

Comparative Analysis of the Main Particle-Based Methods Used for Free Surface Flow Simulation

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Abstract. *This work comprises a comparative study of the particle methods Moving Particle Semi-implicit (MPS) and Smoothed Particle Hydrodynamics (SPH) in terms of their efficiency and accuracy. The method Volume of Fluid (VOF) was used as reference for determining the accuracy of the particle methods. The methods MPS and SPH were compared with each other by means of simulation of the problem of dam-break. In order to analyze the methods' efficiency, the total processing time as a function of the number of particles was calculated. The results obtained in this work show that both the MPS and SPH methods can be considered good tools for free surface flow simulation.*

Keywords: *Free surface flow simulation, MPS, SPH, Particle method, CFD*

1. INTRODUCTION

Free surface hydrodynamic flows are of significant industrial and environmental importance. In these flows, the shape of the interface can continuously change and large deformations of fluid should be considered. Therefore, it can be difficult to analyze these flows using the traditional grid based methods such as finite elements, finite volume and finite difference, since it is difficult to continuously fit and move a grid. In order to overcome these problems, the particle methods, in which each particle is followed in a Lagrangian manner, can be used. In this way, moving interfaces and boundaries can be analyzed by particle methods in a much easier manner than with the traditional grid based methods. In addition, in Lagrangian formulations the convection terms are calculated by the motion of particles without any numerical diffusion.

In this context, two particle methods play an important role: the Smoothed Particle Hydrodynamics (SPH) method and the Moving Particle Semi-implicit (MPS) method. The SPH method was originally introduced by Gingold and Monaghan (1977) in order to solve gas dynamics problems in astrophysics. However, only in 1988 was the SPH method used by Monaghan (1988) to solve problems in fluid mechanics. Monaghan (1994) extended the SPH method to simulate free surface incompressible flows. Monaghan's work (1994) was based on the observation that real fluids, such as water, are compressible, but with a speed of sound which is much greater than the speed of bulk flow. Morris et al. (1997) extended the SPH method to model incompressible flows for low Reynolds number. For such flows, Morris et al. (1997) proposed a new equation of state as a function of sound speed and of fluid density. Shao and Lo (2003) used the method of incompressible SPH for simulating Newtonian and non-Newtonian flows with free surfaces. This method was tested in a 2D dam break problem and the results were in good agreement with experimental data. Using a 3D version of the smoothed particle hydrodynamics method, Gómez-Gesteira and Dalrymple (2004) simulated the impact of a single wave generated by a dam break with a tall structure. Ataie-Ashtiani et al. (2008) proposed an incompressible smoothed particle hydrodynamics formulation to simulate free surface incompressible fluid problems. In that work, a new type of source term for the Poisson equation was proposed and a modified Poisson equation of pressure was used to satisfy the incompressibility condition of free surface particle.

Koshizuka and Oka (1996) and Koshizuka et al. (1998) proposed a modified particle method called the Moving Particle Semi-implicit (MPS) method. This method was able to model, in good agreement with the experimental data, the fluid fragmentation and the free surface deformation in 2D cases such as the dam break problem and the breaking waves problem. Ataie-Ashtiani and Farhadi (2006) proposed a stable moving particle semi-implicit method for free surface flows. In their paper, various kernel functions were considered and applied to improve the stability of the MPS method. Based on these studies, a kernel function was introduced and the method's stability was improved. Furthermore, a fractional step method, which split each time step in two steps, was applied. Shibata and Koshizuka (2007) simulated the three-dimensional impact of shipping water on a deck using the moving particle semi-implicit method. The fluid motion, the surface elevation and the impact pressure on a deck were in good agreement with the experimental data.

In this paper, the particle methods MPS and SPH are compared with each other, in terms of their accuracy and efficiency, through analysis of free surface flows. Thus, the dam break problem is simulated using both methods. The volume of fluid (VOF) method is used as reference for determining the accuracy of the particle methods. In order to analyze the methods' efficiency, the total processing time as a function of the number of particles is determined.

2. GOVERNING EQUATIONS

In this study, incompressible non-viscous flows are considered. Thus, the mass conservation and momentum conservation are presented in Eqs. (1) and (2), respectively.

$$\frac{1}{\rho} \frac{D\rho}{Dt} = -\nabla \cdot \mathbf{v}, \quad (1)$$

$$\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho} \nabla p + \mathbf{g}, \quad (2)$$

where t (s) is the time, ρ (kg.m^{-3}) denotes the density, \mathbf{v} (m.s^{-1}) is the velocity vector, p ($\text{kg.m}^{-1}.\text{s}^{-2}$) is the pressure and \mathbf{g} (m.s^{-2}) is the acceleration of gravity.

In particle methods, mass and momentum conservation equations are transformed into a particle interaction equation, where all interactions between particles are limited to a finite distance. In Eq. (2), the left side represents the Lagrangian time differentiation involving advection terms. In MPS and SPH methods, the advection terms are directly incorporated into the calculation by moving particles.

3. THE MPS METHOD

3.1. Particle interaction models

The interaction between a particle and its neighboring particles is represented by a kernel function $w(r)$, where r denotes the distance between two particles. Thus, the influence exerted by particles that are within this neighborhood is determined by the kernel function. In this work, the following kernel function (Fig. 1) was employed:

$$w(r) = \begin{cases} \frac{r_e}{r} - 1 & 0 \leq r < r_e \\ 0 & r \geq r_e \end{cases} \quad (3)$$

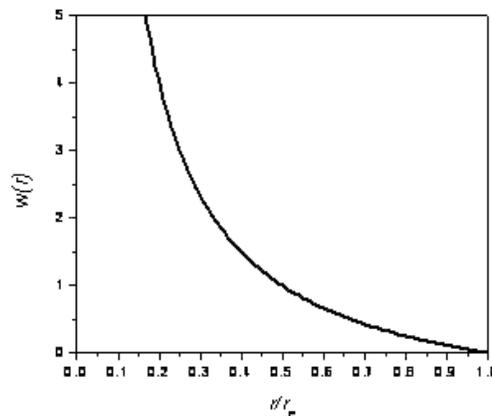


Figure 1. Kernel function used in this study

In this kernel function, the parameter r_e is the radius of the interaction area, which means that the area covered by the function is bounded (Fig. 2). Therefore, a particle interacts with a finite number of neighboring particles. Note, by analysis of Fig. 1, that the kernel function tends to infinity as r tends to zero. According to Koshizuka and Oka (1996), this is good for avoiding clustering of particles.

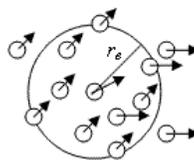


Figure 2. Conceptual image of the particle interaction domain

The MPS method uses a concept called particle number density, n , which replaces fluid density in order to ensure the incompressibility property. Thus, the fluid density will be constant if the particle number density is constant. This constant value is denoted by n^0 . When a particle i and its neighbors j are located at \mathbf{r}_i and \mathbf{r}_j , the particle number density is defined as:

$$\langle n \rangle_i = \sum_{j \neq i} w(|\mathbf{r}_j - \mathbf{r}_i|) \quad (4)$$

According to Koshizuka and Oka (1996), the constant value of particle number density (n^0) for incompressibility condition is determined by using $r_e = 2.1l_0$, where l_0 is the initial spacing between particles. This constant value is also used for judging free surface (an explanation of this use will be presented later).

The gradient vectors between a particle i and its neighboring particles j are weighted with the kernel function and averaged to obtain a gradient vector at particle i :

$$\langle \nabla \phi \rangle_i = \frac{d}{n^0} \sum_{j \neq i} \left[\frac{\phi_j - \phi'_i}{|\mathbf{r}_j - \mathbf{r}_i|^2} (\mathbf{r}_j - \mathbf{r}_i) w(|\mathbf{r}_j - \mathbf{r}_i|) \right], \quad (5)$$

where ϕ is a scalar quantity and d is the number of the space dimension. The value of r_e used by the kernel function in the gradient model is the same value that is used to determine n^0 .

According to Koshizuka and Oka (1998), in Eq. (5) ϕ'_i is used in place of ϕ_i to improve the numerical stability of the MPS method. Thus, the value of ϕ'_i is calculated by:

$$\phi'_i = \min(\phi_j), \text{ for any } j \text{ satisfying } w(|\mathbf{r}_j - \mathbf{r}_i|) \neq 0 \quad (6)$$

The gradient model is not sensitive to absolute pressure. This feature is consistent with the property of incompressible fluids, which depends on the relative pressure distribution. This model is applied to determine the pressure gradient term in MPS method.

The Laplacian model is derived from the physical concept of diffusion. Thus, this model, presented in Eq. (7), is conservative because part of a quantity at particle i is distributed to neighboring particles j .

$$\langle \nabla^2 \phi \rangle_i = \frac{2d}{n_{iccg}^0 \lambda} \sum_{j \neq i} (\phi_j - \phi_i) w(|\mathbf{r}_j - \mathbf{r}_i|) \quad (7)$$

In Eq. (7), the constant value of particle number density for the Laplacian model, $n^0 = n_{iccg}^0$, is determined using $r_e = 4.0l_0$, the same condition that was used by Koshizuka and Oka (1996). This value of r_e is also used by the kernel function present in the Laplacian model. The parameter λ is introduced so that the increase in variance is equal to the analytical solution of a diffusion problem (Koshizuka and Oka, 1998). The parameter λ is defined as:

$$\lambda = \frac{\int_V w(r) r^2 dV}{\int_V w(r) dV} = \frac{\int_0^{r_e} \left(\frac{r_e}{r} - 1 \right) r^2 2\pi r dr}{\int_0^{r_e} \left(\frac{r_e}{r} - 1 \right) 2\pi r dr} = \frac{r_e^2}{12} \quad (8)$$

3.2. Description of the MPS method

In incompressible flows, the fluid density should be constant. According to the MPS method, this means that the particle number density should be constant and equal to n^0 . If the particle density number n^* is different from n^0 , n^* should be implicitly corrected to n^0 by the following equation:

$$n^* + n' = n^0 \quad (9)$$

In Eq. (9), n' is the correction value of particle number density. This value is related to the velocity correction \mathbf{v}' by the mass conservation equation:

$$\frac{1}{\Delta t} \frac{n'}{n^0} = -\nabla \cdot \mathbf{v}' \quad (10)$$

The particle velocity \mathbf{v} is calculated as the sum of the correction velocity \mathbf{v}' and the temporal velocity \mathbf{v}^* . The temporal velocity is obtained directly by applying gravity acceleration. Thus, the correction velocity is obtained from the implicit pressure term present in the momentum conservation equation:

$$\mathbf{v}' = -\frac{\Delta t}{\rho} \nabla P^{n+1} \quad (11)$$

From Eqs. (9), (10) and (11), a Poisson equation of pressure is obtained:

$$\langle \nabla^2 P^{n+1} \rangle_i = -\frac{\rho}{\Delta t^2} \frac{\langle n^* \rangle_i - n^0}{n^0} \quad (12)$$

The right side of Eq. (12) represents the deviation of the particle number density from the constant value n^0 . The left side in Eq. (12) is discretized by the Laplacian model presented in Eq. (7). In this way, a symmetric and sparse linear system of equations is obtained. This system has order N , where N denotes the number of particles, and it can be solved by the incomplete Cholesky conjugate gradient (ICCG) method (Hirsch, 1988). Finally, the correction velocity can be determined using the gradient model by:

$$\mathbf{v}'_i = -\frac{d\Delta t}{n^0 \rho} \sum_{j \neq i} \left[\frac{P_j^{n+1} - P_i^{n+1}}{|\mathbf{r}_j - \mathbf{r}_i|^2} (\mathbf{r}_j - \mathbf{r}_i) w(|\mathbf{r}_j - \mathbf{r}_i|) \right] \quad (13)$$

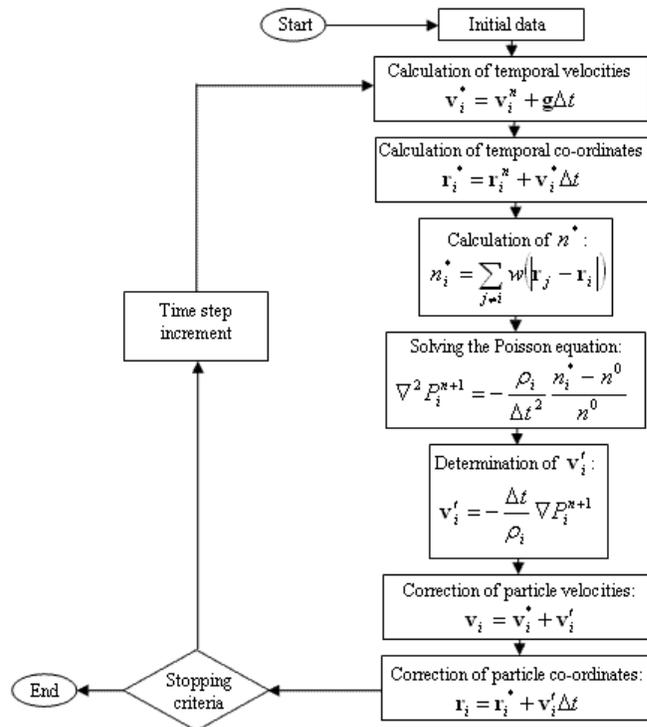


Figure 3. Algorithm of MPS method

A simplified flowchart of the MPS algorithm is shown in Fig. 3. In each time step, the temporal velocities are determined by application of gravity acceleration. Afterwards, the temporal co-ordinates are calculated. Thus, the particle number density of each particle is obtained. Then, the Poisson equation of pressure is solved using the ICCG method. With the pressure values, correction velocities are determined. Finally, new velocities and co-ordinates are obtained.

The value of the particle number density decreases for particles on the free surface. In the MPS method, a particle is considered to be on the free surface when it satisfies the following condition:

$$\langle n^* \rangle_i < \beta n^0, \quad (14)$$

where β is a parameter less than 1.

Pressure zero is given to particles on the free surface, as boundary condition, when solving the Poisson equation of pressure. According to Koshizuka and Oka (1996), the value of parameter β can be chosen from 0.8 to 0.99. In this study, the value used was 0.97, as recommended by Koshizuka and Oka (1996). Solid boundaries such as walls or other fixed objects are represented by fixed particles. These fixed particles have velocity equal to zero. Three layers of particles are used to represent fixed objects in order to keep the particle number density of the first inner wall layer around n^0 . Pressures are calculated at these particles to repel fluid particles from the wall. On top of that, the collision between particles is used to avoid superposition of particles.

4. THE SPH METHOD

4.1. Particle interaction models

The main idea behind the SPH method is to replace the fluid by a set of particles. Just as in the MPS method, the interaction between a particle, at a specific position \mathbf{r} , and its neighboring particles, at surroundings positions \mathbf{r}' , can be evaluated using a kernel function W . Thus, according to the SPH method, a scalar field $A(\mathbf{r}_i)$ and its associated gradient vector field $\nabla A(\mathbf{r}_i)$ are interpolated using the particles j within a circle of radius kh around \mathbf{r}_i , where h denotes the smoothing length and k is a constant value, as follows:

$$A(\mathbf{r}_i) = \sum_j \frac{m_j}{\rho_j} A(\mathbf{r}_j) W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (15)$$

$$\nabla A(\mathbf{r}_i) = \sum_j \frac{m_j}{\rho_j} A(\mathbf{r}_j) \nabla W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (16)$$

where m is the particle mass.

On top of that, the divergent of a vector \mathbf{u} at position \mathbf{r}_i can be approximated, using the SPH approximation, as follows:

$$\nabla \cdot \mathbf{u}(\mathbf{r}_i) = \sum_j \frac{m_j}{\rho_j} \mathbf{u}(\mathbf{r}_j) \cdot \nabla W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (17)$$

In this study, the quintic spline function (Morris et al., 1997) is used (Fig. 4):

$$W(R, h) = \alpha_d \times \begin{cases} (3-R)^5 - 6(2-R)^5 + 15(1-R)^5 & 0 \leq R < 1 \\ (3-R)^5 - 6(2-R)^5 & 1 \leq R < 2 \\ (3-R)^5 & 2 \leq R < 3 \\ 0 & R > 3 \end{cases} \quad (18)$$

In this function, $R = \frac{|\mathbf{r} - \mathbf{r}'|}{h}$, where $|\mathbf{r} - \mathbf{r}'|$ denotes the distance between particles. The values of α_d in one, two and three dimensions are $\alpha_d = 120/h$, $\alpha_d = 7/478\pi h^2$ and $\alpha_d = 3/359\pi h^3$, respectively.

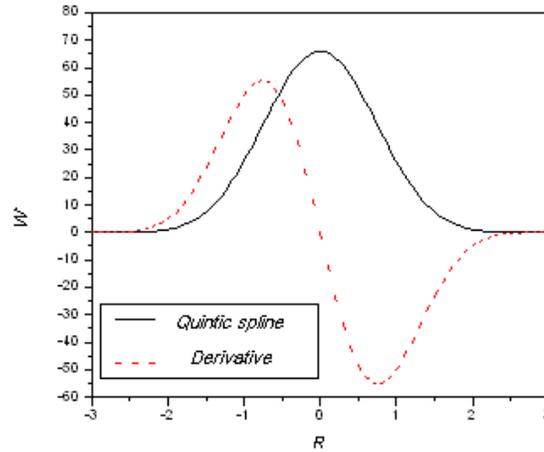


Figure 4. Quintic spline function

4.1. Description of the SPH method

In flow simulations using the SPH method, it is necessary to calculate the particle density. Using Eq. (15) to determine the fluid density, the following equation can be obtained:

$$\rho(\mathbf{r}_i) = \sum_j m_j W(R, h) \quad (19)$$

Equation (19) gives the summation density. Since the mass is carried by particles, this equation conserves mass in a precise manner. However, this equation can lead to computer errors, because surface particles in free surface scenarios have fewer neighbors and, in this case, an erroneous lower density can be computed. To overcome this problem, an approach introduced by Monaghan (1994) is used, which consists in solving the continuity equation and results in the following SPH approximation:

$$\frac{D\rho(\mathbf{r}_i)}{Dt} = \sum_j m_j v_{ij}^b \cdot \nabla^b W(R, h), \quad (20)$$

where $v_{ij}^b = v_i^b - v_j^b$ and the superscript b denotes the direction. In this work, Eq. (20) was used to determine particle density.

Pressure determination is a delicate issue for simulations of incompressible fluids using the SPH method, because the pressure is calculated explicitly using an equation of state. In this work, the following equation of state (Batchelor, 1967) is used, which, according to Monaghan (1994), is an appropriate choice for simulating incompressible fluids such as water:

$$p = B \left[\left(\frac{\rho}{\rho_0} \right)^\gamma - 1 \right], \quad (21)$$

where $\gamma = 7$, $B = \frac{c_0^2 \rho_0}{\gamma}$ is a parameter which depends on the problem, $\rho_0 = 1000 \frac{kg}{m^3}$ is the reference density and c_0 denotes the speed of sound in the fluid.

After determining particle pressure, the pressure term in the momentum conservation equation can be determined. In this paper, the following symmetric SPH formulation is applied to determine the gradient of pressure (Monaghan, 1988):

$$-\frac{1}{\rho(\mathbf{r}_i)} \nabla p(\mathbf{r}_i) = -\sum_j m_j \left(\frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \nabla W(R, h) \quad (22)$$

The acceleration of gravity is applied over all fluid particles directly without the need to use the SPH approximation. Thus, the following SPH approximation for the momentum conservation equation is obtained:

$$\frac{D\mathbf{v}(\mathbf{r}_i)}{Dt} = -\sum_j m_j \left(\frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2} \right) \nabla W(R, h) \quad (23)$$

During free surface simulations, an unphysical particle motion may occur. In order to overcome this situation, the XSPH technique (Monaghan, 1989), which consists of computing an average velocity from the velocities of the neighboring particles, is used. This technique helps to keep the motion of particles in a more ordered way when simulating incompressible flows. Thus, according to the XSPH technique, each particle moves in the following way:

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i - \varepsilon \sum_j \frac{m_j}{\rho_j} (\mathbf{v}_i - \mathbf{v}_j) W(R, h), \quad (24)$$

where ε is a constant which varies from 0 to 1.

The SPH equations are integrated using the second order accurate Leap-frog scheme (Hirsch, 1988). In this work, the time step is determined using the following equation:

$$Cr = \frac{v_{\max} \Delta t}{l_0} \leq 0.2, \quad (25)$$

where Cr is the Courant number, Δt is the time step, l_0 is the distance between particles in the initial configuration and v_{\max} denotes the maximum velocity of all particles in the current time step. The maximum time step allowed is 10^{-3} s. This criterion was also adopted in MPS method.

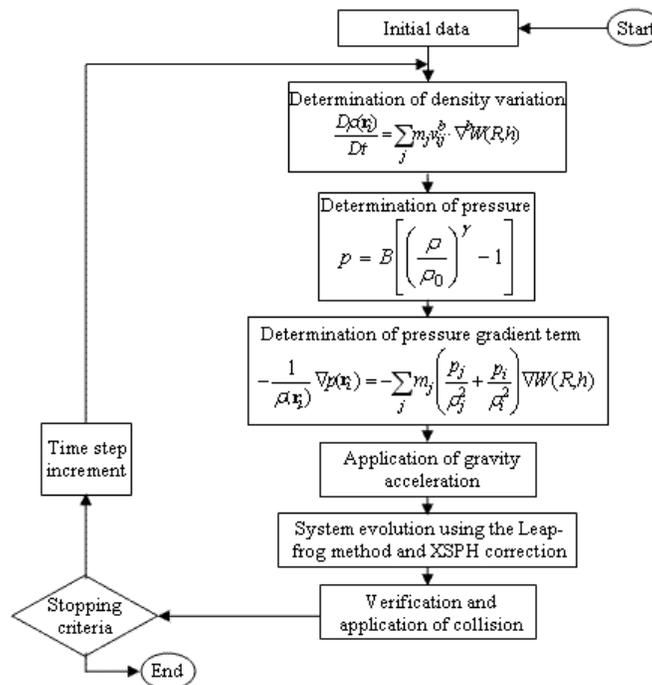


Figure 5. Algorithm of SPH method

A simplified flowchart of SPH method is presented in Fig. 5. First, the variation of density is calculated using the SPH approximation of the continuity equation (Eq. 20). After that, the pressure is obtained using the equation of state (Eq. 21). With the values of pressure, the pressure gradient term is determined by the SPH approximation presented in Eq. (22) and the gravity acceleration is applied directly over all fluid particles without using the SPH approximation. Afterwards, the evolution of the system is performed by the Leap-frog method and by application of the XSPH technique. Finally, collision tests are applied and corrections are executed.

Solid boundaries such as walls are represented by fixed particles which have velocities equal to zero. Collisions between solid boundaries and fluid particles may occur. Therefore, an algorithm to detect and treat collision between fluid particles and solid boundaries was developed and implemented. This algorithm is sufficiently robust to consider not only the position of each particle, but also its trajectory, simulating the correct behavior.

5. RESULTS

5.1. Broken dam analysis

According to Ataie-Ashtiani and Farhadi (2006), dam-break flows are an important practical problem in civil engineering and their prediction is now a required element in the design of a dam and its surrounding environment. On top of that, this problem has been used as a verification problem of the codes for the free surface (Koshizuka and Oka, 1996). In the dam-break problem, a water column located on the left vertical wall is initially supported by a barrier (Fig. 6). At the beginning of computation, the barrier is instantaneously removed and the water column starts to collapse. In order to simulate the fragmentation of the fluid, a right vertical wall is added to the model.

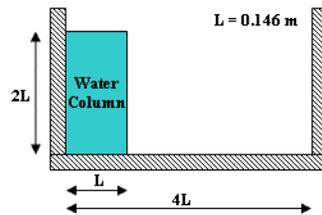


Figure 6. Geometry of dam-break problem

During the simulation, the number of fluid particles totaled 1682, corresponding to a particle spacing of 0.005 m in the initial configuration. The fluid particles have an initial density of 1000 Kg.m^{-3} and they are initially arranged in a regular and equally-spaced grid. For computation, an initial time step of 0.0001 s is employed. These conditions are used for both MPS and SPH methods.

Using the SPH method, the initial value of particle density needs to be adjusted to give the correct hydrostatic pressure when the pressure is calculated from the equation of state. In this work, the following equation (Monaghan, 1994) is used to correct the value of particle density:

$$\rho = \rho_0 \left(1 + \frac{\rho_0 g (H - y)}{B} \right)^{1/\gamma}, \quad (26)$$

where y is the particle's co-ordinate.

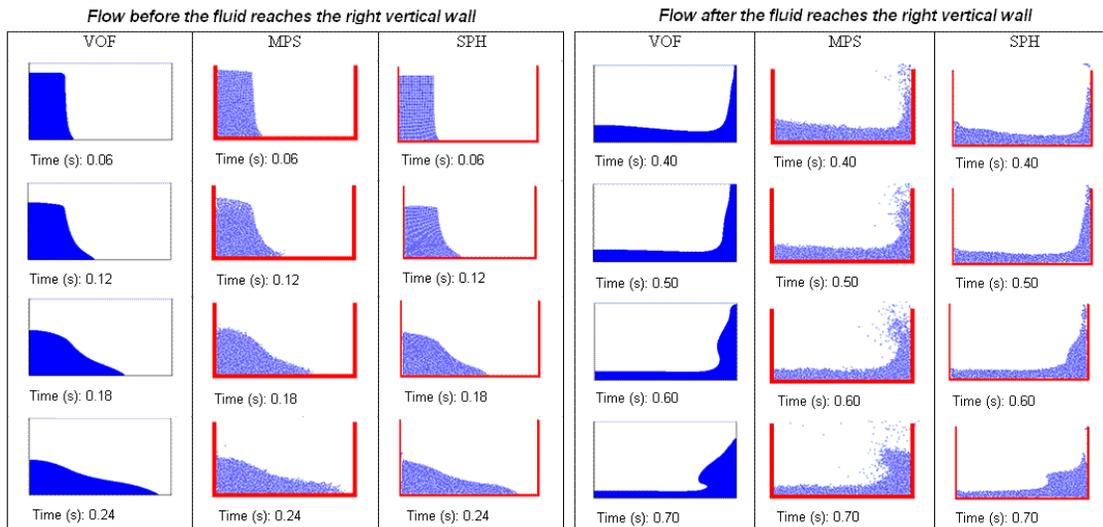


Figure 7. Dam-break flow at different times

The evolution of the dam-break flow is shown in Fig. 7. The results obtained in dam-break flow simulation using the MPS and SPH method are compared, in terms of accuracy, with the results obtained by the Volume of Fluid (VOF) method. The VOF is used because, according to Shao and Lo (2003), it has been successfully applied to a wide variety of flow problems involving free surfaces such as dam-break and wave break in the surf zone. Thus, this work uses FLUENT® (2008), a state-of-the-art CFD package which is widely used in both industry and academia, in order to simulate the dam-break problem using the VOF method.

Analyzing Fig. 7, it can be observed, in a qualitative manner, that the simulated flow patterns obtained by MPS, SPH and VOF method are very similar. It is important to note that, after the flow reaches the right vertical wall, only the MPS method is able to simulate fluid fragmentation.

Figure 8 presents a quantitative comparison in which the change in the leading edge's position (Z/L) is shown with respect to time. It can be seen that the results obtained by MPS and SPH methods are in good agreement with the results obtained by the VOF method in the simulation of the dam-break problem. However, the MPS method seems to be more accurate to simulate this problem, when compared with the results obtained by the VOF method.

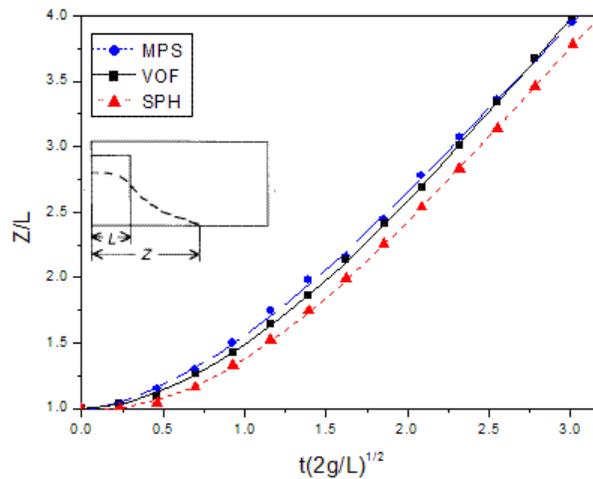


Figure 8. Motion of the leading edge in dam-break problem

5.2. Analysis of efficiency between the MPS and SPH methods

In this work, an analysis of efficiency between the MPS and SPH methods was also performed. In order to analyze the efficiency, the total processing time as function of the number of fluid particles is calculated. For this computation, a Pentium 4 (3.00GHz), with 2 GB of RAM memory, has been used. The total simulation time of the dam-break problem was 1s.

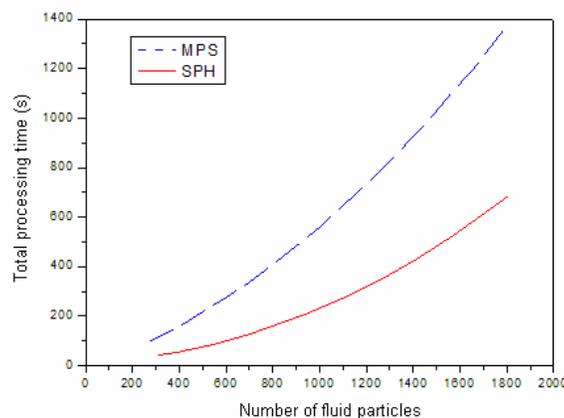


Figure 9. Total processing time as a function of the number of fluid particles

Figure 9 shows a plot of the total processing time as a function of the number of fluid particles. The MPS method has a larger computational cost, which is due to the fact that this method needs to solve a linear system for determining the pressure, resulted from the Poisson equation, using the ICCG method. In the SPH method, the pressure is

determined by an equation of state and, in this way, the computational cost is smaller. In this work, it was not used any technique to improve the determination of neighborhood. Thus, the processing time is proportional to N^2 (Shibata and Koshizuka, 2007), where N is the total number of particles.

6. CONCLUSION

The paper presents a comparative study between the MPS and SPH methods. Both methods employ particles to discretize the governing equations, such that interactions between particles simulate the flows. The dam-break problem was simulated using both methods and the results obtained are in good agreement with the results obtained by the VOF method. The MPS and SPH methods are effective in dealing with larger deformation of free surfaces. However, the fluid fragmentation is better represented by the MPS method. The SPH method presents a smaller computational cost when compared with the MPS method in simulation of the dam-break problem because the SPH method uses an equation of state to determine the pressure. In sum, based on the results obtained in this work, it can be said that the MPS method is a more robust method for simulating incompressible free surface flows. However, good results can also be obtained, at a lower computational cost, using the SPH method. Thus, the SPH method can be considered as a good alternative for applications that do not require a high accuracy, such as those in the field of computer graphic simulations.

Future works include simulation of 3D models, implementation of algorithms to optimize the determination of neighboring particles, simulation of the viscous term present in momentum equation and applications of these methods to others physical processes.

7. ACKNOWLEDGEMENTS

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