

A COMPUTATIONAL BIOFLUID DYNAMIC APPROACH USING THE GENERAL LATTICE BOLTZMANN EQUATION

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Abstract. *The lattice Boltzmann method (LBM) is a modern numerical technique, very efficient, flexible to simulate different flows within complex/varying geometries. The LBM has evolved from the lattice gas automata (LGA) in order to overcome the difficulties with the LGA. The core equation in the LBM turns out to be a special discrete form of the continuum Boltzmann equation, leading it to be self-explanatory in statistical physics. In contrast with the traditional computational fluid dynamics (CFD) based on a direct solution of flow equations, the lattice Boltzmann method provides an indirect way for solution of the flow equations. This method is characterized by simple calculation, parallel process and easy implementation of boundary conditions. This feature makes the lattice Boltzmann method a very promising computational approach in different areas. A computational code is described for numeric simulations of blood flow using the Cellular Automata theory, applying the lattice Boltzmann general equation (GLBE). The algorithm and user's environment are also described. The mathematical theory required for the program code is also included and a formal example is included to show the versatility and power of the method.*

1 INTRODUCTION

The fluid dynamic behavior in human heart valves has marveled many researchers including Leonardo da Vinci¹, who described a technique to produce an aortic valve model. After Hufnagel had successfully implanted a heart valve device in a human in 1952², several *in vitro* research studies were carried out to find out the flow characteristics through these artificial devices.

The good results obtained with heart valve devices in humans have contributed to continue experimental work and to develop new designs and materials. Experimental successes with different kinds of devices show that artificial valves do not necessarily imitate the biological valve. However, the unsteady flow development as well as the presence of large Reynolds numbers in valve devices has caused haemolysis with significant undesirable effects. Therefore it is essential to achieve the functional and geometric optimizations of these artificial devices. Additionally to the experimental work, computer simulation was carried out in sophisticated and powerful computers to obtain the whole flow dynamic description³.

The fluid-structure interaction is a very interesting point in the blood flow simulation. Tang *et al.*⁴ have analyzed a nonlinear three-dimensional thick-wall model with fluid-structure interaction to simulate blood flow in carotid arteries. A non symmetric stenosis was included to quantify the effects of stenosis severity, eccentricity, and pressure conditions on blood flow and artery compression. De Hart *et al.*⁵ use the Lagrange multiplier based fictitious domain method in a three-dimensional finite element model of a stented aortic valve. An arbitrary Lagrangean–Eulerian (ALE) formulation is adopted in many recent studies, which must be compatible with the fluid–structure motion interface^{6,7,8,9}.

Different techniques, based on the exchange of momentum and the integration of stress tensor, for the evaluation of the hydrodynamic forces in the lattice Boltzmann simulations are investigated on the curved and moving boundaries in two and three dimensions^{10,11,12}. All of them propose a LBE boundary condition for moving boundaries by combination of the bounce-back scheme and spatial interpolations of first or second order.

A three-dimensional computational fluid-structure interaction model of the mechanical aortic valve prostheses is presented. The merits and demerits of the applied numerical techniques are given in this work. Fluid and structure modeling, fluid-structure interaction modeling, boundary conditions and solution strategies are briefly discussed.

2 PROBLEM DEFINITION AND GOVERNING EQUATIONS

A three-dimensional representation of the valve is shown in Fig. 1, where two rotating leaflets are immersed in a pulsatile flow inside a rigid channel. The channel includes a simplified representation of left ventricle and contains the sinus cavity downstream the heart valve fixed ring.

2.1 Generalized lattice Boltzmann equation (GLBE)

The lattice Boltzmann equation (LBE) is a marching time related moving model of finite differences based on Boltzmann discrete equation (in time and space)¹³. The LBE method is

usually used in a Cartesian prefixed latticework space (non dimensional), as a result of the symmetry array of the discrete velocities, and latticework space δx is related to time δt multiplied by $\delta x = c \delta t$, where c is the basic unit of the velocities discrete arrangement. Thus, this method works basically following two main steps: collision and propagation. During collision the interaction between the fluid particles is modelled in a simple manner and in propagation, the fluid particles simply move from one point of the latticework to the next according to its velocity direction (discrete array e).

The method used in this research is based on the well known fact that fluids movement can be described by Boltzmann's equation¹⁴. As a matter of fact, Navier-Stokes equation is just the second degree approximation to Boltzmann's equation^{15,16}. When the distribution function is known, the macroscopic velocity and stress can be calculated automatically from these two first moments.

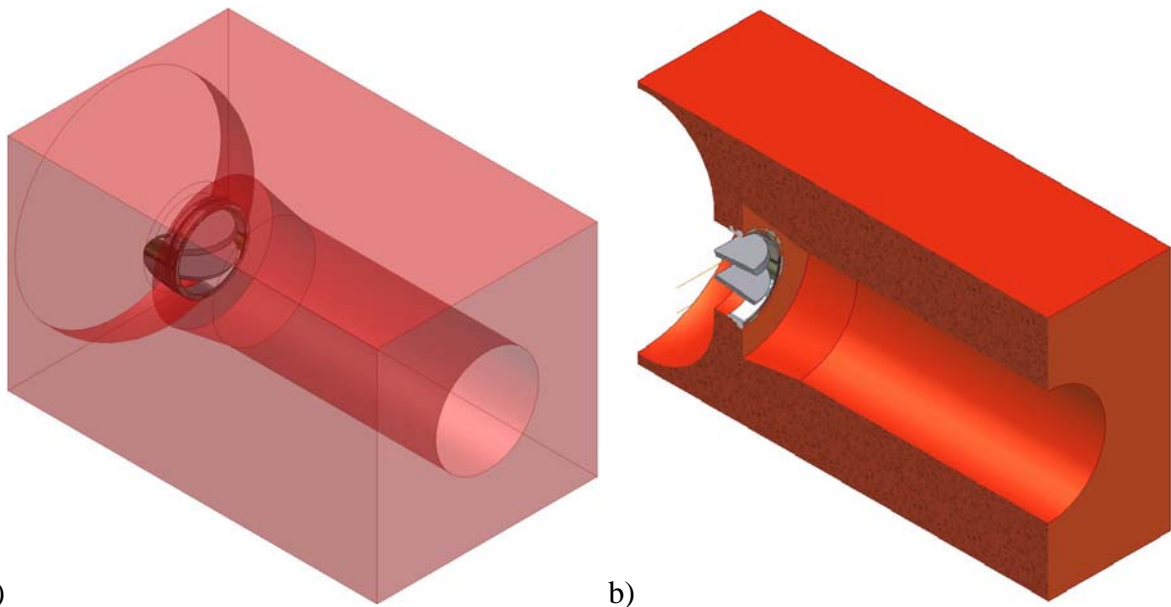


Figure 1: Assembly defined for the lattice Boltzmann simulation, including mechanical heart valve, left ventricle and aortic segment. The figure shows a) end section view, b) xz half section view¹⁷.

The fluids state evolution in time is represented by the general equation

$$|f(r_j + e_\theta \delta t, t_n + \delta t)\rangle = |f(r_j, t_n)\rangle + \Omega |f(r_j, t_n)\rangle \quad (1)$$

where collision is symbolized by the operator Ω . For each point the system state is represented by a vector defined in equation (2) in a 15-dimensional space \mathbf{F} ($\theta \in \{0, \dots, 14\}$):

$$|f(r_j, t_n)\rangle \equiv (f_0(r_j, t_n), f_1(r_j, t_n), \dots, f_{14}(r_j, t_n))^T \quad (2)$$

The main difficulty when using the LBE method to simulate a real isotropic fluid is how to systematically eliminate as much as possible the effects due to the symmetry of the underlying lattice. We shall proceed to analyze some simple (but nontrivial) hydrodynamic

situations and to make the flows as independent as possible of the lattice symmetry¹⁸.

The typical subroutines included in the main lattice Boltzmann loop with fluid-structure interaction are summarized in table 1.

Table 1. Main loop for lattice Boltzmann code for moving boundary.

1	Propagation subroutine
	The population f is distributed from a macroscopic way to its neighbouring environment ¹⁹ .
2	Re-meshing subroutine
	Each lattice-cell is redefined as fluid or as structure type, according to the displacement of the solid through the flow ¹⁷ .
3	Collision subroutine
	The collision operator of the Boltzmann equation is calculated ²⁰ .
4	Set Boundary Conditions subroutine
	In agreement with the pulsatile flow the conditions are assigned for fixed walls, inflow and outflow limits and the moving boundary interpolations ¹¹ .
5	Solve Structure movement subroutine
	Displacement and Rotation movements for solids in the flow are obtained from classical dynamic equations for solids ²² .

We can make a linear transformation from ψ space to some other space that may be more convenient. In particular, we shall use physically meaningful moments of the quantities f_{θ} that span space \mathbf{M} . As proposed by d'Humières²³, we shall use the generalized lattice Boltzmann equation in which the collision process is executed in moment space \mathbf{M} .

The mapping between moment space \mathbf{M} and discrete velocity space ψ is defined by the linear transformation \mathbf{M} which maps a vector $|f\rangle$ in ψ to a vector $|m\rangle$ in \mathbf{M} :

$$|m\rangle = \mathbf{M}|f\rangle \quad \text{and} \quad |f\rangle = \mathbf{M}^{-1}|m\rangle \quad (3)$$

The rows of the transformation matrix \mathbf{M} are organized in the order of the corresponding tensor, rather than in the order of the corresponding moment. The local state in \mathbf{M} space

$$|m\rangle = (\rho, e, \varepsilon, j_x, q_x, j_y, q_y, j_z, q_z, 3p_{xx}, p_{ww}, p_{xy}, p_{yz}, p_{zx}, m_{xyz})^T \quad (4)$$

can be physically interpreted: $m_1 = \rho$ is the density, $m_2 = e$ is related to the kinetic energy, $m_3 = \varepsilon$ is related to the kinetic energy square, $m_{4,6,8} = j_{x,y,z}$ are components of the mass flux, $m_{5,7,9} = q_{x,y,z}$ are proportional to the components of the energy flux; the symmetric traceless viscous stress tensor $m_{10} = 3p_{xx}$, $m_{11} = p_{ww} = p_{yy} - p_{zz}$, with $p_{xx} + p_{yy} + p_{zz} = 0$, $m_{12,13,14} = p_{xy,yz,zx}$; and an antisymmetric third order moment $m_{15} = m_{xyz}$.

2.2 Multiple-relaxation-time lattice Boltzmann model (MRT)

The relaxation lattice Boltzmann equation (RLBE) was introduced by Higuera and Jiménez²⁴ to overcome some drawbacks of *lattice Gas Automata* (LGA) such as large statistical noise, limited range of physical parameters, non-Galilean invariance, and implementation difficulty in three dimensions. The general RLBE model has three components: The first component is the discrete phase space defined by a regular lattice in D dimensions together with a set of judiciously chosen discrete velocities e_θ connecting each lattice site to some of its neighbors. The main aspect in the theory is the set of velocity distribution functions f_θ defined on each node r_j of the lattice. The second component includes a collision matrix S and $N+1$ equilibrium distribution functions $m_\theta^{(0)}$, which are functions of the local conserved quantities. The third component is the evolution equation in discrete time $t_n = n \cdot \delta t$, $n=0, 1, \dots$,

$$|f(r_j + e_\theta \delta t, t_n + \delta t)\rangle - |f(r_j, t_n)\rangle = -\mathbf{M}^{-1} \hat{S} [|m(r_j, t_n)\rangle - |m^{(0)}(r_j, t_n)\rangle] \quad (5)$$

The collision process is naturally accomplished in the space spanned by the eigenvectors of the collision matrix, the corresponding eigenvalues being the inverse of their relaxation time towards their equilibria. The $N+1$ eigenvalues of S are all between 0 and 2 as to maintain linear stability and the separation of scales, which means that the relaxation times of non-conserved quantities are much faster than the hydrodynamic time scales. The LBGK models are special cases in which the $N+1$ relaxation times are all equal, and the collision matrix $S = \omega I$, where I is the identity matrix, $\omega = 1/\tau$, and $\tau (> 1/2)$ is the single relaxation time of the model¹⁸.

2.3 Boundary conditions

Unlike other CFD methods (computational fluid dynamics), lattice Boltzmann methods require a defined boundary condition for the density distribution instead of pressure and velocity. In other words, the density distribution must be known for each one of the cells of the boundary. In order to represent the valve opening and closing movement within the lattice Boltzmann mesh, the leaflet new position is recalculated at each time step and the cell definitions are only updated for those cells that were assigned previously as a solid to a fluid and viceversa.

Ginzburg and d'Humières²⁶ present a unified approach of several boundary conditions for lattice Boltzmann models. The multi-reflection boundary condition is a generalization of previously introduced schemes such as the bounce-back rule, linear or quadratic interpolations, etc.

After the propagation step at t , the post-collision population in the fluid-structure interface can be thought to be on the outside boundary node. At the same time the population corresponding to the opposite direction (boundary node) is unknown and has to be supplied by the boundary condition. Ginzburg and d'Humières had proposed an approach based on the reconstruction of the unknown populations from a second-order Chapman-Enskog expansion in Ginzburg and d'Humières²⁷, and extend the results of Bouzidi *et al.*²⁸ in order to derive formally third-order accurate boundary conditions for general flows. For details, see Ginzburg

and d'Humières²⁶. The present work uses this model to simulate the blood - valve's leaflet interaction.

3 PARALLEL COMPUTATIONAL SIMULATION

3.1 Parallel code

The code was developed using explicit parallelism²⁹ that works in the software and the operating system. Using the concept of *partition of the domain* the code was organized so that the program was executed simultaneously in n different tasks and using *partition of data* the code distributed the numerical array in the cluster's nodes.

The parallel code was carried out following the Foster's method^{30,31}, the passing of information among teams of the cluster works under the *overlaps of border's method*.

3.2 Configuration of the cluster

A non-dedicated cluster was implemented, configured by six computers of high yield (nodes) connected by two switches Planet FSNW 1601 (figure 2). Table 1 summarizes the selected teams specifications.

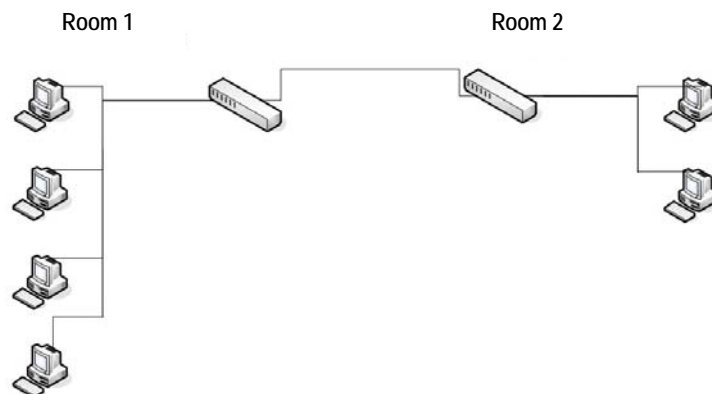


Figure 2: Cluster implemented in the laboratory to solve the parallel version of the lattice Boltzmann code : one master/slave node and five slave nodes³².

The solution was developed in MS Windows. The *single program multiple data* model (SPMD) was used, under the *master-slave* scheme²⁹. The parallel library installed in each node was WMPI 1.3.

Table 1. Cluster configuration³²

	Galileo	Newton	Keppler	Atenea	Heracles	Sirius
CPU	AMD Athlon Xp 2600+ 1.917 GHz					
Cache L1 Instructions	64 KB					
Cache L1 Data	64 KB					
Cache L2	512 KB					
RAM Memory	1.5 GB DDR2700	1GB DDR2700 960 MB operatives		512MB DDR2700 448 MB operatives		
Hard disk	Serial ATA 120 GB 7200 RPM	ATA100 80 GB 7200 RPM			ATA100 40 GB 7200 RPM	
Motherboard	DFI AD77 Infinity (Serial ATA, Raid)	MSI KM400 – 8235				
OS	Windows XP Professional Service Pack 2					

3.3 Validation of the cluster

Figure 3 shows different CPU times in a three-dimensional example using the lattice Boltzmann D3Q15 cellular model. A homogeneous behavior is observed; certain fluctuations at the beginning indicate a bigger CPU consumption that later are stabilized. The cluster offers its biggest yield with 6 nodes and it reflects that the yield can continue improving with the incorporation of new nodes to the process. The decrease is located between a 70 and 80% in time of computation for a lattice evaluated of almost 3.5 million cells. Future works could be focused in an internal parallelism of the code, working with *control partition*³³.

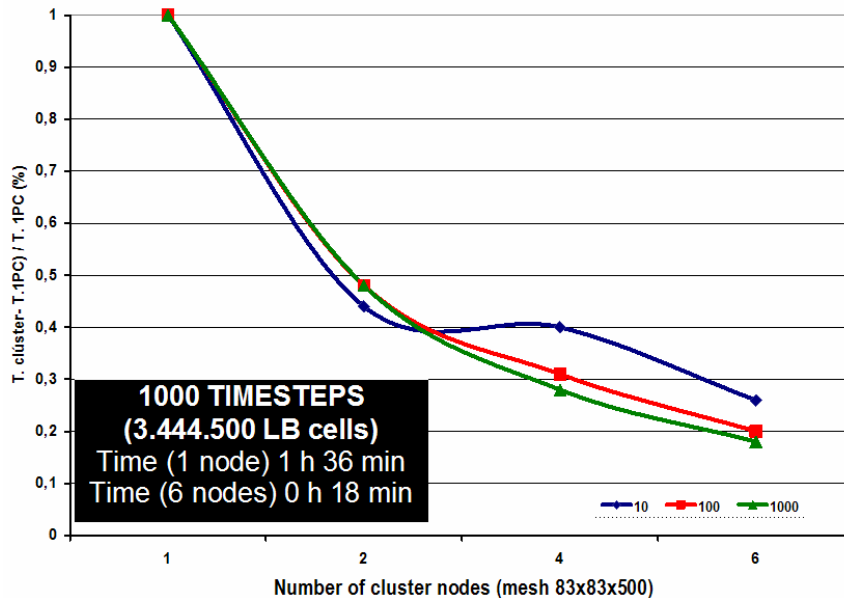


Figure 3: Percentage of CPU time reduction using a MPI cluster for a three-dimensional lattice Boltzmann simulation. Curves to 10, 100 and 1000 timesteps³²

4 LATTICE BOLTZMANN ANALYSIS

The model under study is formed basically by a self-regulating cell population of the D3Q15 type of voxel geometry (see Figure 4). For cell D3Q15, the fifteen discrete velocities are defined

$$\{e_{\theta}\} = \begin{pmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \end{pmatrix} \quad (6)$$

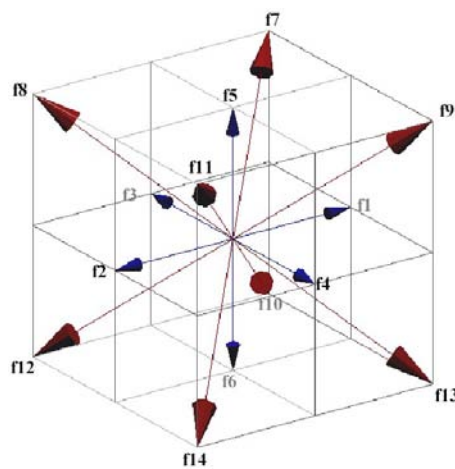


Figure 4: D3Q15 lattice Boltzmann cell¹⁷.

For each one of the mechanical devices being simulated, a cell's group was taken and individual characteristics were given to fixed and to mobile components. The cells ordered in a regular and uniform way were classified one by one according to their function within the simulation process, i.e. FLUID, STATIC-WALL and BOUNDARY cells. This allows tile completely the control volume defined by the boundary which represents the portion of the left ventricle, the aortic valve segment and part of the aortic artery, as shown in Fig. 5. As it can be observed in the image, the valve geometry adapted itself to the regular geometry of the lattice. The fluid-structure coupling is straightforward (nodes and element boundaries coincide along the fluid-structure interface).

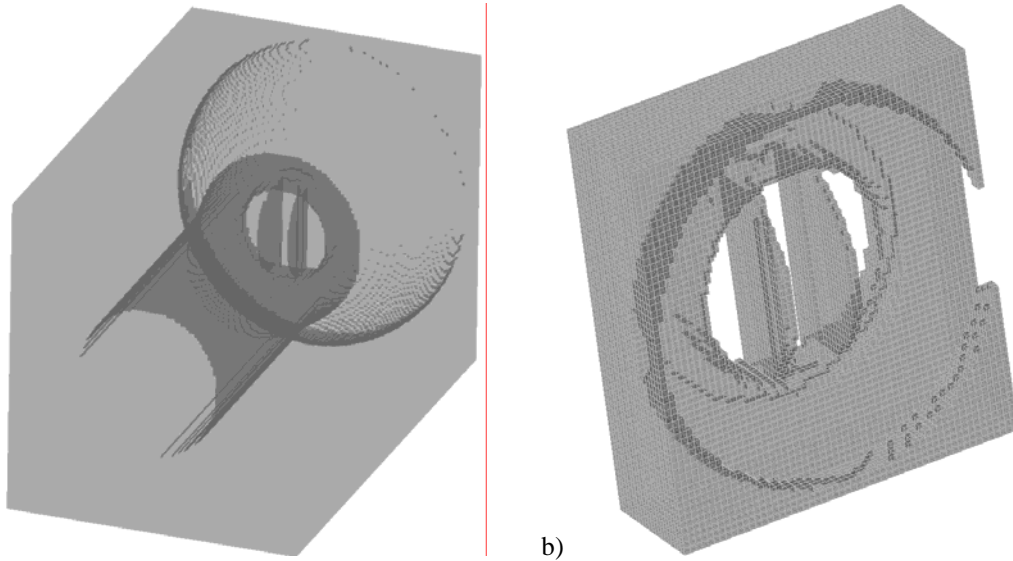


Figure 5: Three-dimensional lattice using D3Q15 lattice Boltzmann cells. a) End section view, and b) detail of the mechanical heart valve.

4.1 Preprocess configuration

To set up inflow boundary conditions in the model, a laminar profile was defined to the left ventricle. A period of time (cardiac cycle) was defined as $T = 227$ iterations ($\omega = 2\pi / T$). The initial velocities distribution in the domain was zero for the whole system and then the simulation was developed in $40T$ to define time zero ($t = 0$) of the numerical calculation.

Three boundary conditions were required in this model: one on the first cells column where the left ventricle is and begins the pulsatile blood flow, another in the fixed walls (ventricle, aortic artery and the fixed ring of the valve), and finally another in the valve dynamic boundary. From the left ventricle a flow comes out with a laminar profile which is variable in time and it is based on the heart cycle. Its peak velocity was also adapted to the information obtained from King³⁴. The density distribution for each one of the cells based on the velocity components was estimated and registered for that boundary. For the static boundary, the simple bounce-back method was implemented. In this analysis the fluid-structure interaction is considered between the fluid domain (blood) and the immersed structures, *i.e.* the valve leaflets, while assuming the aortic root to be rigid.

The density of the leaflet material is taken equal to the fluid density, so that buoyancy forces can be neglected. The effects of heart valves substitution with mechanical valvular implant were simulated by blood flow through mechanical device using time step analysis. A St. Jude Medical Valve (SJM) was evaluated in this work. The physiological conditions around the device implant were carefully modeled and the geometry of the aortic cavity was modeled according to the pulsatile *in vitro* test equipment used by King³⁴. Blood physical

properties were used for the model such as fluid density $\rho = 1.05 \cdot 10^3 \text{ kg/m}^3$ and $\nu = 3.4 \text{ mm}^2/\text{s}$. Numerical simulations were carried out in the mesh with a flow output of 5.5 l/min and a heart pulse of 72 bpm (0.82 s , Womersley $\alpha^2 = D^2\omega/\nu = 256.4$). Time related velocity values were selected as the system input condition from a periodic curve $Q = Q_p \sin(\omega t)$, where Q_p is the flow by stroke used in the experimental simulation³⁴. The velocity values were non-dimensionalized by using the Reynolds number. Additionally, the aortic segment was enlarged four times its diameter size in order to eliminate numeric effects on the output boundary. The aortic diameter was considered about 29 mm .

The leaflets movements are governed by the solid body dynamics and are only free to rotate on a fixed axis which is defined by the device own geometry; each leaflet movement is studied separately.

The code was implemented on a cluster of six machines AMD Athlon Xp 2600+ 1.917 GHz , with a global lattice of $137 \times 62 \times 57$ cells (133 644 fluid cells and 960 moving boundary cells).

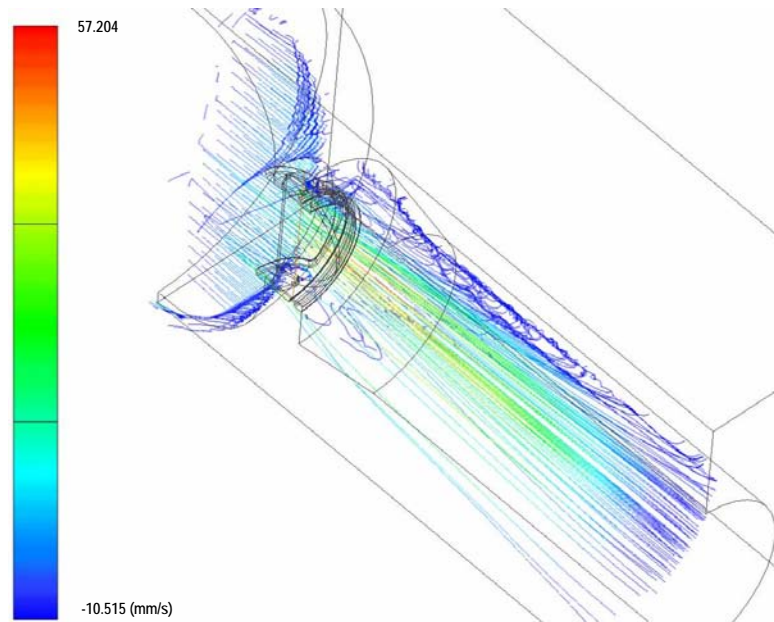


Figure 6: Numerical lattice Boltzmann streamlines in a pulsatile blood flow through a SJM heart valve, beginning the systole $0.10T$ ($t = 0.08 \text{ s}$); xy half section view.

4.2 Numeric results

In Fig. 6 streamlines through the bileaflet valve are reported. In the profile closest to the valve, the leaflets' influence on the flow field is evident, with three jets, one central and two laterals. This is a characteristic feature of bileaflet valves. In the Valsalva sinus, there is an intense fluid recirculation generated by the interaction between jet, valve structure and

geometry of the aorta.

Results were compared with King *et al.*³⁵. They used computational fluid dynamics models to predict the flow through a bileaflet mechanical heart valve during the first half of systole and were compared with flow visualization and laser Doppler anemometry *in vitro* experiments. Direct comparison of the LB and flow visualization results was difficult because one was displayed as particle pathways and the other as velocity vector. However, comparison of the global flow features was promising.

Fig. 7 shows the absolute value of xy , yz and zx shear stress levels in the fluid for the device $|(\tau - \tau_{MAX})/\tau_{MAX}|$.

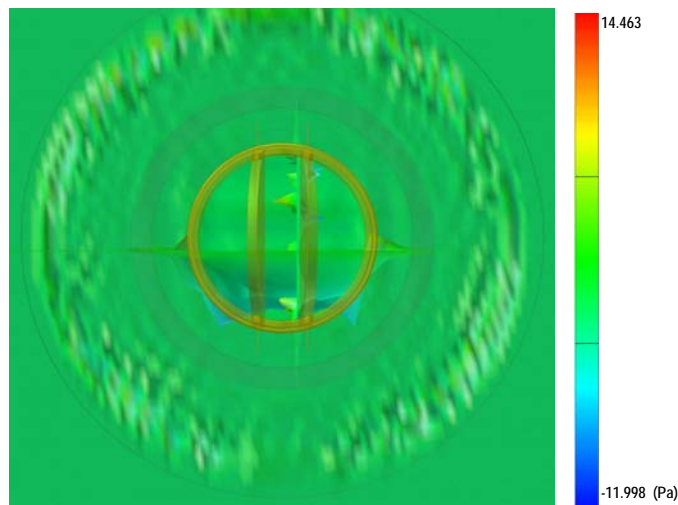


Figure 7: xy , yz , zx shear stresses in the symmetric planes in one leaflet of the mechanical heart valve, beginning the systole $0.10T$ ($t = 0.08$ s).

Some clinical deduction can be made from this work. The ring vortex in the sinus area indicates an area of slow moving fluid. This is a well documented phenomena: the formation of thrombus on the cuff of the valve. The instability of the central orifice jet may well increase the risk of platelet collisions. The impingement of the major orifice jets on the aortic walls may alter the patterns of tissue growth in these areas, however, this has not been reported as a clinical problem and insertion of any valve with a slight miss alignment may result in the jets through the valve orifice impinging on the aortic walls.

5 DISCUSSION

A fully discrete solution strategy is used to solve the blood-leaflet interaction problem. The main advantage of a fully coupled approach is that fluid and structural unknowns are solved simultaneously and, consequently, are completely in equilibrium each time the set of equations is solved.

Computational models such as that presented in this work can be useful in the cardiovascular research for choosing the time and type of surgical intervention. They may

specifically be helpful in giving insight in system responses, which are difficult to capture experimentally. Moreover, their application towards development of clinical hardware, such as new types of prosthetic valve is of great interest. The computational techniques presented here are, as matter of course, not confined to the aortic valve system. They can readily be generalized to be applicable to other fluid-structure interaction systems within the cardiovascular regulation.

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