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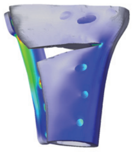

Minisymposium 1: Computational Bioengineering

COMPUTER SIMULATION OF MOTION OF SOLID PARTICLES IN LAMINAR FLOW USING STRONG SOLID-FLUID COUPLING COMPUTATIONAL SCHEME

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Abstract. Lattice Boltzmann method is successfully applied in simulating flows through micro and nano channels, but also in modeling blood flow, motion of particles under shear-thinning blood flow, analysis of leukocytes-erythrocytes interaction, as well as in many other areas in biomedicine. Accurate simulation of fluid flow, with solid particles moving through the fluid domain represents nowadays one of the greatest challenges in computational fluid dynamics. In this study, fluid behavior is modeled using lattice Boltzmann method. Strong coupling approach is used to model solid-fluid interaction. The Immersed Boundary Method (IBM) with enforced no-slip boundary condition is implemented in the in-house developed software. In this study, the developed software was used to model the motion of circular particles in a 2D laminar flow. Examples of motion of one and two particles in stenotic artery are considered. A good agreement with solution found in available literature is obtained. These results show that this approach for computer simulations of solid-fluid interaction can successfully be applied in biomedicine, to model motion of micro/nanoparticles in blood flow.

1. Introduction

Lattice Boltzmann (abbreviated LB) method is a discrete method that is used to simulate fluid flow. LB method observes the physical system in an idealized way, so that space and time are discretized, and the whole domain is made up of a large number of identical cells [1]. Special propagation function is defined, so that it depends on the state of neighboring cells and it has an identical form for all cells. The state of all cells is updated synchronously, through a series of iterations, in discrete time steps.

LB method is successfully applied in simulating multicomponent fluid flow in porous media and simulating flows through micro and nano channels [2,3], but also in modeling blood flow, including simulation of cancer invasion and tumor cell migration [4], motion of leukocytes under shear-thinning blood flow [5], analysis of leukocytes-erythrocytes interaction [6,7,8] as well as in many other areas in biomedicine.

During the last few years and decades modeling solid-fluid interaction has become one of the greatest challenges in computational fluid dynamics. There are several approaches in modeling the motion of solid bodies through a fluid domain [9-11]. In this paper Immersed Boundary Method (IBM) is used to model solid-fluid interaction [12].

In this paper the results of several simulations are shown. These simulations are performed using specifically designed software based on LB method, with additionally implemented IB method for simulation of solid-fluid interaction. The obtained results are compared to the results published in literature and a good agreement of results is obtained, that confirms that the developed LB solver can be successfully used to simulate fluid flow, with complex boundaries and with coupled movements of solid particles through the fluid domain.

The rest of the paper is organized as follows. Section 2 gives the basic equations of lattice Boltzmann method. Section 3 briefly discusses the details of the method used to model solid-fluid interaction. Results of simulations are presented in section 4. Section 5 concludes the paper.

2. Theoretical background of lattice Boltzmann method

The Boltzmann equation is a partial differential equation that describes the behavior and movement of particles in space and is valid for continuum. The basic quantity in Boltzmann equation is single distribution function 1, that is defined such that $f(\mathbf{x},\mathbf{v},t)$ represents the probability for particles to be located within a space element $d\mathbf{x}\,d\mathbf{v}$ around position $(\mathbf{x},\mathbf{v})$, at time t, where $\mathbf{x}$ and $\mathbf{v}$ are the spatial position vector and the particle velocity vector, respectively. BGK model of the continuous Boltzmann equation is given by:

$$\frac{\partial f}{\partial t}+\mathbf{v}\frac{\partial f}{\partial \mathbf{x}}+\mathbf{g}\frac{\partial f}{\partial \mathbf{v}}=-\frac{1}{\tau}\left(f-f^{(0)}\right) \tag{1}$$

where τ is the relaxation time (the average time period between two collisions), $\mathbf{g}$ is external force field, $f^{(0)}$ is the equilibrium distribution function, the so-called Maxwell-Boltzmann distribution function and Ω is the collision operator. Here a simplified model is introduced, initially proposed by Bhatnagar, Gross and Krook [13]. This model is known as the single relaxation time approximation or the Bhatnagar-Gross-Krook (BGK) model.

The original BGK Boltzmann equation is continuous in space domain and is related to continuous velocity field and it is not suitable for numerical implementation. In order to develop a program that numerically solves this equation, the discretization procedure has to be performed. But, this has to be conducted carefully, ensuring that the Navier-Stokes equations can still be derived from the newly obtained equations, in order to preserve the possibility to apply this method on fluid flow simulations.

The equation that represents LB numerical scheme and that is used in all the solvers based on LB method is given by:

$$f_i(\mathbf{x}+\xi_i,t+1)-f_i(\mathbf{x},t)=-\frac{1}{\bar{\tau}}\left(f_i(\mathbf{x},t)-f_i^{eq}(\mathbf{x},t)\right)+\left(1-\frac{1}{2\bar{\tau}}\right)F_i \tag{2}$$

where $\bar{\tau}$ is the modified relaxation time (given by $\bar{\tau}=\tau+\frac{1}{2}$).

When LB method is implemented on a computer, equation (2) is solved in two steps – collision and propagation step. Each one of these steps must be applied to the whole system (to all particles) before the next one starts.

2.1. Definition of macroscopic quantities

LB method describes the fluid on a molecular level and the characteristics of the fluid from the continuum aspect are implicitly contained in the model. Fluid density and velocity can be calculated using evaluated values of distribution function as weighted sums over a finite number of discrete abscissae that were used to discretize the space domain:

$$\rho = \sum_{i=0}^{q-1} f_i \tag{3}$$

$$\overline{\mathbf{u}} = \frac{1}{\rho} \sum_{i=0}^{q=1} \xi_i f_i = \frac{1}{\rho}\left(\rho\mathbf{u} - \rho\,\mathbf{g}/2\right) \tag{4}$$

3. Modeling solid-fluid interaction

The basic idea of strong coupling approach of solid-fluid interaction is to solve the complete domain (both fluid flow and particle motion) in every time step, so all quantities are changing simultaneously. The method used in this paper is called Immersed boundary method (abbreviated IBM) and it was first developed and presented by Peskin [14]. It uses a fixed Cartesian mesh to represent the fluid domain, so that the fluid mesh is composed of Eulerian points. IBM represents solid body as an isolated part of fluid, with a boundary represented by a set of Lagrangian points. The basic idea is to treat the physical boundary between two domains as deformable with high stiffness [15]. Force exerted from the fluid is acting on the boundary surface of the solid body and tends to deform the boundary. However, this deformation produces a force that tends to return the boundary to its original shape. These two forces have to be in equilibrium. Practically, using the law of action and reaction (Newton's third law) the force exerted from the fluid and acting on the solid is acting on the fluid near the boundary too, and is distributed through a discrete delta function. The entire solid-fluid domain is solved using Navier-Stokes equations, with external force term. There are several ways to determine this force representing the interaction between solid and fluid [16-18]. The approach used in this paper was proposed by Wu and Shu [19]. This method ensures that the non-slip condition is satisfied, i.e. ensures the equality of fluid and solid velocities in boundary points, by introducing a fluid velocity correction in boundary points. Using velocity corrections, it is also easy to evaluate the forces exerted from the fluid, acting on the immersed body and thus to solve particle motion.

4. Simulation results

Specialized and in-house developed software that numerically simulates fluid flow is used to simulate several problems of particle movement through fluid domain. Obtained results were compared with results that were found in literature. All examples are related to two-dimensional (plane) problems.

4.1. Simulation of movement of circular particle through a stenotic artery

The efficiency of the strong coupling approach in simulations of solid-fluid interaction becomes obvious when the flow is simulated in geometrically complex domain. Simulation of particle motion through a stenotic artery (artery with constriction) is one example. Li et al. [20] have analyzed the fluid flow in a mildly or severely stenotic artery and Wu and Shu simulated the motion of particles through stenotic artery [15]. In this paper results obtained using LB solver will be compared with results found in literature.

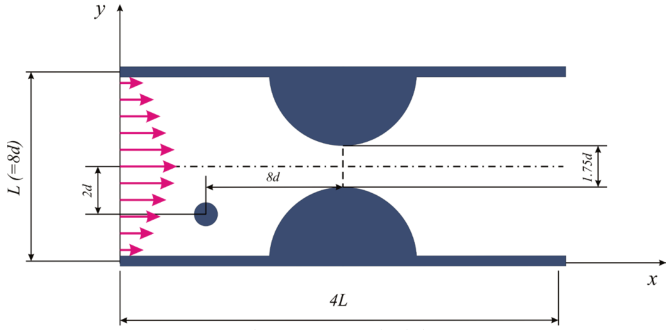

Figure 1. Example 1 – Geometrical data

All the necessary geometrical parameters are shown in Figure 1. In the fluid domain as initial condition the pressure difference on the inlet and outlet is prescribed and the boundary condition is set such that the velocity of the upper and lower wall is equal to zero. The stenosis is implemented using the bounce-back method. Fluid velocity field for the specific moment in time when particle is passing through the stenotic artery is shown in Figure 2a. Figure 2b represents a schematic diagram of particle trajectory (in several steps) from the initial position to the final position symmetrically on the other side of the stenosis.

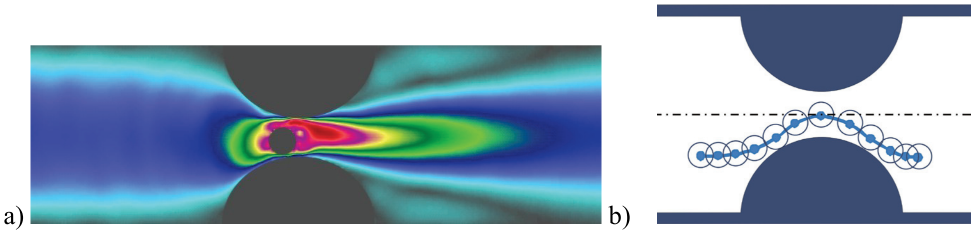

Figure 2. Example 1 – Motion of one particle through stenotic artery; a) Fluid velocity field; b) Trajectory of the particle through a stenotic artery

The comparative diagrams for x and y components of particle velocity for this example are shown in Figure 3 (results obtained using LB solver and results obtained by Wu and Shu [15] are plotted).

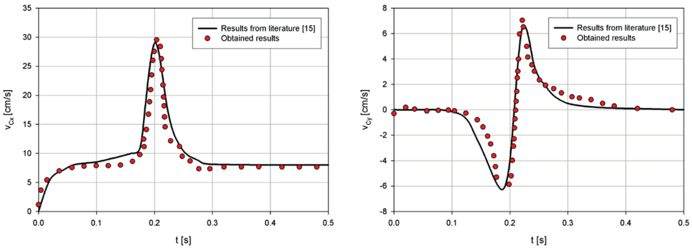

Figure 3. Example 1 - Comparison of results for x component of particle velocity (left) and for y component of particle velocity (right)

4.2. Simulation of movement of two circular particles through a stenotic artery

This example has exactly the same boundary and initial conditions like example 1 and was simulated based on a similar example presented in literature [15]. Here the movement of two particles is simulated. Also, it is necessary to implement the interaction force between two particles as proposed in [15].

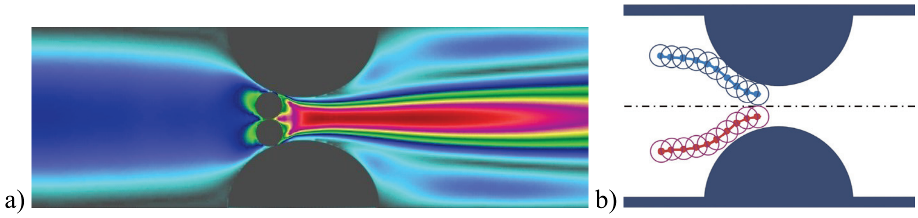

Figure 4. Example 2.1 – Motion of two particles through stenotic artery; a) Fluid velocity field; b) Trajectories of particles

Considering that the free space in the artery (the gap between two protuberances) is less than $2d$ (as it is shown in Figure 1), it is obvious that both particles cannot pass through the stenosis at the same time. If both particles are initially placed symmetrically to the centerline of the artery, they will start moving towards the throat, but will stay stuck at the entrance and block the throat. Figure 4a shows the fluid velocity field and Figure 4b shows the schematic diagram of particles' trajectories for this case.

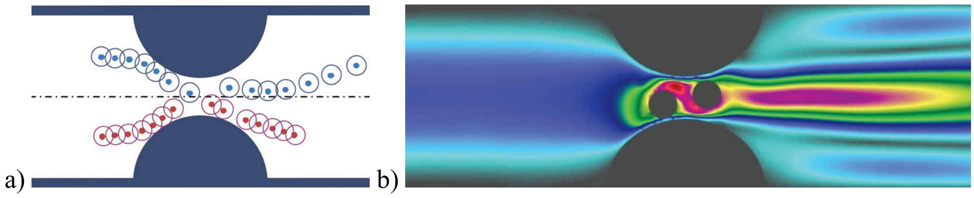

Figure 5. Example 2.2 – Motion of two particles through stenotic artery; a) Trajectories of particles; b) Fluid velocity field

If one of the particles is initially moved for a very small distance towards the centerline (e.g. for only 1 lattice unit), the particles will be able to pass the stenosis and move on through the artery. This is shown schematically in Figure 5a, while Figure 5b shows the fluid velocity field in the moment of passing through the throat.

5. Conclusion

In this paper lattice Boltzmann method was used to simulate motion of particles through fluid domain with complex boundaries. A specific type of particle-fluid interaction was considered. Agreement between LB method and solutions found in literature demonstrate that this method and the developed software can successfully simulate complex problems of fluid flow and fluid-particle interaction and that it can be applied in the field of particle transport in blood vessels, bio-imaging and drug delivery.

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