Proceedings of the ECCOMAS Thematic International Conference on Simulation and Modeling of Biological Flows (SIMBIO 2011) September 21–23, 2011, VUB, Brussels, Belgium

ISAIF10-042

Study of a Lattice–Boltzmann Immersed Boundary Coupled Method for Fluid-Structure Interactions in Hemodynamics.

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Abstract

The development of most cardiovascular diseases can be associated with certain specific hemodynamic conditions. Hence, a detailed description of such conditions is an important information for the medical community. With this goal in mind, we propose in this work a lattice-Boltzmann Immersed Boundary coupled method to model two and three-dimensional blood flows in deformable vessels. The lattice-Boltzmann (LB) method is a mesoscale method that deals with micro-particles distributions on a regular lattice and approximates the incompressible Navier-Stokes equations under some hypothesis. In the cardiovascular system, besides a detailed blood dynamics description, it is also important to represent the phenomena of pressure wave propagations (by fluid-structure interactions). When coupled, for instance, to an Immersed Boundary (IB) method, the LB method can model the fluid dynamics and its interaction with an immersed structure. Here, the structure represents the arterial walls and the blood is represented by the fluid inside the closed domain defined by the structure. The LB method with BGK approximation is explicit and efficiently parallelizable, therefore, suitable to be implemented in a parallel environment in order to reduce the computing time of complex simulations. In that direction, it is important to point that the use of an IB method has the advantages of permitting the description of different constitutive laws for the wall arteries and also of preserving the efficiency of the parallelization of the LB method, without having to create and destroy nodes as the structure moves. We validate this implementation by simulating an elastic stretched membrane oscillating towards an equilibrium state. In addition, we present the pressure wave propagation phenomena in two and three-dimensional vessels. These last two cases are used to study the sensitivity of the problem to changes in some of the new parameters introduced by the coupled method.

Keywords: Navier–Stokes, Incompressible fluids, Physiological flows, Fluid-structure interaction.

Introduction

The development of many cardiovascular diseases is associated to certain specific hemodynamic conditions. Hence, a detailed description of the blood flow in the target vessels of the human body and the associated hemodynamic quantities are an important information for the medical community. With this goal in mind, we study in this work a lattice–Boltzmann Immersed Boundary coupled method to model two and three-dimensional fluid (blood) flows in deformable vessels.

Since its introduction in the 80's the lattice–Boltzmann method (LBM) has overcome several refinements and extensions, and has become a promising numerical scheme for simulating complex fluid dynamics in the most varied applications. In particular, LBM has been systematically employed, during the last few years, in several computational hemodynamics applications. Some examples are the simulation of blood flows in heart valves [5, 15], in coronaries [14], in aneurysms [10, 12] and in the abdominal aorta [2], among others.

Differing from the conventional methods, based on the discretization of continuum macroscopic Navier–Stokes equations, LBM is a mesoscopic particle based method derived from the Lattice-Gas Cellular Automata method (LGCA) [16] and the Boltzmann Equation [1]. It approximates the incompressible Navier-Stokes equations under some hypothesis [11].

In the cardiovascular system, besides the detailed blood dynamics description that can be provided by this method, it is also important to take into account the interaction between the blood and the arterial walls. This allows us to represent the wave propagation phenomena, as a consequence of the deformation of the arterial walls. When coupled, for instance, to an Immersed Boundary (IB) method [4], the LB method can model the fluid dynamics and its interaction with an immersed structure. Here, the structure represents the arterial walls and the blood is represented by the fluid inside the closed domain defined by the

structure. It is important to recall here that the LB method with BGK approximation is explicit and efficiently parallelizable, therefore, suitable to be implemented in a parallel environment in order to reduce the computing time of complex simulations. In that direction, the use of an IB method has the advantages of permitting the description of different constitutive laws for the wall arteries and also of preserving the efficiency of the parallelization of the LB method, without having to create and destroy nodes as the structure moves.

To accurately represent the involved phenomenology, we present in this work a study of the fluid-structure interaction model proposed by [4] in terms of mass conservation, influence of the external non-physical fluid, walls rigidity and the relevance of an implicit coupling. This analysis can provide a good insight on the correct application of this coupled method. The coupling between fluid and solid problems can be made in an implicit or explicit manner. In any case, the immersed structure moves with the same velocity as the fluid and, as a reaction, the structure responds with a force that depends on the local strains through a given constitutive law. We also extend this model to the three-dimensional counterpart, where the immersed fibers (one-dimensional structures) are replaced by two-dimensional structures.

We validate this implementation by simulating an elastic stretched membrane oscillating towards an equilibrium state (see [4]). In addition, we present the hemodynamics area problem of pressure wave propagation in two and three-dimensional vessels. A discussion about the sensitivity of these problems to the parameters variations is presented.

The structure of the paper is as follows. In Section Methods, the governing equations of LBM with BGK approximation and the chosen methods for implementing boundary conditions, as well as, its coupling with an immersed boundary are presented. In Section Numerical Results, we present the numerical validation and study the results of the three proposed problems. Finally, the conclusions are outlined in the Conclusions Section.

Methods

From the numerical point of view, the lattice–Boltzmann Method with BGK approximation (referring to the work of [3]) is an explicit method with Eulerian description. It is based on the movement and collision of micro-particles distributions described by the lattice–Boltzmann equation (LBE):

$$f_i(\vec{x} + \Delta x\, \vec{e_i}, t + \Delta t) - f_i(\vec{x}, t) = \frac{1}{\tau}\left[f_i^{\text{eq}}(\vec{x}, t) - f_i(\vec{x}, t)\right],\ i = 0, \ldots, \ell, \quad (1)$$

where, $f_i(\vec{x}, t)$ represents the micro-particles distribution density at position $\vec{x}$ and time t, moving towards the direction $\vec{e_i}$ of the lattice, Δx is the lattice spacing, Δt is the time step and ℓ is the dimension of the discrete velocity space. The relaxation parameter (τ) is related to the kinematic viscosity of the fluid (ν) through the expression: $\nu = (2\tau - 1)\Delta x^2/(6\Delta t)$. It has been demonstrated that the LBE approximates the Navier-Stokes equations by means of an asymptotic expansion [11].

The equilibrium distribution chosen for this work was introduced by [11], and is devised to minimize the compressibility effects of the method. It is described as:

$$f_i^{\text{eq}} = \omega_i \left\{ \rho + \rho_0 \left[3\frac{(\mathrm{v}\vec{e_i} \cdot \vec{u})}{\mathrm{v}^2} + \frac{9}{2}\frac{(\mathrm{v}\vec{e_i} \cdot \vec{u})^2}{\mathrm{v}^4} - \frac{3}{2}\frac{(\vec{u} \cdot \vec{u})}{\mathrm{v}^2} \right] \right\},\ i = 0, \ldots, \ell, \quad (2)$$

where, $\mathrm{v} = \Delta x/\Delta t$ is the particles speed, the weights ω_i are lattice dependent, ρ_0 is the average density (constant), ρ and u are the density and velocity of the fluid, calculated from the distribution density as:

$$\rho(\vec{x}, t) = \sum_{i=0}^{\ell} f_i(\vec{x}, t), \quad \rho_0 \vec{u}(\vec{x}, t) = \sum_{i=1}^{\ell} \mathrm{v}\vec{e_i} f_i(\vec{x}, t). \quad (3)$$

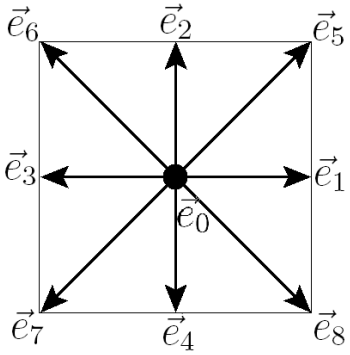
In this model, the pressure is calculated as function of the density

$$P = \rho c_s^2, \quad (4)$$

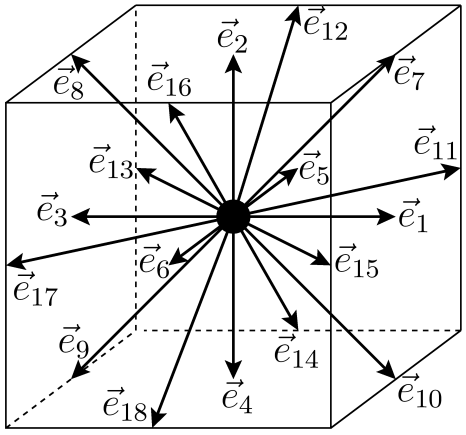
where $c_s = \mathrm{v}/\sqrt{3}$ is the speed of sound in the lattice.

Several 2D and 3D lattice models were proposed in the literature for the LBM. The most commonly used were adopted in the current work, namely the $D2Q9$ for 2D problems and the $D3Q19$ for 3D problems (both shown in Fig 1). The characteristic directions of the lattice model $D3Q19$ are: $e_0 = (0,0,0)$, $e_1 = (1,0,0)$, $e_2 = (0,1,0)$, $e_3 = (-1,0,0)$, $e_4 = (0,-1,0)$, $e_5 = (0,0,-1)$, $e_6 = (0,0,1)$, $e_7 = (1,1,0)$, $e_8 = (-1,1,0)$, $e_9 = (-1,-1,0)$, $e_{10} = (1,-1,0)$, $e_{11} = (1,0,-1)$, $e_{12} = (0,1,-1)$, $e_{13} = (-1,0,-1)$, $e_{14} = (0,-1,-1)$, $e_{15} = (1,0,1)$, $e_{16} = (0,1,1)$, $e_{17} = (-1,0,1)$, $e_{18} = (0,-1,1)$. And the directions of the lattice model $D2Q9$ are: $e_0 = (0,0)$, $e_1 = (1,0)$, $e_2 = (0,1)$, $e_3 = (-1,0)$, $e_4 = (0,-1)$, $e_5 = (1,1)$, $e_6 = (-1,1)$, $e_7 = (-1,-1)$, $e_8 = (1,-1)$. The mentioned weights for the equilibrium distribution (see Eq. (2)) of the lattice model $D3Q19$ are $\omega_0 = 1/3$, $\omega_{1-6} = 1/18$, $\omega_{7-18} = 1/36$ and of the lattice model $D2Q9$ are $\omega_0 = 4/9$, $\omega_{1-4} = 1/9$, $\omega_{5-8} = 1/36$.

As mentioned before, the fluid-structure interaction (FSI) is essential to model pressure wave propagation phenomena in the cardiovascular system, as this happens due to the deformation capacity of the arterial vessels. As the LBM is based on a rigid mesh, we have basically two alternatives to model the FSI: to create and destroy fluid nodes as the structure moves [7, 13] or to use a structure immersed in the fluid domain (immersed boundary) [5, 17]. This second approach has the advantages of using fixed number of nodes, making its implementation and parallelization easier and more balanced, besides the fact that it allows the modeling of heart valves and other immersed deformable objects. But it carries the drawback of using more nodes for the area external to the vessel.



(a) 2D lattice model $D2Q9$



(b) 3D lattice model $D3Q19$

Figure 1 Characteristic directions of the lattice models $D2Q9$ and $D3Q19$.

In a simplified approach one can model the arterial walls as 1D or 2D massless structures (for 2D and 3D problems, respectively) that have a constitutive law to relate their force response to a local deformation. These structures (immersed boundaries) are composed by connected nodes that can be described in a Lagrangian manner. To clarify this idea we expose the macroscopic coupled equations, as proposed by [8], for the fluid–structure interaction (with comments on how the coupling equations are interpreted by the model):

$$\begin{cases} \text{Mass conservation:} \\ \quad \nabla \cdot \vec{u} = 0, \\ \text{Momentum conservation with force term:} \\ \quad \rho(\vec{u}_t + (\vec{u}\cdot\nabla)\vec{u}) = -\nabla p + \mu\Delta\vec{u} + \vec{f}, \\ \text{Interaction fluid}\rightarrow\text{structure:} \\ \quad \dfrac{\mathrm{d}\vec{X}(\vec{s},t)}{\mathrm{d}t} = \displaystyle\int_{\Omega_f} \vec{u}(\vec{x},t)\delta(\vec{x}-\vec{X}(\vec{s},t))\mathrm{d}\vec{x}, \\ \text{Constitutive law of the structure:} \\ \quad \vec{F}(\vec{s},t) = \mathcal{S}_f\vec{X}(\vec{s},t), \\ \text{Interaction struture}\rightarrow\text{fluid:} \\ \quad \vec{f}(\vec{x},t) = \displaystyle\int_{\Gamma_b} \vec{F}(\vec{s},t)\delta(\vec{x}-\vec{X}(\vec{s},t))\mathrm{d}\vec{s}, \end{cases} \quad (5)$$

where, P and μ are the pressure and the kinematic viscosity of the fluid, $\vec{f}$ represents the force term (Eulerian description) of the structure acting on the fluid, $\vec{F}$ is the reaction force of the structure (Lagrangian description), $\vec{s}$ is the fiber length (or the area in 3D) of the structure segment, $\mathcal{S}_f$ is the constitutive law, δ is the Dirac delta function, $\vec{X}$ and $\vec{x}$ represent the spatial positioning of the structure and the fluid and $\vec{U}$ and $\vec{u}$ their respective velocities. In the system above, the Eulerian variables (fluid) were described by lower case letters and the Lagrangian ones (structure) by upper case letters.

In a discrete version of equations (5) the force term $\vec{f}$ is the mapping of the force $\vec{F}$ from the structure by means of interpolations that make use of a discrete Dirac delta function, namely δ_h, which approximates δ when $h \to 0$ (see [4]). And, as we intend to apply $\vec{f}$ using the LB equation, this force has to be distributed, inside each node, among the lattice directions. The force term acting on each direction will be called $g_i(\vec{x},t)$. This distribution has to be done in a way that equations (5) are recovered, such as the following model [4]:

$$g_i = 3\omega_i \left\{ \vec{f}\cdot[(\vec{e}_i - \vec{u}) + 3(\vec{e}_i\cdot\vec{u})\vec{e}_i] \right\}, \quad i = 1,\ldots,\ell. \quad (6)$$

Many authors [6, 8, 17] include this force such that the LB equation remains explicit (first order convergence [4]):

$$f_i(\vec{x}+\Delta x\,\vec{e}_i, t+\Delta t) - f_i(\vec{x},t) = \frac{1}{\tau}\big[f_i^{\mathrm{eq}}(\vec{x},t) - f_i(\vec{x},t)\big] + \Delta t\, g_i(\vec{x},t),\ i = 1,\ldots,\ell. \quad (7)$$

But when we need to model structures that move fast or that are exposed to great pressure gradients it is more recommended the use of higher order methods. In [4] a second order implicit approach was proposed:

$$f_i(\vec{x}+\Delta x\,\vec{e}_i, t+\Delta t) - f_i(\vec{x},t) = \frac{1}{\tau}\big[f_i^{\mathrm{eq}}(\vec{x},t) - f_i(\vec{x},t)\big] + \frac{\Delta t}{2}\left[g_i(\vec{x},t) + g_i(\vec{x}+\Delta x\,\vec{e}_i, t+\Delta t)\right], \quad (8)$$

for $i = 1,\ldots,\ell$. This implicit equation can be solved by Piccard iterations (as detailed in [4]). This model was implemented in the present work to have a second order approach, but we also tested the explicit approach, even proposing the use of different time steps for the fluid and the structure.

The constitutive law of the structures reaction force may include, for example, coefficients of tension (k_t), bending (k_b), fastening (k_f), among others, as shown bellow:

$$\vec{F} = k_t\frac{\partial^2\vec{X}}{\partial s^2} - k_b\frac{\partial^4\vec{X}}{\partial s^4} - k_f(\vec{X}-\vec{Z}). \quad (9)$$

In hemodynamics simulations it is a common practice to impose the value of the pressure at the inlets/outlets.

Thus, in order to impose the pressure boundary conditions, we adopted the model propose by [18], designed for flat surfaces. In addition, we chose the model proposed by [9] to impose the boundary conditions for the velocity field. Both method are of second order.

Numerical Results

This section presents results from the implementation of three problems: a stretched pressurized membrane immersed in a viscous fluid and the wave propagation phenomena in two and three dimensions. The first problem is a benchmark that allow us to check the volume conservation of the closed structure and the moving structure behavior. The other two subsections show the analysis of the hemodynamic problem of pressure wave propagation in vessels. A more detailed study of the involved parameters is presented for these problems as they are of great interest in the modeling physiological blood flows in the main vessels of the human body.

Immersed membrane in 2D

To validate the implementation, we simulated a stretched pressurized membrane immersed in a viscous fluid. This choice was made because in this problem the interaction of fluid and boundary is intense, there is an abrupt pressure jump across the boundary, and the fluid leakage is easy to be measured in the close boundary. This membrane is a closed massless fiber (as shown in Fig 2) that was stretched to assume an initial elliptic conformation, with major and minor radii r_x = 0.75cm, r_y = 0.5cm, respectively. The constitutive law that describes the boundary force of the membrane is determined by its local configuration as:

$$\vec{F} = k_t \frac{\partial^2 \vec{X}}{\partial s^2}, \tag{10}$$

where k_t is the fiber tension stiffness. Driven by the restoring force of the elastic boundary and the reaction of fluid inside, the shape of the membrane should converge to an equilibrium circular steady state after a period of oscillations of pressure, velocity, fiber length and enclosed fluid volume (area).

The parameters of the simulated problem are (as proposed in [4]): ρ_0 = 1g/cm^3, k_c = 0.02g cm^2/s^2, ν = 0.002cm^2/s, the boundary condition is p = 100/3 dyn/cm^2 and the initial condition is the same with $\vec{u}$ = 0. It is important to remark that the equilibrium distribution used on the present work is devised to minimize compressibility effects, so the area enclosed by the membrane (as the mass) is expect to have small oscillations. In fact, until the simulation reaches the stationary phase the area inside the membrane changes less than 0.32%. So the fluid leakage is almost negligible in this case.

In Figure 3 are the variations of the horizontal and vertical radii of the membrane until the simulation reaches a the stationary phase. The pressure in the center of the domain is presented in Figure 4 along the same period. Here,

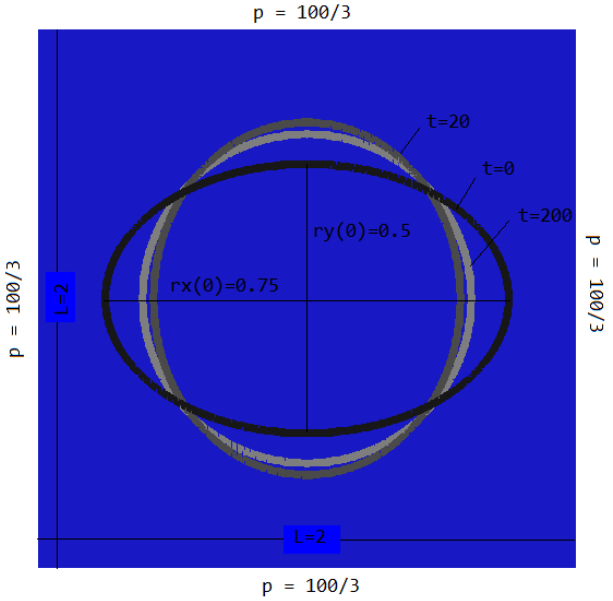


Figure 2 Description of the geometry of the immersed membrane in 2D and its deformation at the instants 0s, 20s and 200s.

we notice that the pressure (and the density, see Eq (4)) presents a variation of less than 0.1%.

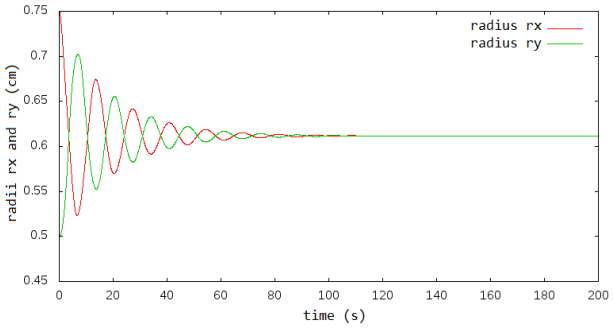


Figure 3 Variation of the two radii of the immersed membrane until the stationary phase.

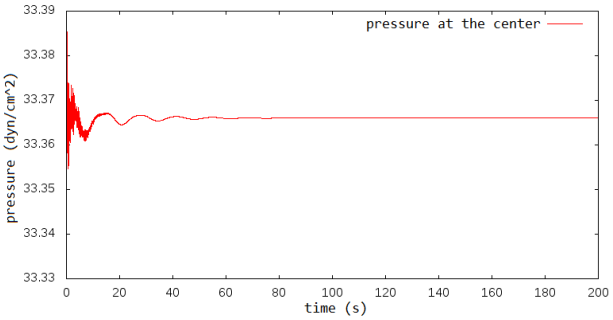


Figure 4 Oscillations of the pressure at the center point C until the stationary phase.

Wave propagation in 2D

The pressure wave propagation problem modeled in the present work takes place in a vessel with distensible walls and is driven by a short period inflow that increases the pressure an the inlet and forms the pressure wave. The walls are modeled by two massless immersed fiber, as shown in Fig 5. The external area allows the walls to move (along with the internal and external fluids) and on the boundary a reference pressure is imposed. While in the outlet of the vessel a condition of null velocity is imposed to have a conservation of the vessel's area after the inlet flow. The inflow condition is a parabolic profile with maximum velocity given by:

$$u_{max}(t) = \begin{cases} U\dfrac{D_i}{D(t)}\sin^2\left(\dfrac{\pi t}{T}\right), & t \leq T \\ 0, & t > T \end{cases} \quad (11)$$

where U = 93.33cm/s, D_i = 0.015cm is the initial vessel diameter, $D(t)$ is the inlet diameter at instant t and T = 2.805×10^{-4}s in the period of the inflow. The fluid parameters are: ρ_0 = 1.05g/cm^3 and ν = 0.035cm^2/s.

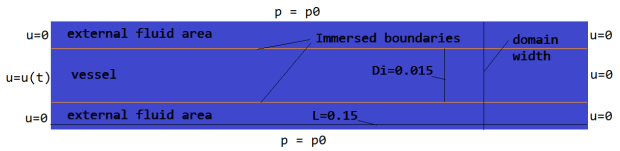


Figure 5 Description of the geometry of the wave propagation in 2D problem.

The constitutive law that describes the boundary force of the immersed fibers is dependent of the local fiber displacement from its initial position ($\vec{Z}$):

$$\vec{F} = k_f(\vec{Z} - \vec{X}), \quad (12)$$

where k_f is the fastening stiffness coefficient.

Figure 6 shows the pressure wave positioning along two periods, from which we can measure its propagation speed. Also, this figure shows the change in the wave speed as the wall fastening coefficient (k_f) changes. The greater k_f is, the more rigid are the walls of the vessel and the wave speed tends to infinity.

Table 1 shows the pressure wave speed for different external area sizes and different values of k_f. Notice that the wave speed increases as k_f increases, but also, that the wave speed has a dependency on the external area size. As this external area has an auxiliary role in the problem modeling, it should be as small as possible and the wave speed should be characterized as a function of k_f. It is important to remark that the wave speed is the information that allows us to model elastic arterial walls.

As a complementary test, we checked if a change in the proportion between structure nodes and fluid nodes would affect the simulation. Most authors, including this work, use $dx/ds \approx 4$ (proportion between the fluid nodes spacing and the structure nodes spacing) as the theoretical limit

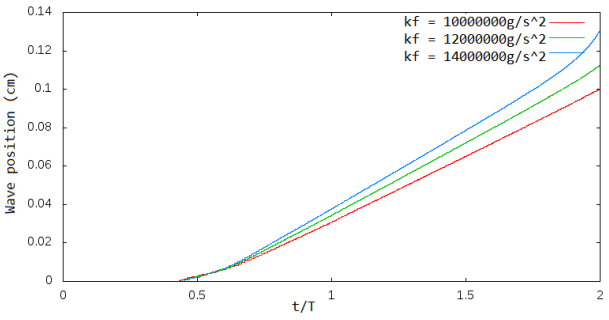


Figure 6 Wave dislocation along two periods for simulations with k_f = 1×10^{7}g/s^2, 1.2×10^{7}g/s^2 and 1.4×10^{7}g/s^2.

Table 1 Wave speed of different problems in 2D.

k_f (g/s^2)	domain width (cm)	wave speed (cm/s)
10000000	$1.5D_i$	256.5
10000000	$2.0D_i$	249.0
10000000	$4.0D_i$	230.6
12000000	$2.0D_i$	268.3
14000000	$2.0D_i$	292.2

is 2, but we decided to test $dx/ds = 3$ and noticed that for the wave propagation problem the changes in the results are negligible. But, when using $dx/ds = 2$ the fluid leakage through the walls became significant.

Wave propagation in 3D

This problem is similar to the previous one, with the difference that it takes place in a cylindrical three-dimensional vessel with the walls modeled by an immersed two-dimensional structure. To represent the walls of the vessel we used an immersed structured mesh with four connections at each node. This problem required a straightforward extension of the coupling proposed by [4] to three-dimensions, extending δ_h to the $\vec{z}$ coordinate.

The modeled vessel has an initial diameter (D_i) of 0.3cm and a length of 3cm. The inlet flow is a parabolic profile with maximum velocity given by Eq. (11), where where U = 0.525cm/s and T = 1.122s. The fluid parameters are: ρ_0 = 1.05g/cm^3 and ν = 0.0035cm^2/s. And the immersed structure has the same constitutive law as in the previous case (see Eq.(12)). The external volume is defined as a surrounding rectangular box (as shown in Fig 7) because the pressure imposition method is designed for flat surfaces. As in the previous case a reference pressure is imposed in the boundaries parallel to the planes XY and XZ.

Table 2 presents the calculated wave speeds for different values of the fastening stiffness coefficient (k_f) with a fixed external volume. From this table we find an almost linear relation between the wave speed and the coefficient k_f. Therefore, one could estimate the value of k_f that would model the behavior of an elastic three-dimensional arterial wall with a given wave propagation speed (usually around 5m/s).

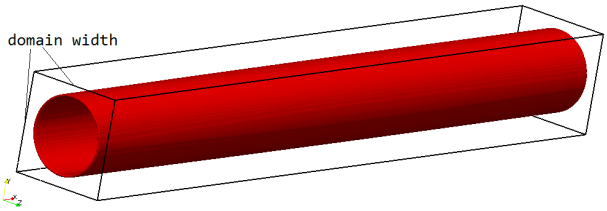


Figure 7 Geometry of the wave propagation in 3D problem.

Table 2 Wave speed of problems with different coefficients k_f in 3D.

k_f (g/s^2)	domain width (cm)	wave speed (cm/s)
150	$1.3D_i$	3.07
200	$1.3D_i$	3.52
300	$1.3D_i$	4.32
400	$1.3D_i$	5.11
600	$1.3D_i$	6.59

The computational cost of detailed 3D simulations is quite high, if compared to 2D simulations. In part because the number of fluid nodes and lattice directions increase, but also because the number of structure nodes increases and the coupling becomes more costly, as there are more nodes in the support of δ_h function (64 in 3D compared to 16 in 2D). In order to reduce the computational cost of these simulations we have tested the use of different time steps for the fluid and the structure, using a larger time step for the structure. That is reasonable if the structure moves at a low velocity and the time step of the fluid is very small, as in the present case. The tests showed that by using a time step 2 times bigger for the structure the wave propagation was not affected during the simulation. When we used a time step 4 times bigger there were a few differences in the wave positioning (close to 1%), and with it 8 times bigger some spurious oscillations appeared but the wave propagation was still very similar. A further analysis is required to determine the ideal structure time step for a general case, but for this problem we found an indication that it should be at most 4 times bigger than the fluid time step.

Conclusions

This work presented three problems of interest in the hemodynamics field with fluid-structure interactions. We propose here the modeling of incompressible fluid flows in vessels with elastic walls by the coupling of the lattice–Boltzmann method and the Immersed Boundary method.

In the wave propagation problems we checked that the external area (that allows the displacement of the vessel's walls) affects the wave speed but, once it has been set, we can analyze and propose a function that relates the wave speed and the fastening stiffness coefficient (k_f). This analysis shall be done in a future work.

This study represents a step towards a better description of the hemodynamics that takes place in arterial segments of interest. The studied model and its extension made to three-dimensional cases can detail the blood flow and its interaction with the arterial walls. This work also opens a door to the study of blood flow in more complex geometries, for which the consideration of an unstructured mesh for the immersed boundary is advised.

Acknowledgements

This work was partially supported by the Brazilian agencies CNPq and FAPERJ. Also, we would like to thank the great support provided by the National Institute of Science and Technology - Medicine Assisted by Scientific Computing (INCT-MACC). Finally, the first author was supported by the Brazilian agency CNPq through process 140234/2009-8. The support of these agencies is gratefully acknowledged.

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