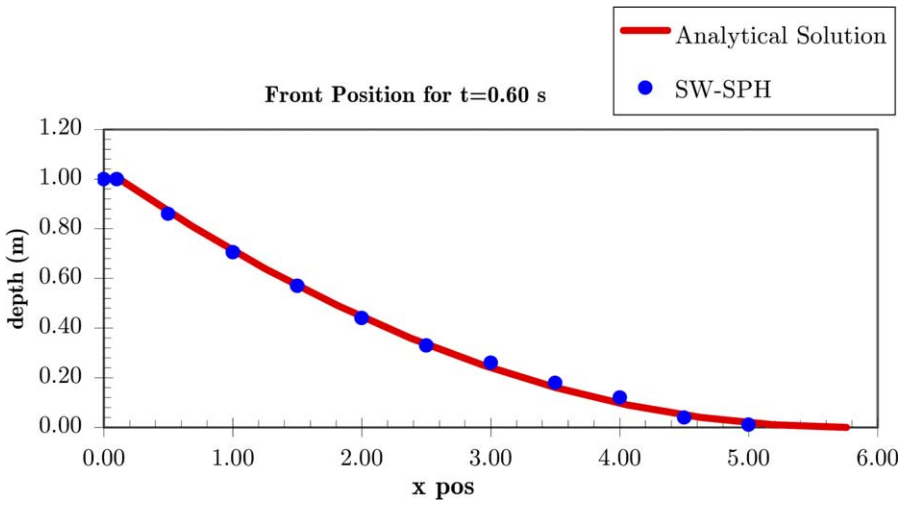

Fig. 9. Profile of the solution at $t = 0.60$ s.

8.2. Circular dam

8.2.1. Case a: Collapse of a circular dam on dry surface

In this case, the dam is a cylinder and the initial radius of the suffers an expansion due to the dam breaking. With constant h the particles near the perimeter of the dam will get fewer neighbours as the simulation progresses. This will lead to poor interpolations of those particles and consequently to non-accurate results.

Using the variable-h approach described in this paper for the density and internal forces, the problem can be solved more accurately, as it is shown in Fig. 10(b), comparing the results for the same time for both approaches.

In Fig. 11 the results for the simulation of the collapse of a circular dam of $r = 0.5$ m and initial height $h = 1.0$ m are shown. It is important to note that even after an expansion of 7 times the initial radius the simulation does not break-up, as it is the case for constant h SPH (Fig. 10(a)).

8.2.2. Case b: Collapse of a circular dam on a wet surface

Consider a column of water of radius $R_1 = 0.5$ m with an initial water depth $h_1 = 1.0$ m. The column of water represents a circular dam enclosed by an infinitely thin circular wall. This dam is located inside another circular dam of radius $R_2 = 5$ m for which the depth is $h_2 = 0.5$ m. This example studies the wave propagation phenomena associated with the sudden collapse of the interior dam wall. At time $t = 0.0$ s the wall of the small dam collapses, causing a wave propagation throughout the bigger dam. The initial conditions for the problem are

$$\begin{aligned} &h = 1.0\ \text{m} && \text{if } x^2 + y^2 \leqslant R_1^2, \\ &h = 0.5\ \text{m} && \text{if } R_1^2 < (x^2 + y^2) \leqslant R_2^2, \\ &v_x = v_y = 0.0. \end{aligned}$$

The interior dam is assumed to collapse instantaneously. In Figs. 12 and 13, the wave propagation pattern is shown for different time steps. Note the smooth boundary due to the correction factor as well as the smooth wave patterns. This problem is simulated using only 7987 particles. The results compare well with similar simulations [16].

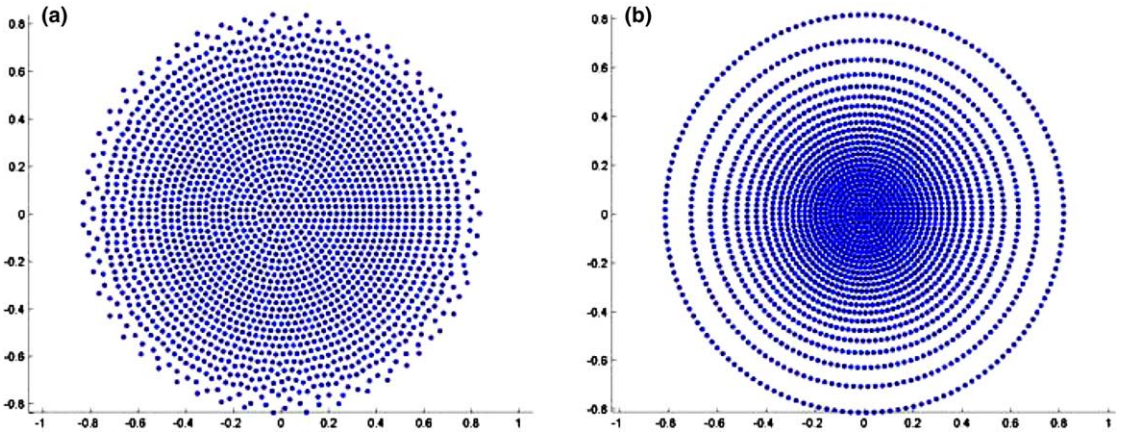

Fig. 10. (a) Standard SPH for a collapsing column of water, (b) variational SPH.

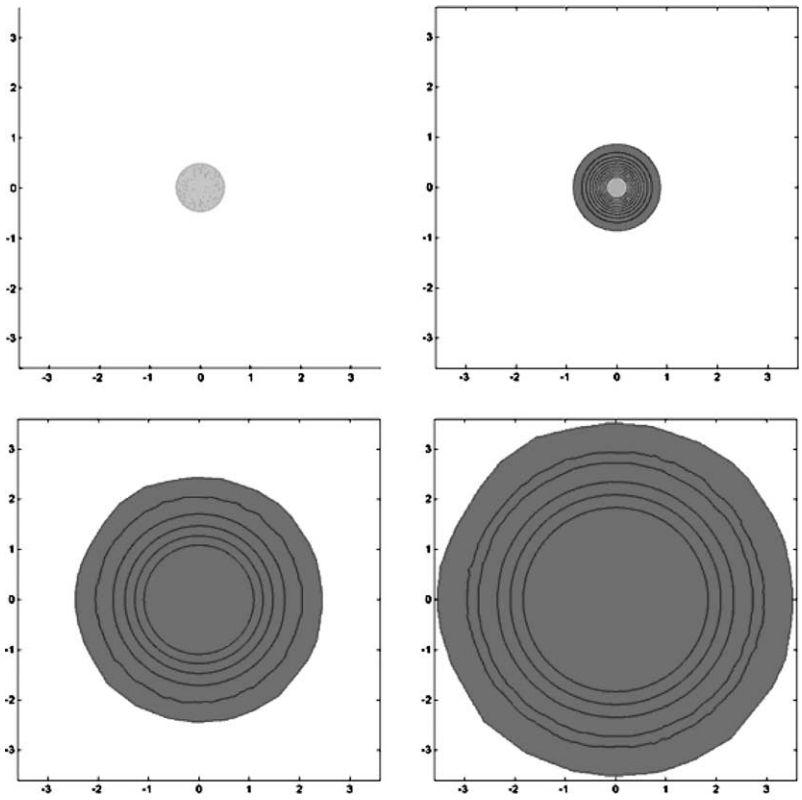

Fig. 11. Variable-h SPH for a collapsing column of wate at times $t = 0$, 0.10, 0.40 and 0.60 s, respectively.

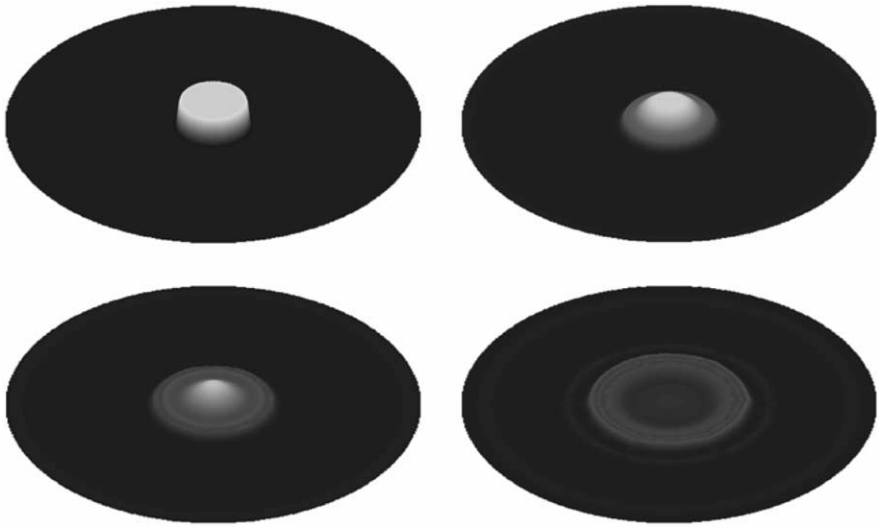

Fig. 12. Travelling waves at times $t = 0.0$, 0.20. 0.40 and 0.80 s. Note the smooth boundary.

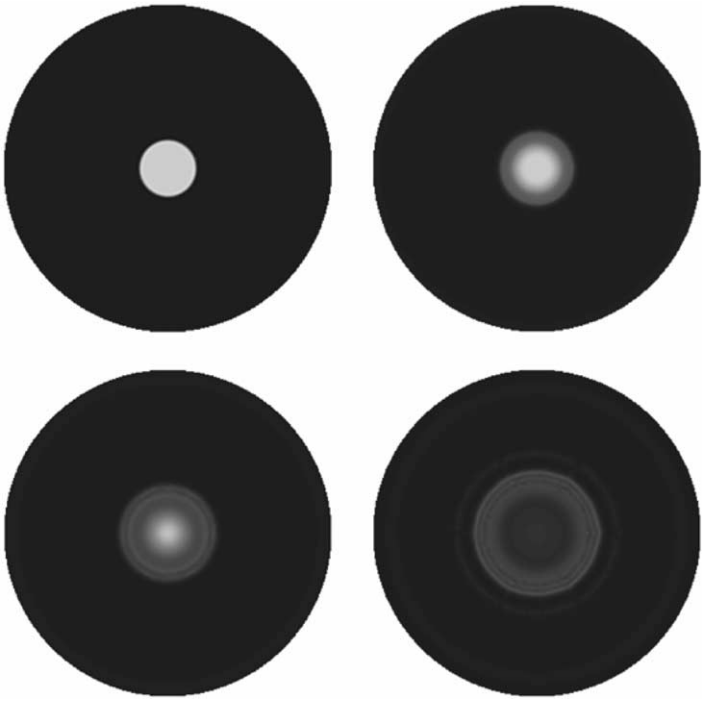

Fig. 13. Top view at times $t = 0.0$, 0.20. 0.40 and 0.80 s. Only 11,469 particles were used.

9. Concluding remarks

This paper has introduced a formulation of the SPH equations for dynamic problems that allows for the use of variable smoothing length and introduces some corrections for the case of rigid boundaries. The results show the improvements of the method over traditional SPH schemes. This new methodology overcomes problems faced by SPH when the nature of the problem makes the number of neighbouring particles vary significantly in time. Since the energy terms are independent of rigid body rotations and translations, this formulation ensures the preservation of physical constants of the motion such as linear and angular momentum for the non-dissipative case.

Although the iterative procedure to evaluate the density is more computationally expensive than the non-iterative techniques, the results show that its performance is better in terms of accuracy. In general, the time spent in each time step is in the order of 2–3 times of that in a non-iterative procedure. However, this technique also allows the use of fewer particles since the variable-h somehow adapts according to the problem's nature.

This variational SPH method is not restricted to fluids and can also be applied to solid mechanics problems.

Acknowledgement

The authors acknowledge the financial support received from EPSRC through contracts GR/R72013 and GR/M84312.

References

[1] L.B. Lucy, A numerical approach to the testing of the fission hypothesis, Astron. J. 82 (1977) 1013.
[2] R.A. Gingold, J.J. Monaghan, Smooth particle hydrodynamics: theory and application to non-spherical stars, Mon. Not. R. Astron. Soc. 181 (1977) 375.
[3] R.A. Gingold, J.J. Monaghan, Kernel estimates as a basis for general particle methods in hydrodynamics, J. Comput. Phys. 46 (1982) 429–453.
[4] J.J. Monaghan, Smoothed particle hydrodynamics, Annu. Rev. Astron. Astrophys. 30 (1992) 543–574.
[5] J. Bonet, S. Kulasegaram, Correction and stabilization of smooth particle hydrodynamics methods with applications in metal forming simulations, Int. J. Numer. Meth. Eng. 47 (2000) 1189–1214.
[6] J.J. Monaghan, Simulating free surface flows with SPH, J. Comput. Phys. 110 (1994) 399–406.
[7] J. Bonet, T.S. Lok, Variational and momentum aspects of smooth particle hydrodynamics formulations, Comput. Meth. Appl. Mech. Eng. 180 (1999) 97–115.
[8] J.J. Monaghan, SPH without a tensile instability, J. Comput. Phys. 159 (2000) 290–311.
[9] J. Bonet, S. Kulasegaram, A simplified approach to enhance the performance of smooth particle hydrodynamics methods, Appl. Math. Comput. 126 (2002) 133–155.
[10] W. Benz, Smooth particle hydrodynamics: a review, in: J.R. Buchler (Ed.), The Numerical Modelling of Nonlinear Stellar Pulsations, Kluwer Academic Publishers, Dordrecht, 1990, pp. 269–288.
[11] P.W. Randles, L.D. Libersky, Smooth particle hydrodynamics: some recent improvements and applications, Comput. Meth. Appl. Mech. Eng. 139 (1996) 375–408.
[12] J.P. Gray, J.J. Monaghan, R.P. Swift, SPH elastic dynamics, Comput. Meth. Appl. Mech. Eng. 190 (2001) 6641–6662.
[13] S. Kulasegaram, J. Bonet, R.W. Lewis, M. Profit, A variational formulation based contact algorithm for SPH applications, Comput. Mech. 33 (4) (2004) 316–325.
[14] R.A. Mann, The Classical Dynamics of Particles: Galilean and Lorentz Relativity, Academic Press, USA, 1974.
[15] J. Bonet, S. Kulasegaram, M.X. Rodriguez-Paz, M. Profit, Variational formulation for the smooth particle hydrodynamics (SPH) simulation of fluid and solid problems, Comput. Meth. Appl. Mech. Eng. 193 (12) (2004) 1245–1256.
[16] E. Toro, Shock-capturing Methods for Free-surface Shallow Flows, Wiley, UK, 2001.
[17] E.P. Fahrenthold, J.C. Koo, Hamiltonian particle hydrodynamics, Comput. Meth. Appl. Mech. Eng. 146 (1) (1997) 43–52.
[18] J.J. Stoker, Water Waves, Interscience, New York, 1965.
[19] J.P. Vila, On particle weighted methods and smooth particle hydrodynamics, Math. Models Methods Appl. Sci. 9 (2) (1999) 161–209.