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Smoothed particle hydrodynamics simulation of confined viscous flows

José Gustavo Coelho^{a1}, Taygoara F. Oliveira^b,

Antonio C. P. Brasil Junior^b and Pierre Maruzewski-Gaud^c

^a Federal University of Triângulo Mineiro, Institute of Technological and Exact Sciences Avenida Doutor Randolfo Borges Junior, 1250, Uberaba, MG, Brazil.

^bUniversity of Brasília, Department of Mechanical Engineering, Campus Darcy Ribeiro, Brasília, Df, Brazil.

^c EDF CIH FM ED, 73373, Le Bourget du Lac, France

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Abstract

In this work the Smoothed Particle Hydrodynamics methodology (SPH) is used to simulate incompressible and confined viscous flows of Newtonian fluids. The SPH is a meshfree Lagrangian method which simulates the flow using moving fluid particles that interact one with others by hydrodynamics forces. The forces acting on each particle are evaluated using a spatial filtering process, taken over a certain region in the neighbourhood of the particle which is defined by a smoothing length, h . The filter kernel function and the ratio of the mean spatial displacement of the particles, and the smoothing length, h , are both of central importance for the accuracy of this methodology. A study of the relative importance of this parameters and also of the boundary condition scheme and pressure constitutive model are performed in a context of low Reynolds number flows. The model is validated by comparison with analytical solution of the Stokes equations. Additionally, the cases $Re = 1$ and $Re = 100$ are simulated. Good agreement of the results of the simulations and the reference theoretical data was observed.

Keywords: *smoothed particle hydrodynamics, meshfree methods, low Reynolds number flow.*

1. Introduction

Smoothed Particle Hydrodynamics (SPH) is a meshfree lagrangean method which may be used to simulate a variety of physical phenomena. Originally, SPH was designed by Monaghan [1] to simulate galaxy dynamics. Currently, it is employed to simulate continuum phenomena like elastic materials behavior [2], fluid dynamics [3] and [4], explosions [5] and non-Newtonian fluid flows [6]. In the case of fluid flow simulations, the SPH method look for numerical solutions of the equations of fluid dynamics by replacing the continuum medium by a set of discrete Lagrangian particles or control points. In this sense, each control point represents a material particle which is allowed to interact with its neighbourhood. This interaction occurs by pairwise systems of hydrodynamics forces acting between the particles. The computation of this forces are performed by using some spatial average procedure which favours the nearest neighbours. Mathematically, it can be reached by using spatial interpolation functions (kernels) to evaluate the properties of a particular material point in the flow. More details about this procedure are given in sections below.

One of the most important characteristics of the SPH is its adaptive nature. SPH is meshfree method and does not need no connected mesh. Actually, in order to find the hydrodynamic properties (velocity, pressure, density, etc.) of a particle we only need to know the state of the neighbours particles. So, the problem is solved always by a local analysis and there are no rigid restriction to the spatial distribution of particles

¹E-mail Corresponding Author: josegustavo@icte.uftm.edu.br

over the domain. Those features leads a very natural treatment of free surface, very large deformations or moving boundaries problems [5]. The price to be paid for this feature is the determination the neighbour particles at each new configuration (or each time step of the time evolution). In the case of incompressible flows, an additional difficulty appears from the determination of the pressure field. The SPH formulation is designed to treat all the quantities of the problem by an explicit approach, in a framework of compressible flow. In this sense, even in incompressible fluid flows, a state equation for the pressure is need in order to keep the solution local and to avoid the global determination of the pressure field by coupling algorithms like the projection methodologies, for instance.

Nowadays, there are a relatively wide bibliography about SPH. Some featured work are [7] which suggest some variations of state equations for liquid fluid flows simulations in order to accommodate the low Reynolds number condition. Monaghan ([3] and [8]), make a wide revision about the subject showing the recent advances in the field and the main issues to be studied and developed. A deep analysis about the importance of the kernel function was made by Hongbin and Xin [9].

The goal of this work is to apply the SPH method for the simulation of viscous confined flows. In all addressed cases, the flow is incompressible, permanent and completely shear-driven, in such a way that the pressure has a secondary role. This situation is quite different of the most applications of SPH on Fluid Mechanics ([2] and [10]), where the velocity of the particles depends basically on its inertia and of the pressure field. This work is a first step in the definition of a meshfree methodology to study flows over solid boundaries which are moving and interacting with the flow (fluid-structure interactions). A computational code was developed based on a typical SPH model for incompressible flows. The accuracy of the model is evaluated by comparison of the velocity fields with results obtained by constructed solutions for the Stokes equations, in the case of $Re \ll 1$. For more moderate Reynolds numbers, experimental results are used like reference to our simulations.

2. Governing Equations

The principle of mass and momentum conservation for a Newtonian fluid flow can be written in the Lagrangian form as:

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

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho}\nabla P + \frac{1}{\rho}\nabla\cdot\mathbf{F} \quad (2)$$

In those equations ρ is the density of the fluid, the velocity field (which is the velocity of the material particle), P the pressure field, an external force by unity of mass and $\mathbf{F}$ is the deviatoric component of the stress tensor of the fluid. The nabla operator, ∇ , have the conventional meaning and the material derivative is defined by $D/Dt = \partial/\partial t + \mathbf{u}\cdot\nabla$. We employ the compressible form of the continuity equation (1) because de SPH methodology was designed for treat all quantities explicitly [5]. In such a case, even for incompressible flows we need a constitutive equation for the pressure field, in order to close the problem in the mathematical point of view. In practice, it means that even for incompressible flow, we have a level of artificial compressibility, which must be carefully tracked along the simulations. In general, for high Reynolds numbers flows, the following state equation can be considered:

$$P = \frac{\rho_0 c^2}{\gamma} \left[\left(\frac{\rho}{\rho_0} \right)^\gamma - 1 \right] \quad (3)$$

where $\gamma = 7$, gives a good approximation of the pressure field for liquids, subjected to small density variations [11] and [8]. By using these state equation for the pressure typically we find a sound velocity throughout the medium, c , about ten times the maximum velocity in the domain. For low Reynolds number flow, Morris [7], has proposed a linear relation between the pressure, P , and the density, ρ , in an alternative form written as:

$$P = c^2 \rho. \quad (4)$$

This approach potentially leads to great variation of pressure, depending on the sound speed in the medium, c . Morris [7], recommends to set the value of c in such a way that the density variation keep below 3%. By using some scaling arguments, Liu [5] shows that an initial approximation for c may be obtained by:

$$c^2 \approx \max \left(\frac{\mathbf{U}_0}{\delta_*}, \frac{\nu \mathbf{U}_0}{L \delta_*}, \frac{\mathbf{F} L}{\delta_*} \right) \quad (5)$$

where $\delta_* = \frac{\Delta \rho}{\rho_0}$, ρ_0 is a reference density, U_0 a characteristic velocity and L a characteristic length. But these estimation must be taken like an initial guess only. The final value of c must be carefully adjusted in order to keep $\Delta \rho / \rho_0 < 0.03$.

3. SPH Formulations

3.1 Core SPH

In SPH formulation the fluid is represented by a set of discrete point particles. Each particle have physical properties like density, mass, volume, pressure and velocity. The only invariant parameter is the mass of the particle. All other quantities are allow to vary during the temporal evolution. The particle properties actually represents a spatial average over a certain portion of the domain. Considering a generic property α (which can be any scalar, vectorial or tensorial quantity) it value for a particle in a specific position is given by:

$$\alpha() = \int_{\Omega} \alpha()' W(-') d', \quad (6)$$

where W is an interpolation, or kernel, function, which obey all properties of a typical probability density function [12], and Ω is the domain. In practice, this integration is taken only over a portion of the domain, which defines the neighbourhood of the particle. In this work we use the cubic spline kernel, defined by:

$$W(s) = \begin{cases} 1 - \frac{3s^2}{2} + \frac{3s^3}{4} & \text{if } 0 \leq s < 1; \\ \frac{2-s^3}{4} & \text{if } 1 \leq s < 2; \\ 0 & \text{if } s \geq 2; \end{cases} \quad (7)$$

where $s = \frac{r}{h}$, h is the so called smoothed length and $r = \sqrt{(-') \cdot (-')}$. The integration in the equation (7) actually is approximated by a summation over the discrete particles in the neighborhood of the particle. By this way, considering a particle a , in the position a , equation (6) reduces to:

$$\alpha(a) \approx \sum_b \frac{m_b}{\rho_b} \alpha_b W(r_{ab}) \quad (8)$$

where b indicate that the summation is taken over the neighborhood of the particle, m is the mass and r_{ab} is the distance between the particle a and the particle b .

In order to write the governing equations in the discrete form in the SPH way, we must to know how the convolution defined in the equation (6) operate over the differential operators in the governing equations. It is possible to show [5] that the gradient of a quantity α can be approximated by:

$$\nabla \alpha(\mathbf{r}_a) \approx \sum_b \frac{m_b}{\rho_b} \alpha_b \nabla_a W(r_{ab}) \quad (9)$$

where $\nabla_a W(r_{ab})$ denotes the gradient of the kernel function in relation to the particle a . Others forms for the gradient can be derived by using the vectorial identities (10) and (11), bellow:

$$\nabla \alpha = \rho \left[\nabla \left(\frac{\alpha}{\rho} \right) + \frac{\alpha}{\rho^2} \nabla \rho \right], \quad (10)$$

$$\nabla \alpha = \frac{1}{\rho} (\nabla (\rho \alpha) - \alpha \nabla \rho). \quad (11)$$

Combining equations 9 and 10 one can show that:

$$\nabla \alpha(\mathbf{r}_a) \approx \rho_a \sum_b m_b \left(\frac{\alpha_a}{\rho_a^2} + \frac{\alpha_b}{\rho_b^2} \right) \nabla_a W(r_{ab}). \quad (12)$$

Furthermore, if we combine equations 9 and 11, one obtains:

$$\nabla \alpha(\mathbf{r}_a) \approx \frac{1}{\rho_a} \sum_b m_b (\alpha_b - \alpha_a) \nabla_a W(r_{ab}). \quad (13)$$

The important distinctive difference between the approximations for the gradient given by equations (12) and (13) is that (12) is symmetric and (13) is anti-symmetric to change in the positions of the particles indices a and b [13]. Similar formula may be derived to the divergent operator. Examples of utilization of gradient and divergent SPH operators in the governing equations are:

$$\nabla P_a \approx \rho_a \sum_b m_b \left(\frac{P_b}{\rho_b^2} + \frac{P_a}{\rho_a^2} \right) \nabla_a W(r_{ab}) \quad (14)$$

and

$$\nabla \cdot_a \approx -\frac{1}{\rho_a} \sum_b m_{bab} \cdot \nabla_a W(r_{ab}) \quad (15)$$

where $ab = a - b$. Other way for the approximations for the gradient and divergent operator are developed by Monaghan [1].

Most implementations of SPH uses an artificial viscosity to simulate the viscous effect. In this sense, the momentum equations (2) takes the form:

$$\frac{D_a}{Dt} = - \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Pi_{ab} \right) \nabla_a W(r_{ab}) +_a \quad (16)$$

where Π_{ab} is the viscous contribution and $_a$ is the body force evaluated at the particle a . The original expression for Π_{ab} was empirically design to permit the stabilization of shock simulations [1], and typically doesn't work well for the estimation of the velocity profile in low, or even moderate, Reynolds number flows. Several others approximations can be found in the literature [13], [5] and [8]. In this work, we uses the artificial viscosity proposed by Morris *et. al.* [7] where the viscous forces are calculated in a separated summation and the discrete momentum equations becomes:

$$\frac{D_a}{Dt} = - \sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) \nabla_a W(r_{ab}) + \sum_b \frac{m_b(\mu_a + \mu_b)_{ab}}{\rho_a \rho_b} \left(\frac{1}{r_{ab}} \frac{W_{ab}}{r_a} \right) +_a \quad (17)$$

The continuity equation in the SPH discrete form becomes:

$$\frac{D\rho_a}{Dt} = \sum_b m_{bab} \cdot \nabla_a W_{ab}. \quad (18)$$

The equations (17) and (18) are integrated in time by an Euler method restricted to the condition:

$$\Delta t = \min \left\{ 0.25 \frac{h}{c}, 0.25 \min_a \sqrt{\frac{h}{f_a}}, 0.125 \min_a \frac{h^2}{\nu} \right\} \quad (19)$$

3.2 Boundary conditions

The application of the boundary conditions in SPH has been subject of several developments in the last few years. A very popular method consist in to set a repulsive force in particles just over the solid walls of the domain. Some molecular models, like Leonard-Jones like models [5], was used to prevent penetration of

inter particles through the boundaries. So, the particles at the walls interact with their neighbors by a force given by:

$$FP_{ab} = \begin{cases} D \left[\left(\frac{r_o}{r_{ab}} \right)^1 2 - \left(\frac{r_o}{r_{ab}} \right)^4 \right] \frac{x_{ab}}{r_{ab}^2} & \text{if } \frac{r_o}{r_{ab}} \leq 1; \\ 0 & \text{if } \frac{r_o}{r_{ab}} > 1; \end{cases} \quad (20)$$

The constant D is of the magnitude of the square of the maximum velocity in the domain. The distance r_0 is approximately equal to the initial separation between the particles. Both these parameters are of crucial importance to stability of the boundary condition. If D is too big, particles which becomes so closed to the wall may be violently putted back, causing oscillations and eventually, the crashing of the simulation. In the other hand, small values of D may allow the particles to pass through the walls and to be putted out of the domain [5]. Other options for boundary condition implementation are the so called ghosts (or virtual) particles created with symmetric properties in relation to the real ones, inside the domain ([7] and [14]). Recent development was made by Crespo [10] in the treatment of fixed wall particles. In the present work, we employ the standard formulation given by equation (20).

4. Constructed Solutions

In the present work, a C++ computational code was developed in order to simulate incompressible flows in closed domains and in low Reynolds numbers regimes. This code is based in Liu [5] e more information can be found in Coelho [15]. Like a first benchmark, we employ some constructed solution of the Stokes equations. We set Re to be much less than the unity, in a such way that the governing equation can be well approximated by the Stokes equation, given by:

$$= \frac{1}{\rho} \nabla P - \nu \nabla^2, \quad (21)$$

$$\nabla \cdot = 0. \quad (22)$$

where the domain is defined by all positions such that $\in [0, 1] \times [0, 1]$. In other words, the flow domain is a 2D unity square cavity. The flow bind to the solid wall providing a non-slip boundary condition. An analytic solution of the equations (21) and (22) is obtained by choosing a velocity field $= (u_1, u_2)$ which respect the continuity equation. We choose a polynomial form of u_1 and u_2 given by:

$$u_1 = x_1^2 (1 - x_1)^2 (2x_2 - 6x_2^2 + 4x_2^3), \quad (23)$$

$$u_2 = -x_2^2 (1 - x_2)^2 (2x_1 - 6x_1^2 + 4x_1^3). \quad (24)$$

It can be observed that the velocity field given by equations (23) and (24) keep the non-slip condition over the edges of the square domain. The pressure is set to constant throughout the flow field. The velocity field is replaced into equation (21) and the body force $= (F_1, F_2)$ is then determined, resulting:

$$\begin{aligned} F_1 &= (-24x_2 + 12)x_1^4 + (48x_2 - 24)x_1^3 + (-48x_2^3 + 72x_2^2 - 48x_2 + 12)x_1^2 \\ &+ (48x_2^3 - 72x_2^2 + 24x_2 - 2)x_1 + (1 - 4x_2 + 12x_2^2 - 8x_2^3), \end{aligned} \quad (25)$$

$$\begin{aligned} F_2 &= (48x_2^2 - 48x_2 + 8)x_1^3 + (-72x_2^2 + 72x_2 - 12)x_1^2 \\ &+ (24x_2^4 - 48x_2^3 + 48x_2^2 - 24x_2 + 4)x_1 + (-12x_2^2 + 12x_2^3 - 12x_2^4). \end{aligned} \quad (26)$$

So, in this way, the velocity field given by (23) and (24), the body force given by (25) and (26) and a constant pressure field are an analytic solution of the Stokes equation in the square domain $[0, 1] \times [0, 1]$.

In order to use these solution as a benchmark to the computational code, we program the body force in the equation (17) in such manner to obey the expressions (25) and (26). We expect to recover a velocity field equal to given by (23) and (24).

5. Results and Discussions

5.1 Cavity with constructed analytical solution

A simulation were performed considering a low Reynolds number of 10^{-6} . We use cavity size $(L)/40$, resulting in 1600 fluid particles uniformly spaced at the beginning of the simulation. It was necessary 320 particles to establish the walls. The smoothing length, h , is a central parameter in SPH simulations. Large values of h favors a good spatial average, because the influence radio of the kernel function becomes wider and a more particles are used in the mean processes. In other hand, to keep the local character of the model, the neighborhood should be narrow. Large values for h also tends to impose some over diffusion. In this work, we made a sensitive analysis in which we vary h and track the mean square deviation of the velocity components of the particles, defined by:

$$\epsilon = \frac{1}{n} \sum_{i=1}^n (u_{sp} - u_a)^2 \quad (27)$$

where n is he number of particle in the domain, u_{sph} is the simulation result, u_a is the analytical value for the u component of the velocity vector. Figure 1 shows the velocity vectors of a simulation with $h = 1.1\Delta x_o$, where Δx_o is the initial separation between the particles.

Figure 1: Velocity vectors for $h = 1.1\Delta x_o$ (Cavity flow with constructed solution).

Figures (2a) and (2b) shows the velocity profile at the horizontal central line compared with the analytical solution. It is possible to observe that for $h = 1.3\Delta x_o$ the results qualitatively agree more closely.

Figure 2: (a) Velocity profile at the horizontal central line for $h = 1.1\Delta x_o$ (Cavity flow with constructed solution). (b) Velocity profile at the horizontal central line for $h = 1.3\Delta x_o$ (Cavity flow with constructed solution).

The table (1) shows the results for the mean square deviation, ϵ , like a function of h . We can observe that ϵ reach a minimum approximately for $h = 1.6\Delta x_o$. The same behavior repeats for the maximum deviation between the analytical and numerical solutions.

Table 1: Mean square and maximum deviation as a function of the smoothing length for 1600 particles. (Cavity flow with constructed solution).

$h/\Delta x_o$	ϵ	maximum deviation
1.1	0.03430	0.0630
1.2	0.03100	0.0567
1.5	0.00380	0.0115
1.6	0.00048	0.0110
1.7	0.00590	0.0130
2.0	0.07210	0.1518

Monaghan [8], stress the importance of the number of particles for SPH simulation. Actually, in a wider sense, discrete methods must to preserve an invariance in relation of the number of particles. To examine the influence of spatial resolution the initial particle distance between the closest neighbouring particles is $L/20$, $L/30$, $L/40$, $L/50$ and $L/60$, resulting in 400, 900, 1600, 2500 and 3600 particles. In each case, we look for the optimum smoothing length too. For 400 particles we cannot to stabilize the simulation. For 900 particles we find out that the optimum smoothing length is different that we have found for 1600 particles, like can be seen in the table (2).

Table 2: Mean square and maximum deviation as a function of the smoothing length for 900 particles. (Cavity flow with constructed solution).

$h/\Delta x_o$	ϵ	maximum deviation
1.2	0.0045	0.0157
1.3	0.0011	0.0144
1.6	0.1078	0.2249
2.7	10.517	21.509

Figure (3) shows ϵ as a function of the number of particles. We can observe that ϵ appears to approximate to a plateau for large number of particles. Probably, the residual which still remains came from the temporal

integration.

Figure 3: Mean square deviation as a function of the number of particles.

It is important to alert that for each new value of n (number of particles) we proceed with a new optimization procedure. In these sense, we plot the optimum smoothing length as a function of the number of particles. In the Figure (4) we can observe that these relation is very close to linear in the interval we has studied.

Figure 4: Optimum smoothing length as a function of number of fluid particles.

5.2 Shear driven cavity flow

The other test case considered in the present work is the classical situation of the shear driven cavity flow. It is benchmark which has been used as reference for numerical studies of low and moderate Reynolds number flows. In the present case, the flow domain is a 2D square box with length of the edge $L = 10^{-3}m$. The upper wall of the cavity moves from left to right with constant velocity $U = 10^{-2}m/s$. We change the Reynolds number, $Re = UL/\nu$, by varying the kinematic viscosity, ν . The most important difference in the present flow in relation to the previous one is the fact that here the driven force comes from the shear stress term, while in the other case was a body force. To simulate the constant velocity plate at the top of the cavity, we create a line of particles which velocity is always equal to U but don't are allowed to change its positions. We perform two different simulations for $Re = 1$ and $Re = 100$, respectively. Experimental and numerical data available in the literature was employed in quantitative comparisons.

For $Re = 1$, 1600 fluid particles and 320 wall particles are used. The smoothing length, h , is equal to the initial separation between the particles. We compare our results with numerical data from finite element simulations obtained by Liu [5].

Figure 5: Shear-driven cavity flow. Velocity vectors for $Re = 1$.

Figure (5) shows the velocity vectors after the steady state. For quantitative validation, we extract the profile of horizontal component of the velocity vector at the central vertical line in the cavity and compare with the reference data. This comparison is shown in Figure (6). We can observe a good agreement between results.

Figure 6: Horizontal component of the velocity at the central line in the cavity for $Re = 1$. Red thick line is SPH results and black thin line is the numerical data from Liu (2003)

For $Re = 100$, 6400 fluid particles and 320 wall particles are used. The smoothing length, is $h = 1.3\Delta x_o$. We compare our results with numerical finite difference data obtained by Ghia [16].

Figure 7: Shear-driven cavity flow. Velocity vectors for $Re = 100$.

Figure (7) shows the velocity vectors after the steady state. We can observe a numerical oscillation at the upper right corner. One more time, we extract the profile of horizontal component of the velocity vector at the central vertical line in the cavity and compare with the Ghia data [16]. This comparison is shown in Figure (8). We can observe a good agreement between results in the bottom portion of the plot, but as we approximate to the moving plate the results turns away one each other. It is clear that the numerical oscillation has negative effects over the results of the simulation.

Figure 8: Horizontal component of the velocity at the central line in the cavity for $Re = 100$. Red thick line is SPH results and black thin line is the data from Ghia (1982).

6. Conclusions

A SPH numerical code for the simulation of incompressible Newtonian fluid flows confined at low Reynolds number was implemented. In this type of flow the viscous stress is mainly responsible for the fluid motion.

Initial tests were carried out by comparing numerical results with constructed analytical solutions of the Stokes equations where the studied domain is the cavity. In the study the smoothing length, h , and the spatial discretization (particles number) with different configurations were tested. To quantify the results were calculated the mean square and maximum deviation for each configuration. It noticed that, in the case studied, there is an approximately linear relationship between the smoothing length, h , and the particles number, n , so the optimal value of h depends on the n . Another case analyzed was the 2D shear driven cavity with $Re = 1$ and $Re = 100$, where both were compared with literature data. For the first case ($Re = 1$) we used an discretization with 1600 fluid particle and the SPH code obtains satisfactory results. For the simulation with $Re = 100$, we use an extended discretization, totaling 6400 fluid particles. The results were also good, but due to instabilities occurring in the upper right corner, the result in this region showed a small discrepancy compared with the literature. Thus, the SPH code was able to calculate satisfactorily confined flows with low Reynolds number.

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