The Lattice Boltzmann Equation for Modelling Arterial Flows: Review and Application

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Abstract
The lattice Boltzmann model is a relatively new development in computational fluid dynamics. Here we review the technique with particular emphasis on its application to biological systems. Further, we consider its application to arterial flows and discuss its potential for simulating flow on length-scales where traditional numerical approaches can be troublesome. Finally we present results from a preliminary investigation which demonstrate the suitability of the lattice Boltzmann model for simulating oscillatory flow.

1 Introduction

The study of arterial blood flow has many important applications. For example, the buildup of plaque deposits on blood vessel walls and its subsequent rupture can lead to acute coronary syndromes such as sudden ischaemic cardiac death[1]. It is therefore important to understand how blood flow affects both the buildup of the deposits and the rupture. In many cases *in vivo* measurements are extremely difficult and so numerical simulation and *in vitro* techniques become the main investigative tools.

Traditionally numerical techniques such as the finite element or finite difference methods have been applied, however to model arterial blood flow there are a number of important features which must be considered. Firstly, the blood flowing in the artery is not a simple Newtonian fluid; it transports particles such as red and white blood cells and this needs to be simulated in any realistic model. Secondly, the artery wall is far from being the solid no-slip boundary which is applied in most computational fluid dynamics (CFD) simulations. In reality the endothelium, which lines the blood vessels, contains many complex features from a computational view point. It is not smooth or regular, and it is not stationary in time due to the compliant nature of the blood vessel and the ability of the cells which form the endothelium to move with time. Further, the geometry of the artery can change significantly due to the build up of plaque, a complex process which may depend on shear stress rates in the fluid[2,3]. Thus any realistic model must be able to simulate flows which have complicated evolving boundaries and which contain suspended particles. It is also desirable that the models are capable of simulating a range of length scales down to the micro-sized arterioles.

2 Objectives

Here we consider and evaluate a novel approach to fluid simulation which can incorporate the different features which are required for arterial flow modelling: the lattice Boltzmann model (LBM). The LBM has been widely applied in the field of fluid dynamics over recent years and has been found to be particularly well suited to flows with complex boundary conditions[4-6] as well as multi-phase[7,8] and suspended particle problems[9,10]. It is therefore potentially a very useful tool for investigating physiological flows and may be especially useful for nano-scale problems[11,12] where the application of traditional methods is not straightforward.

3 Method

The LBM has recently been developed as an alternative numerical method for studying fluid flow. The LBM has evolved from the lattice gas model (LGM) and it is useful to consider this first.

3.1 *The lattice Gas Model*

The lattice gas model was first considered as a serious approach to fluid modelling about fifteen years ago[13]. It can be viewed as a simplification of the molecular dynamics approach which considers the motion of individual fluid molecules; an approach which is in general too computationally intensive to be applied to a large simulation. On the other hand, it also relies on some of the continuum ideas which are applied in deriving the Navier-Stokes equation which is the starting point of traditional CFD.

Rather than considering a large number of individual molecules, the molecular dynamics approach, a much smaller number of fluid `particles' are considered. A fluid `particle' is a large group of molecules which although much larger than a molecule is still considerably smaller then the smallest length scale of the simulation. This reduces the amount of data which needs to be stored since large simulations can be performed using less than one million `particles'. This is justified on the grounds that the macroscopic properties do not depend directly on the microscopic behaviour of the fluid. This can be seen in low Mach flows where, provided the Reynolds number is the same, experiments carried out in a water tank and a wind tunnel produce the same results. These two fluids have different microscopic structures, but they both exhibit the same macroscopic features. A lattice gas model is further simplified by restricting the `particles' to move at unit speed on the links of a regular underlying grid and limiting the number of particles which are allowed at each grid site. With these assumptions the model becomes totally discrete in space (particles are only considered at the grid sites) and in time (since all the particles move between the sites at the same speed). At each site the particles collide in such a way that the local mass and momentum are conserved. This is found to be sufficient for the model to produce physically correct results. Given the restrictions already applied the number of possible collisions is small and does not require significant computation, often they are simply found from a look-up table. These two time saving advantages of the lattice gas model allow simulations of a significantly large scale to be performed. The simulation evolves in two steps: streaming of the particles from one site to a neighbouring site; followed by particle collision at the new site. Thus the evolution of site $\boldsymbol{r}$ at time t can be expressed as

$$n_i(\boldsymbol{r}+\boldsymbol{e}_i,t+1)-n_i(\boldsymbol{r},t)=\Delta_i(\boldsymbol{r},t), \qquad (1)$$

where i labels each link of the grid, $\boldsymbol{e}_i$ is a unit vector along link i, n_i is the population of the link (n_i = 1 if a particle is present on the link or = 0 otherwise), and Δ_i represent the change to n_i due to the collision. Defining the local density and momentum to be the sum of the mass and momentum of each of the particles at a site, it is possible[14] to show that such a system satisfies the correct macroscopic equation for fluid motion.

The lattice gas models have been used to simulate many different flow situations. These include single fluid simulation such as Poiseuille flow in a pipe[15]; Von Karman street formation behind a flat plate[16-18]; flow over a step[19]; jet simulation[20]; injected flow from a pipe into a transverse flow[21] and multiple fluid simulations such as the Kelvin-Helmholtz instability[22]. There are, however, a number of problems with the lattice gas technique. These include a lack of Galilean invariance and noisy simulations which require significant averaging to provide meaningful results.

3.2 The lattice Boltzmann model

Given the initial success of the LGM a number of researchers devised approaches which maintained the advantages of the LGM approach while overcoming some of the shortfalls. The outcome of this evolution was the LBM which can be expressed as

$$f_i(\boldsymbol{r}+\boldsymbol{e}_i,t+1)-f_i(\boldsymbol{r},t)=\frac{-1}{\tau}\left(f-f_i^{\mathrm{eq}}\right). \qquad (2)$$

In terms of practical implementation this differs from the LGM, equation (1) in two ways. Firstly, we are no longer considering the Boolean particles, n_i, but f_i[23] which is a real number varying in the range 0 - 1 and is the particle distribution function which can be thought of as an ensemble average of the n_i. Secondly, the collision term[24] on the right hand side of equation (2) is the Bhatnagar Gross Krook (BGK) operator[25]. It assumes that the particle distribution functions relaxes to their equilibrium state, f_i^{eq}, at a constant rate determined by the relaxation time τ. In practice $\tau > ½$ and can be varied in the simulation to affect the viscosity of the fluid. The form of the equilibrium distribution function in 2D is commonly taken to be[26]

$$f_i^{\mathrm{eq}}(\boldsymbol{r},t)=w_i\rho\left(1+3\boldsymbol{e}_i\cdot\boldsymbol{u}+\frac{9}{2}(\boldsymbol{e}_i\cdot\boldsymbol{u})^2-\frac{3}{2}u^2\right), \qquad (3)$$

where w_0 = 4/9, w_1=w_2=w_3=w_4=1/9 and w_5=w_6=w_7=w_8 = 1/36, and the link directions are shown in figure 1. The equations of motion for a LBM model can be found, see for example[27], following a similar approach to the LGM. LBMs are masoscopic fluid models which fit between the microscopic molecular dynamics and the macroscopic Navier-Stokes solvers.

In any simulation the implementation of suitable boundary conditions is essential if the results are to be meaningful. In the LGM[28] a solid no-slip wall was implemented by ensuring that any particle approaching the boundary is reflected back along the direction from which it has come. A free-slip boundary was applied by reflecting the particle such that the momentum parallel to the wall is conserved and the momentum perpendicular to the wall is reversed. The bounce back concept is easily carried forward to the LBM model and found to give good results in many applications. Other, higher-order schemes have also been devised, see for example[29-31].

The LBM approach is becoming increasingly popular[27,32] and it has been applied to a wide range of problems including flow in porous media[4,5], flow through particulate suspensions[9], interfacial[33] and acoustic[34] waves, turbulence[35] and multi-phase fluids[7,8].

3.3 Applications of the LBM relevant to arterial flow simulations

3.3.1 Blood Flow

Despite the wide application of the LBM there have been relatively few studies of blood flow. The most noticeable exception to this is the work of Krafczyk *et al*.[36,37] who consider flow through an artificial aortic valve. A three-dimensional simulation[36] is presented for transient flows through a geometry representing a CarboMedics bileaflet heart valve. To find the transient behaviour the valve is fixed at different opening angles and all boundaries are considered to be fixed. The simulation predicts complex flow patterns within the valve. Further the resulting shear stresses were calculated and found to be of the same order of magnitude as observed in similar *in vitro* experiments[38]. The peak shears were found to be about 10 N m^{-2} which is well below the critical shear stress range to cause necrosis of red blood cells or lethal erythrocyte and thrombocyte damage. This work has been extended[37] by allowing the leaflets of the valve to move while being driven by blood flow over a complete heart cycle. Due to the complexity of the simulation it was performed in two-dimensions and as before all other boundaries were considered to be rigid. Complex flow patterns were again observed during the cycle and peak shear stresses of 10-15 Nm^{-2} were found in the vicinity of the front and back end of the leaflets. Both simulations have demonstrated the ability and suitability of LBM in physiological blood flow simulations. Despite certain limitations, such as the rigid structure of the wall, the results are promising and generally in good agreement with results from other sources.

The advantages of the LBM for simulating blood flow have been realised by Belleman and Sloot[39]. They propose using the LBM in an ambitious project to build a `Virtual Laboratory' in which LBM simulations will be combined with imaging techniques such as magnetic resonance angiography (MRA). This will be used, for example, to aid a surgeon in deciding on the best treatment for a vascular disorder such as stenosis. Members of the same group also investigated flow through a centrifugal elutriation chamber using the LBM in a parallel implementation[40]. They present velocity profiles for different flow rates in a fixed geometry and find that as the flow rate is increased the effective volume of the chamber is decreased due to the formation of vortices.

3.3.2 Compliant walls

To fully simulate blood flow the elasticity of artery walls must be taken into account. This has been addressed by Fang *et al*.[41] who propose a LBM model for simulating a system with elastic and moveable boundaries. Fang *et al.*[41] present results of flow in a long thin elastic pipe representing a pulmonary blood vessel in which the fluid pressure and the change in radius of the pipe were found to be in good agreement with analytical expressions. Pulsating flow was also considered in an elastic pipe and simulations were found to be similar to the aortic flow in the left anterior descending coronary. Fang *et al*. further tested the model[42] by considering both steady and pulsating flows. The pulsating flow simulations were compared with experimental results for aortic flow and showed similar features. A direct quantitative comparison was not possible, however, due to the simulations being in two-dimensions.

3.3.3 Suspended particles

A number of authors have considered LBM simulations containing suspended particles. Much of the pioneering work was performed by Ladd[9,43,44] as well as Behrand[45] and Aidun and Lu[46]. This approach involved describing a number of particles each with a radius of at least of few grid points. Each particle is then assigned an initial velocity which comprises of a translational component and a rotational component. At each time step the boundary conditions for the fluid are determined by the position and velocity of the particles and the particles position and velocity are updated respectively according to the particle velocity and the change in the momentum of the fluid distribution functions at the particle surface. This approach has been used to simulate tens of thousands of suspended particles and is fully reviewed in[47]. An alternative approach to modelling a large number of particles has also been considered[10, 48-50]. Here the particles are modelled on the same grid as the fluid and their motion is determined by the local velocity field. This approach has been applied to a range of diverse problems where particle transport and deposition are important.

3.3.4 Micro-scale simulations

A number of LBM investigations have considered fluid simulations in micro-sized systems, referred to as microelectromechanical systems (MEMS)[12,51,52]. In[12] the authors consider 2D micro-channel flow and carefully consider the boundary conditions which need to be applied. The results show that the LBM is an efficient approach for simulating micro-flows, provided the correct boundary conditions are applied. The importance of the correct boundary conditions when modeling micro-flows is also considered in[51]. Here a number of fundamental properties of micro-flows are demonstrated: slip velocity; non-linear pressure drop along the channel; and mass flow rate variation with the Knudsen number. In[52] reactive micro-flows are simulated which again highlight the approach of the LBM at this scale. Although these do not relate directly to blood flow, they indicate that the LBM can be applied to blood flow at a micro-scale.

3.3.5 Flows with complex boundaries

Arguably, the area where the application of the LBM has been most fruitful is to the simulation of flow through porous media. This has largely been due to the simplicity of the bounce back boundary condition in the LBM relative to the treatment of boundaries in other numerical schemes. This is especially advantageous when considering porous media where there are a large number of often irregularly shaped boundaries. Two examples of the simulation of porous media are the work of Michael *et al*.[5] and Manwart *et al*.[6] who both demonstrate the use of the LBM for simulating flows with complex boundaries, a feature which is essential if the technique is to be applied to study arterial flow with a realistic endothelium boundary. Both these applications[5,6] also illustrate the application of the LBM to small scale systems with[5] considering directly micro-scale flow.

3.3.6 Oscillatory flows

Recently a systematic investigation of the applicability of the LBM to simulate oscillating flows[53] has been carried out. These were performed to evaluate the performance of the LBM to oscillatory flows as a prelude to vascular studies. For this reason rigid boundaries and a zero-mean flow were applied since an exact analytic solution is available for comparison. In the remainder of this paper we will present these results and evaluate the LBM approach for true physiological simulations.

4 Results

To validate the LBM for oscillatory flow problems a number of simulations were performed in a two-dimensional channel. This problem was selected because it has a well-established analytical solution which enables the LBM simulation technique to be rigorously verified for an oscillating flow. The results for a simulation performed for a frequency of 2 Hz and a maximum velocity of 10 ms^{-1} in a channel of width 9 mm is shown in figures 2 and 3 for the up-stroke and down-stroke respectively. The simulation was performed with rigid boundaries for a fluid with density 1000 kg/m^3 and viscosity 4 mPa·s. The results are compared to an analytic solution[54] and the agreement was found to be good in all cases. This demonstrates the ability of the LBM in oscillatory flow situations.

5 Conclusions

We have presented a review of the LBM concentrating on the attributes which make it attractive to arterial flow simulation. The main features pf which are highlighted below. The LBM is able to handle complex boundary conditions such as those found on the endothelium. Suspended particles can be incorporated into the flow; this is required to model particles such as red and white blood cells and also the deposition and rupture of plaque during atherosclerosis*s*. The LBM can also be applied to micro-scale flow phenomena; this is essential if a large range of physiological flows is to be studied. The ability of the LBM to accurately simulate non-stationery, oscillatory flows has also been highlighted. These features suggest that the LBM is potentially an important and useful tool for investigating a large range of arterial flow problems. The model used to produce the results in figures 2 and 3 is currently being extended to three dimensions to enable blood flow over realistic vein geometries to be modelled. Further work will involve adapting the model to include many of the features discussed above, as well as investigating the possibility of coupling the LBM with models incorporating plaque deposition[55].

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FIGURES

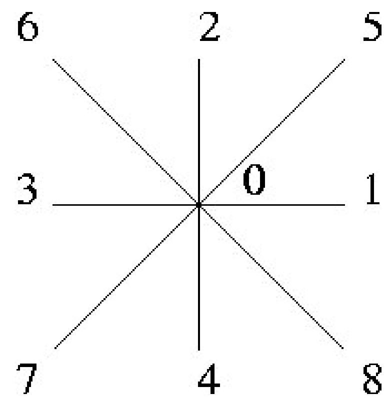

Figure 1: Link directions for a two-dimensional square grid.

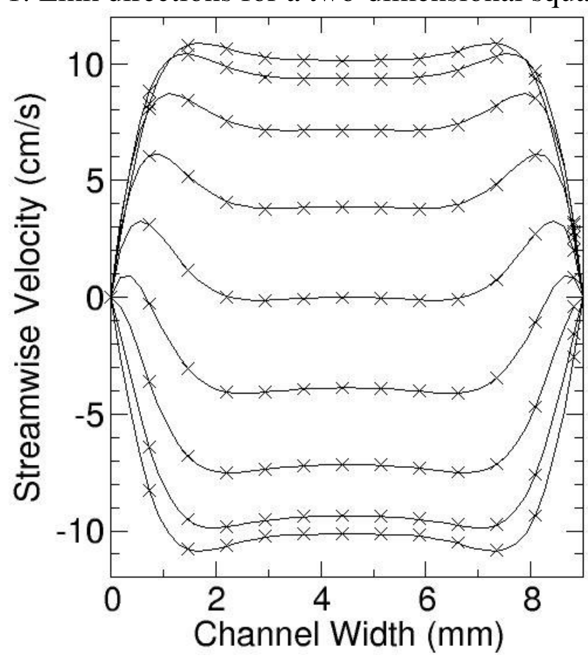

Figure 2: LBM simulation (x) and analytical solution (line) of oscillating flow during an up-stroke.

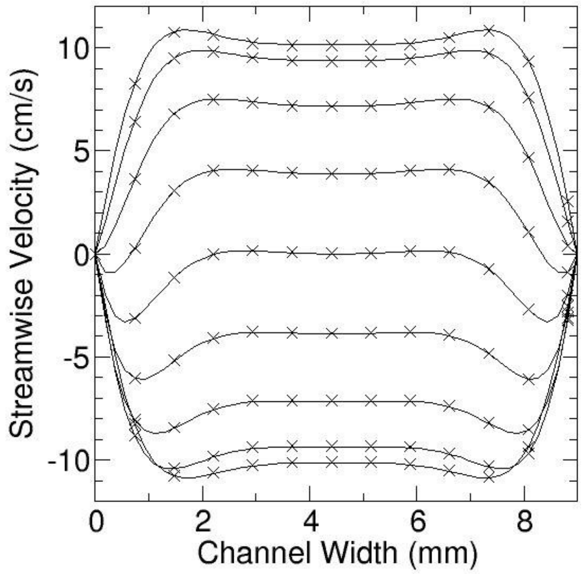

Figure 3: LBM simulation (x) and analytical solution (line) of oscillating flow during a down-stroke.