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VALIDATION OF A SMOOTHED PARTICLE HYDRODYNAMICS CODE FOR INTERNAL FLOW SIMULATIONS: APPLICATION TO HEMODYNAMICS IN A REALISTIC LEFT HEART CAVITY MODEL

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ABSTRACT

A numerical simulation of flow in the left heart cavity, left ventricle, based on Smoothed Particle Hydrodynamics, a meshfree particle method is presented. Most of the works using this numerical method have been dedicated to simulation of free surface flows or internal flows with low Reynolds number. The present study is the first work dedicated to simulate the complex flow in a realistic rigid model of left ventricle applying the realistic pulsatile inlet velocity (having moderate Reynolds number) using a meshfree particle method.

The numerical validation of our code is performed through the simulation of flow in a cavity at a Reynolds number equal to 1000. Also, the comparison of the results of flow simulation in a simplified geometry of left ventricle with the finite volume results is presented. The smoothed particle hydrodynamics method was able to resolve the flow patterns showing its potential to be applied in complex cardiovascular flow simulations.

INTRODUCTION

Numerical simulation plays an important role in the analysis of physical problems in engineering and science and improves understanding new phenomena. In traditional numerical methods such as Finite Difference Methods (FDM), Finite Volume Methods (FVM) and Finite Element Methods (FEM), the physical domain is discretized into meshes (Eulerian approach). They have been used over a wide area in Computational Fluid Dynamics (CFD) and almost clearly understood and associated commercial software tools have been developed.

A new practical application of numerical simulation emerges in the field of biomedical engineering involving

several academic disciplines and professional specializations and integrates engineering and medicine. Investigation of blood flow dynamics in the cardiovascular system is of great interest in biomedical engineering and cardiology. Indeed, cardiovascular diseases are the major cause of death in North America. The heart is the main part in the cardiovascular system. The heart consists of four cavities with their own duty in receiving and pumping blood through the body. The left ventricle (LV) cavity has the most important responsibility in the heart since it receives the oxygen-rich blood and pumps it into the entire body. The detailed investigation of flow patterns inside of the LV can improve our understanding of heart function and provide further insight into the mechanisms of heart failure. Since the access to in vivo data is sometimes difficult, investigators can only rely on experimental measurements and computational simulations. For this purpose, numerical simulations are extremely useful tools since they allow the simulation of a large panel of normal and pathological conditions, however, the specific characteristics of cardiovascular flows represent a great challenge to current existing methods.

The most significant difficulty in traditional numerical methods comes from their mesh dependent nature that is time consuming and numerically expensive especially in the simulation of problems with complex geometries, moving interfaces and large deformable boundaries, such in the cardiovascular system. To overcome these limitations, a new generation of numerical methods called meshfree methods was created. A class of such methods, called particle methods, employs a set of particles in a fluid domain as physical representatives of the fluid. The particles are not connected to each, and therefore no mesh is required. A consequence, no

time is spent in mesh or remeshing the domain. Although all meshfree particle methods are similar in the fundamental idea, there are some differences mainly in the formulation of the approximations and their implementation. These methods are still under development and several improvements are still ongoing. In this study, a specific meshfree particle method, called Smoothed Particle Hydrodynamics (SPH), is used.

In comparison with other meshfree methods, there are some advantages in using SPH method; this method is a completely meshfree method (some meshfree methods need a kind of background cells to integrate the system of equations locally or on the whole the domain), applicable in micro- to macro- scale phenomena and fluid and solid dynamics simulations.

In literature, a limited number of works were dedicated to modeling blood flow in the cardiovascular system using meshfree methods. Krafczyk et al. applied lattice Boltzmann method to simulate the flow through a model of mechanical heart valve [1]. Fang et al. modeled the unsteady pulsatile flow in a simple geometry similar to plane poiseuille flow using Lattice Boltzmann method [2]. With exception to the work of Sinnott et al. on SPH application to blood flow in bifurcation artery presented at CSIRO Minerals conference in 2006 [3], no other work has been dedicated to extend SPH applications to moderate Reynolds number pulsatile flows in geometries similar to the ones found in the cardiovascular system.

All the previous simulations of the flow inside the heart cavities employed grid-based methods, such as finite difference method, finite volume method, and immersed boundary method [4, 5, 6].

Smoothed Particle Hydrodynamics (SPH), a fully Lagrangian meshfree method, was created originally, by Lucy and at a same time by Gingold and Monaghan around 1970s [7, 8], to simulate compressible flows in astrophysics. The applications of SPH method in engineering fields began around 1991. Indeed, most of the incompressible flow simulations using SPH are dealing with free surface or internal low Reynolds number cases. As a primary approach, we performed 2D modeling of the flow inside a simplified model of the LV [9]. The present work is the first work demonstrating the ability of SPH and our home-made code to simulate the flow in a realistic geometry of a LV cavity with a realistic inlet velocity boundary condition.

SPH METHODOLOGY

In SPH, a continuum domain is discretized by a finite number of particles. Each particle has its own physical properties that are approximated using the information of its neighboring particles. The numerical interpretation of this concept leads to

$$A(\vec{r}_a) = \sum_b m_b \frac{A_b}{\rho_b} W(\vec{r}_a - \vec{r}_b, h) \quad (1)$$

The physical properties, A , of a particle, a , located at \vec{r}_a is interpolated by a summation over its neighboring particles, b , located at \vec{r}_b using an Gaussian shape interpolating function of W , characterized by h , called smoothing length. Interpolating function (kernel function) is a symmetric function which is normalized and is analog to a Dirac delta function when h tends to zero.

Many different kinds of kernels are constructed and presented. In this study, a fourth order, quartic, spline kernel for 2D simulations is used because of its high stability as, [10]

$$W_{ab} = \frac{\alpha_d}{h^2} \begin{cases} \left(\frac{5}{2}-q\right)^4 - 5\left(\frac{3}{2}-q\right)^4 + 10\left(\frac{1}{2}-q\right)^4 & 0 \leq q \leq 0.5 \\ \left(\frac{5}{2}-q\right)^4 - 5\left(\frac{3}{2}-q\right)^4 & 0.5 \leq q \leq 1.5 \\ \left(\frac{5}{2}-q\right)^4 & 1.5 \leq q \leq 2.5 \\ 0 & 2.5 < q \end{cases} \quad (2)$$

where $\alpha_d = 96/1199\pi$ and $q = |\vec{r}_{ab}|/h$. Here, we set smoothing length 1.25 times of the initial particle spacing.

Using Eq. (1) and its gradient for scalar properties and divergence operator for vectorial properties, the Navier-Stokes equations can be rewritten in the form of SPH formulation.

The flow inside the heart cavities behaves as an incompressible Newtonian fluid flow [11]. The Lagrangian form of the Navier-Stokes equations are

$$\frac{d\rho}{dt} = -\rho \vec{\nabla} \cdot \vec{V} \quad (3)$$

$$\frac{d\vec{V}}{dt} = -\frac{\vec{\nabla} P}{\rho} + \frac{\mu}{\rho} \nabla^2 \vec{V} \quad (4)$$

here ρ is the fluid density, \vec{V} is the velocity vector, P is the pressure and μ is the fluid dynamic viscosity.

In SPH literature, different types of formulations are presented to approximate each term of the continuity (Eq. 3) and momentum (Eq. 4) equations.

For continuity equation, an appropriate formulation for liquids connecting the rate of change in density to the relative velocity of the particles is employed here as, [12]

$$\frac{d\rho_a}{dt} = \sum_b m_b (\vec{V}_a - \vec{V}_b) \vec{\nabla}_a W_{ab} \quad (5)$$

To approximate momentum equation based on SPH formulation, pressure and viscous forces need to be modeled. In this study, momentum equation is formulated as, [12, 13]

$$\frac{d\vec{V}}{dt}\bigg|_a = -\sum_b m_b \left(\frac{P_b}{\rho_b^2} + \frac{P_a}{\rho_a^2} \right) \vec{\nabla}_a W_{ab} + \sum_b m_b \frac{(\mu_a + \mu_b) \vec{r}_{ab} \cdot \vec{\nabla}_a W_{ab}}{\rho_a \rho_b |\vec{r}_{ab}|^2} \vec{V}_{ab} \quad (6)$$

Finally, the position of each particle is calculated by doing time integration over the velocity.

In SPH method, the pressure is calculated based on a quasi-incompressible equation of state such as, [13]

$$P = c^2 \rho \quad (7)$$

where c is the speed of sound. An artificial sound speed has to be employed to keep density fluctuations within an acceptable range of 1 - 3 % (to maintain incompressible flow behavior). The value of 10 times of maximum bulk velocity of the flow is suggested as a rough value for this sound speed. Indeed, applying the realistic speed of sound results in a very small computational time steps.

NUMERICAL FEATURES

Here, a second order predictor-corrector procedure is employed for time integration of the algebraic equations. This method has three main stages. In predictor stage the explicit time integration is done in a half time step and the corrector part corrects the physical properties using the forces at the half time step. At the end, the properties at new time step are calculated using the previous time step and half time step information. A variable time step is used based on the three criteria controlled by Courant- Friedrichs- Levy (CFL) condition, magnitude of particle acceleration and viscous diffusion.

To Model wall boundaries, different techniques are reported in SPH literature [13, 14, 15]. In this study, a set of number of particles are located on the wall boundaries and three layers of fixed particles are imagined outside of the boundaries parallel to the walls (Fig. 1). In this case, the particles near the boundaries will have enough particles in their neighboring domain to interact with.

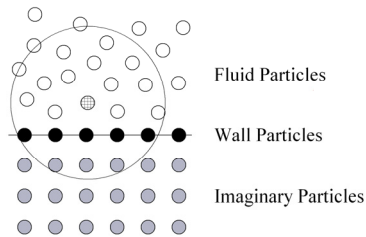


Figure 1. Wall boundary condition implementation

The velocity of particles on the walls are put zero, and an extrapolated velocity is allocated to the imaginary particles in a way to enforce the zero velocity condition on the wall

boundaries [13]. The inlet and outlet boundary conditions (open boundaries) are defined in such a way, the conservation of mass over the domain is satisfied.

As mentioned earlier, to calculate the physical properties of each particle, the information of its neighboring particles are needed and as the position of particles are changing with time, at each instant, the numerical algorithm requires to find neighboring particles within the supporting size of the selected kernel function. The simplest way, but highly computational time demanding, is to calculate the distance of a given particle with all particles in the domain and compare it with the kernel supporting size at each time step. Thus, the computational time is in the order of N^2 , where N is the number of particles.

Here, we applied the idea of linked list method [16] to search the neighboring particles rapidly. In this method, some imaginary cells are constructed with a dimension equal to the support size of the kernel function. Then, for a particle in a cell only the interaction with the particles in the neighboring cells are considered. In this way, the computational time is significantly reduced to $N \log N$. The efficiency of linked list method rises logarithmically with increasing the number of particles.

VALIDATIONS AND RESULTS

The ability of SPH and our home-made code to predict accurately the moderate Reynolds number flows is examined by simulating the flow in lid-driven cavity with physical properties of $L=1(m)$, $\rho_o=1(kg/m^3)$ and $\nu=1/1000(m^2/s)$ leading to $Re=U_o L/\nu=1000$. Here U_o is the lid velocity and L is dimension of the square cavity. This test case is a standard benchmark widely used to validate numerical codes.

The SPH simulated velocity vector map at steady state is shown in Fig. (2).

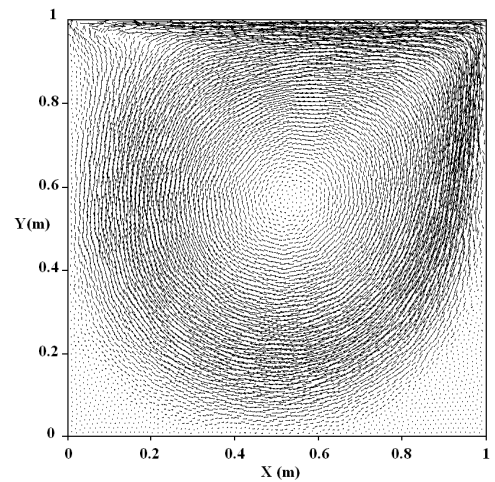
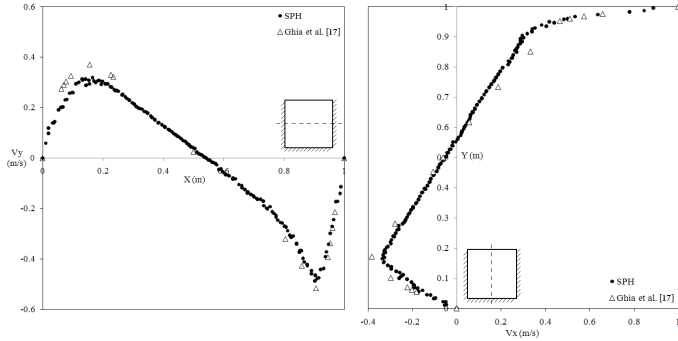


Figure 2. Velocity vector map; Lid-driven cavity flow

The velocity components profiles at the main mid-cross sections of the cavity are plotted in Figs. 3 (a,b) and compared

with the reported results of Ghia et al. [17]. In these figures, the velocity of particles located in a thin strip with a width equal to the initial particle spacing along each cross section are considered. Here, the initial spacing of SPH particle distribution is 1/80 (m).

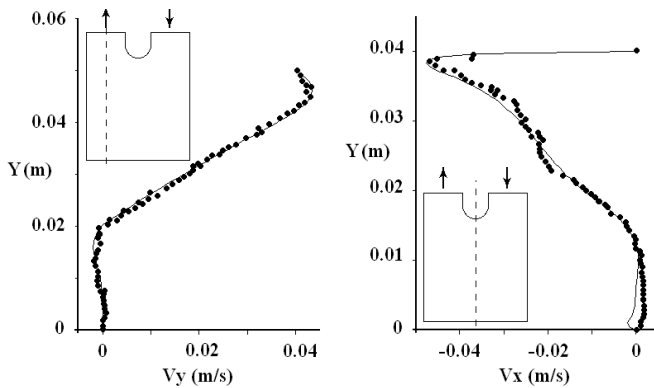


3(a) at the main horizontal cross section 3(b) at the main vertical cross section

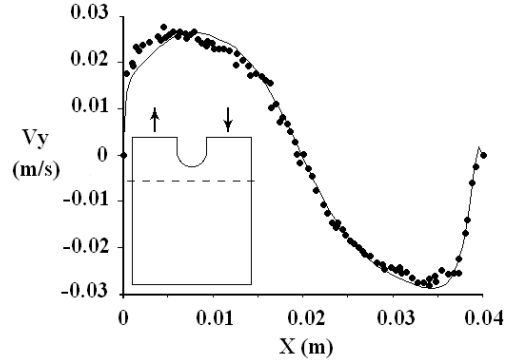
Figure 3. Velocity profiles obtained by SPH against the reference results for a lid-driven cavity flow; Re= 1000

The good agreement between the results of SPH and reference shows that SPH formulations and the code are able to give accurate estimations of the velocity field. The incompressibility stands well in the accepted limit (The maximum density variation is 0.1%).

To simulate the flow inside the LV, as a first approach, a simple 2D model of LV was considered with an unsteady inlet velocity, as a simple parabolic function of the time with a periodic time of 0.6 (s) and peak velocity of 0.4 (m/s) at 0.3 (s) [9]. The velocity profiles at the main vertical and horizontal cross sections of the LV are plotted and compared with the results obtained using FV method in Figs. 4 (a,b) at t=0.3 (s). [9]



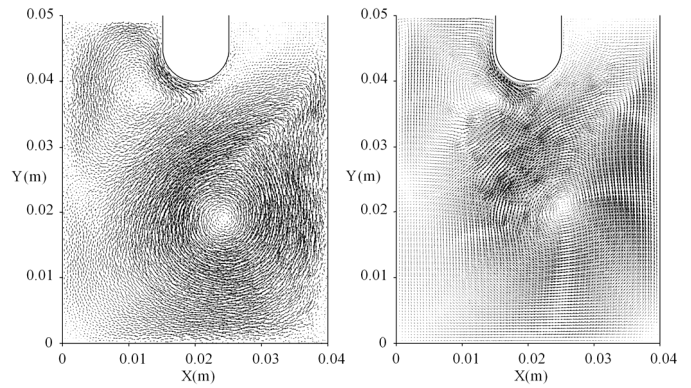
4(a) at vertical cross sections



4(b) at up horizontal cross section

Figure 4. Velocity profiles obtained by SPH against the FV results at t=0.3 (s); simplified model of LV [9]

The simulated velocity vector map at the end of a cycle (0.6 s) is plotted and compared qualitatively with the results obtained using finite volume method (FV) in Fig. 5.



5(a) SPH

5(b) FV

Figure 5. Velocity vector map; Simplified model of LV

The close agreement between our results and the ones obtained using FV method shows the ability of SPH to approximate properly the behavior of unsteady flows having the same range of flow characteristics and geometry as the subject of this study.

To simulate the flow inside a realistic model of LV, a 2D geometry of LV is considered as sketched in Figs. 7 (a-d). The inlet pulsatile velocity is modeled with a time dependent magnitude as shown in Fig. 6 based on in vivo study for filling phase.

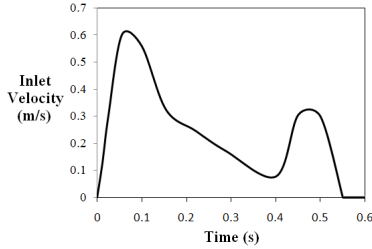


Figure 6. One cycle of pulsatile inlet velocity magnitude

Figures 7 (a-d) show the simulation results of velocity vector maps at different instants of a cycle ($t = 0.2$; 0.4 ; 0.5 ; and 0.6 s). The numerical code runs for three inlet velocity cycles to reach the periodicity and results are extracted after two cycles were completed.

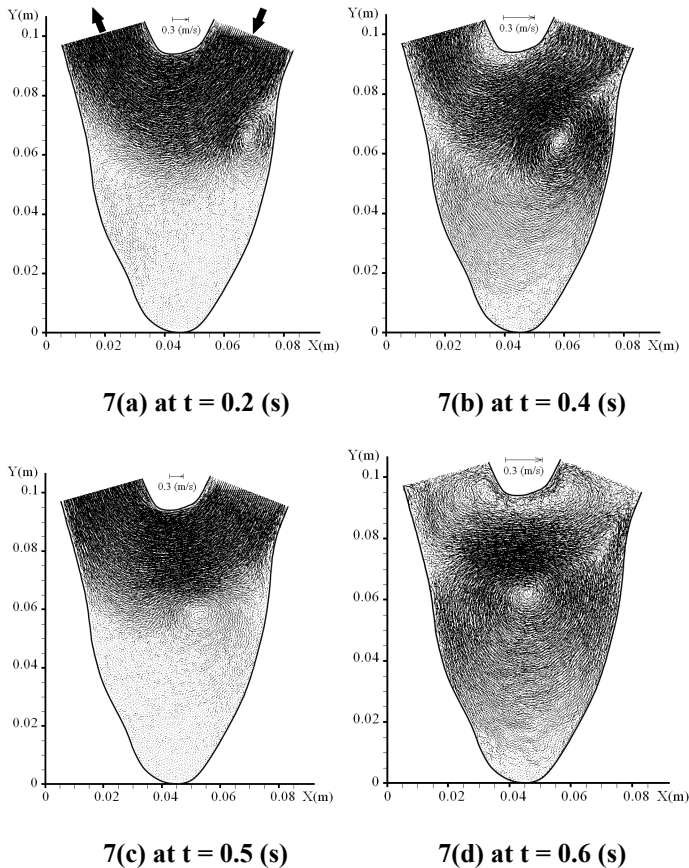


Figure 7. Velocity vector maps at different instants of a cycle; Realistic model of LV

As in our model the outlet (aortic valve) is always in open position, the flow entering from inlet (mitral valve) is directed towards the aortic valve. The acceleration phases show the penetration of the entering jet in the LV and in the deceleration phase, jet breakdown phenomena leads to appearance of a

coherent structure in the LV that is then convected towards the centre of the LV at the end of the deceleration periods.

The Lagrangian nature of the SPH method allows for the tracking of fluid particles easily to obtain the time history of the fluid particles which is important in fluid mechanics studies and biofluid mechanics in particular. In this way the applied shear stresses on individual fluid particles passing from different locations in the domain are able to be achieved at each instant. Figure 8 shows the time history of fluid particles located at different locations until leaving the domain.

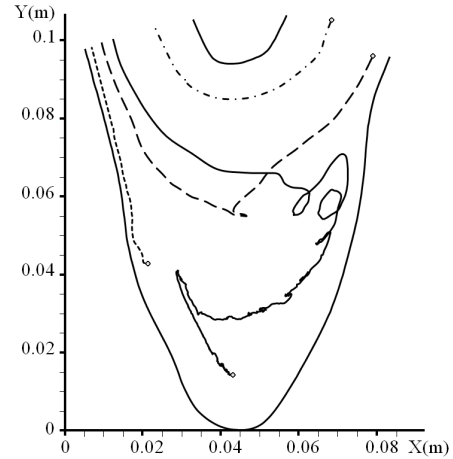


Figure 8. Time history of particles; Realistic model of LV

As it was mentioned previously, the linked list method searches the neighboring particles of each particle faster comparing with the simple search method. Our study shows that the computation time in a case with 6100 fluid particles (initial particle spacing of 1 mm) runs 45 times, 12600 fluid particles (initial particle spacing of 0.7 mm) run 90 times and 25000 fluid particles (initial particle spacing of 0.5 mm) runs 158 times faster than when linked list method is not applied.

CONCLUSION

As a conclusion, despite the fact that in the present simulation the LV wall movements are not considered, the characteristics of the flow, such as main vortex structure in the LV, obtained using SPH method are very close to the ones observed in a LV during the filling phase [18]. This work is the first attempt to simulate the flow in a realistic rigid geometry of LV using a meshfree particle method. To reach physiological conditions, the flow pattern under the effect of LV myocardial deformation is under investigation as well as opening and closure of the heart valves. The realistic dynamic deformation of LV can be captured based on in vitro studies. This allows also the comparison of computed flow velocity field with experimental results using particle image velocimetry (PIV) system.

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