Mesoscopic Computational Haemodynamics

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Chapter 6

Accuracy Versus Performance

The aim of this chapter is to tune the lattice Boltzmann parameters in order to achieve optimum accuracy and performance for time dependent flows. We present detailed analysis of the accuracy and performance of the lattice Boltzmann method in simulating pulsatile Newtonian flow in a straight rigid 3D tube and compare the obtained velocity profiles and shear stress to the analytical Womersley solutions. A curved boundary condition is used for the walls and the accuracy and performance are compared to that obtained by using the bounce-back on the links.

6.1 Introduction

Suitability and accuracy of the lattice Boltzmann method in simulating time dependent fluid flows has been demonstrated in the previous chapter. It was shown that use of curved boundary conditions noticeably enhances the accuracy as compared to using the simple bounce-back on the links.

Here, we further investigate the accuracy by considering the effect of Mach number on the accuracy and performance of the method. The aim of this study is to end up with optimum simulation parameters for a desired accuracy with minimum simulation time. Simulation parameters for fixed Reynolds and Womersley parameters are studied. We will present the relationship between the free parameters of the lattice Boltzmann and the constraints arising from running simulations under fixed Reynolds number and Womersley parameter at different Mach and Knudsen numbers. Then, we will discuss the convergence behaviour under different simulation choices; and set up the optimum conditions for best performance.

Time dependent LBM simulations involve higher density fluctuation, since the density and the unsteady pressure are tied up together through the ideal gas equation of state. Although there are a number of incompressible lattice Boltzmann models in existence, they are not yet popular as they degrade the simplicity and flexibility of the standard method. Therefore, we stick here to the standard quasi-incompressible D3Q19 model, previously described.
6.2 Simulations

In all simulations presented here, the flow rate in the tube is computed from a measured aortic pressure at the entrance; and its unsteady Fourier terms, up to the 8th harmonic, are used to set a suitable time dependent pressure gradient for obtaining an average Reynolds number $Re = \frac{UD}{\nu} = 590$ and a Womersley parameter $\alpha = R \sqrt{\frac{\omega}{v}} = 16$, where $R = d/2$ is the radius of the tube, $\omega = 2\pi/T$ is the angular frequency and $T = 1/f$ is the period, with $f$ being the number of heart beats per second. Pressure boundary conditions are used for the inlet and the outlet boundaries and, for the walls, either the bounce-back on the links (BBL) or the Bouzidi (Bouzidi et al., 2001) boundary condition (BBC) is used. We have performed three different categories of simulations of systolic flow in a 3D rigid tube benchmark. The first set of simulations compares BBL with BBC. The second set deals with error behaviour and the third set investigates the convergence behaviour. They are all subsequently discussed.

6.2.1 Influence of the Wall Boundary Conditions

Since the lattice Boltzmann method is defined only for fluid nodes, distributions streaming into the fluid structure from non-fluid nodes need to always be evaluated. The way in which these distributions are defined imposes a boundary condition. A wall boundary condition is needed to evaluate distributions coming from solid boundaries, while inlet/outlet conditions are needed to drive the flow. For the walls, achieving the macroscopic non-slip boundary condition with correct momentum flux is always desirable. Boundary conditions in lattice Boltzmann algorithm may be evaluated in terms of these two constraints together with their convergence behaviour and viscosity independence. The first and still most popular wall boundary condition is the bounce-back on the links used previously by the lattice gas community (Lavalle et al., 1991; Cornubert et al., 1991). With the bounce-back rule, relevant distributions (coming from wall nodes) are simply reflected back to the direction they came from. The major drawbacks of the bounce-back rule are its slip velocity and first order behaviour. A number of enhanced bounce-back rules successfully increase the accuracy to second order and the slip velocity to zero (Skordos, 1993; Ziegler, 1993; Noble, 1995) but they increase the computational cost. Alternate, more complex and “computationally” more expensive body fitted second order boundary conditions have recently been introduced (Filippova and Hänel, 1998a; Yu et al., 2002; Bouzidi et al., 2001; Fang et al., 2001). Apart from a few exceptions, these boundary conditions are viscosity dependent and slightly violate conservation laws. In the previous chapter, we have used oscillatory pressure gradient to compare the error associated with the body fitted Bouzidi boundary conditions (BBC) and the bounce-back on the links (BBL), in which we have reported that the accuracy associated with BBC is at least three times higher than that with BBL. In this work, we investigate the error behaviour for a complete systolic cycle which contains at least 16 harmonic terms. We find this necessary since the error doesn’t scale linear in these harmonics because they have different ampli-
Simulations

6.2 Simulations

itudes with increasing Womersley parameters. Moreover, we compare here the error behaviour for the two boundary conditions at a fixed Mach number in order to know how much gain we get from using a more accurate, but rather sophisticated boundary condition, such as BBC, over the less accurate but rather simple BBL.

The diameter of the tube is represented by 74 lattice nodes and the tube length is \( L = 148 \) lattice nodes. First, BBL is used to simulate systolic flow in the tube. The simulation parameters are set to yield the required Womersley and Reynolds numbers which are kept fixed to the values mentioned above. For this simulation, \( T = 2000, G = 1.1 \times 10^{-5} \), and \( \tau = 0.55 \). Samples of obtained velocity profiles at different times of the systolic cycle are shown in Fig. 6.1(a) compared to the real part of the analytical Womersley solutions

\[
u(y, t) = \sum_{m=1}^{8} \left[ -\frac{A_m}{\rho m \omega} e^{-i m \omega t} \left( 1 - \frac{J_0 \left( \sqrt{mby} \right)}{J_0 \left( \sqrt{mbR} \right)} \right) \right], \tag{6.1}
\]

where \( J_0 \) is the zeroth order Bessel function of the first type and \( b = -\frac{i \omega}{v} = -im(\alpha/R)^2 \) for the \( m^{th} \) Fourier harmonic. The average Mach number is 0.05 for this simulation. As clearly shown in this figure, the agreement with the analytical solution is quite good. The relative error in velocity at each time-step is defined by

\[
E_v = \frac{\sum_{i=1}^{n} \left| \tilde{u}_{ih}(\bar{x}_i) - \tilde{u}_{lb}(\bar{x}_i) \right|}{\sum_{i=1}^{n} \left| \tilde{u}_{ih}(\bar{x}_i) \right|} \tag{6.2}
\]

where \( \tilde{u}_{ih}(\bar{x}_i) \) is the analytical solution for the axial velocity and \( \tilde{u}_{lb}(\bar{x}_i) \) is the velocity obtained from the lattice Boltzmann simulations. The overall relative error is averaged over the period and will be referred to as the average error. The bounce-back on the links yields an average error of 0.11 at a Mach number of 0.05 for this specific simulation. This indicates that, even with the bounce-back rule, acceptable accuracy can be obtained for engineering applications.

Using the same simulation parameters, we have conducted another set of simulations after replacing BBL with BBC. The agreement with analytical solutions enhances significantly, as shown in Fig. 6.1(b) and the average error reduces to approximately 0.03.

In a separate study (Artoli et al., 2002d), we have shown that it is possible to go for higher Mach numbers with curved boundary conditions while still having better accuracy than that associated with the BBL at a considerably low Mach number. We have shown that, even with a 10 times higher Mach number, the error associated with the curved boundary conditions is still better than that associated with BBL. It was also reported that using a curved boundary condition enhances the stability of the system and can reduce the simulation time since it allows higher Mach numbers than the simple bounce-back rule. It is therefore not recommended to use BBL for such case unless simulation parameters are changed towards low Mach numbers. However, reducing the Mach number slows down the convergence to equilibrium (Maier, 1996), unfortunately, as will be investigated in the next chapter.
Figure 6.1: Obtained samples of velocity profiles (dots) in lattice units during the systolic cycle in a 3D tube, compared to the analytical Womersley solution (lines) with: (a) BBL and (b) BBC2 wall boundary conditions.

6.2.2 Grid Refinement

In order to study the accuracy and convergence behaviour for the same physical problem under fixed Reynolds number \( (R_e) \) and Womersley parameter \( \alpha \), we need to tune our simulation parameters in a special way. The standard lattice Boltzmann method has several free parameters, but for pulsatile flow in rigid tubes, it is more convenient to tune the lattice viscosity \( v \), the Mach number \( M \), the diameter \( D \) of the tube and the period \( T \) of the pulse. Changes in any of these parameters will result in changes in the space and time resolutions of the grid, and accordingly, the Mach and the Knudsen numbers. For lattice Boltzmann simulations the error behaviour is influenced by the Mach number, \( M = \frac{U}{c_s} \), and the Knudsen number \( \varepsilon \sim (2\pi - 1)/D \). The effect of these numbers arises as a compressibility error, given by (Holdych et al., 2002)

\[
\phi = \delta^2 \frac{R_e^2}{\varepsilon^2} c_s^2 c^2 \partial_t \rho
\]  

which increases with increasing Reynolds and Mach numbers, since \( R_e = MDc_s/v \). As a function of Womersley number, the compressibility error can be written as

\[
\phi = \frac{2\delta^2 c_s c^2}{\pi} \frac{\alpha^2 MD}{St} \partial_t \rho
\]  

where \( St = Df/U \) is the Strouhal number. In this simulation, the dimensionless hydrodynamic numbers \( (R_e, \alpha \) and \( St) \) and the Mach and the Knudsen numbers are all fixed. This implies that the grid must be refined, and/or the density gradients shall be small in order to reduce the compressibility error. Time-dependent flow with BGK involves high density gradients, as stated before. Therefore, we are only left with grid refinement. There are three different ways to do this;

1. **fixed M method**: in which the the diameter \( D \), the period \( T \) and the viscosity \( v \) are changed while keeping fixed the Mach number.
2. **fixed \( \tau \) method**: by changing the diameter \( D \), the period \( T \) and the Mach number \( M \) while keeping fixed the lattice viscosity \( \nu \), and

3. **fixed \( D \) method**: by keeping Fixed the diameter \( D \) while changing the viscosity, period and the Mach number.

The effects of these changes on the grid resolution are tabulated in Table 6.1, in which we assume an \( n \) times change in one of the parameters and compute the corresponding changes in the other parameters to return the fixed \( R_e \) and \( \alpha \). From this table, we can predict the computational efficiency of each approach. For instance, the fixed \( M \) approach involves \( n \) times decrement in \( \delta_x \) (which increases the number of grids \( n^3 \) times) and \( n \) times reduction in \( \delta_t \) which scales the simulation time by \( n^4 \). The fixed \( \tau \) method scales the simulation time as \( n^5 \) and the fixed \( D \) method scales it as \( n \). Although it is easy to tell that the last method is faster while the second one is more accurate, a combination of accuracy and performance is not trivial. The fixed \( M \) method does not involve reduction of the Mach number, which is a major contributor to error enhancement when considering time dependent flows and, therefore, it is not attractive in this study. Accordingly, we have performed two sets of simulations corresponding to the two left methods. These are discussed below.

### Table 6.1: Relative changes in simulation parameters under fixed Reynolds and Womersley numbers with respect to an \( n \) times change in one of the parameters of a reference simulation.

<table>
<thead>
<tr>
<th>Lattice Parameter</th>
<th>( D'/D )</th>
<th>( \nu'/\nu )</th>
<th>( T'/T )</th>
<th>( U'/U )</th>
<th>( \delta_x'/\delta_x )</th>
<th>( \delta_t'/\delta_t )</th>
<th>( M'/M )</th>
<th>( \varepsilon'/\varepsilon )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed ( D )</td>
<td>1</td>
<td>1/( n )</td>
<td>( n )</td>
<td>1/( n )</td>
<td>1</td>
<td>1/( n )</td>
<td>1/( n )</td>
<td>1/( n )</td>
</tr>
<tr>
<td>Fixed ( \tau )</td>
<td>( n )</td>
<td>1</td>
<td>( n^2 )</td>
<td>1/( n )</td>
<td>1</td>
<td>1/( n^2 )</td>
<td>1/( n )</td>
<td>1/( n )</td>
</tr>
<tr>
<td>Fixed ( M )</td>
<td>( n )</td>
<td>( n )</td>
<td>( n )</td>
<td>1/( n )</td>
<td>1</td>
<td>1/( n )</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

### Accuracy and Performance with the Fixed \( D \) Method

Based on Table 6.1, we have selected three sets of parameters to study the error behaviour produced by this technique. First, we have performed a reference simulation at \( M = 0.5 \) and \( \varepsilon = 1/74 \) with \( \tau = 1 \) and \( T = 200 \). Then, two other parameter sets are selected with the aid of Table 6.1. These parameters are listed in Table 6.2 which also lists the changes in \( M \) and \( \varepsilon \) and their multiplication for each simulation set. In Table 6.2, \( n = 1 \) represents a reference simulation, in which we set \( \tau = 1 \), the magnitude of the pressure gradient as \( G = 0.0011 \) and \( T = 200 \) to yield a resulted Mach number \( M = 0.50 \). The Mach number is reduced \( n \) times through increasing the period \( n \) times, reducing the pressure gradient \( 1/n^2 \) times, and \( \tau \) by a factor \( 1/\sqrt[3]{n} \) in order to have the same Reynolds and Womersley numbers. In all simulations, the system is initialised from rest and the simulation ends after 40 complete periods. The BBL, BBC with first order interpolation (BBC1) and BBC with second interpolation (BBC2) were used separately for each parameter set to end up with 9 simulations. The simulations were
performed on 8 nodes of a Beowulf cluster using slice decomposition. The mean time per iteration is about 0.45 seconds using BBL and 0.47 seconds using BBC.

Table 6.2: Simulation parameters with respect to the reference simulation for which \( \tau = 1, M = 0.50 \) and \( \varepsilon = 1/74 \). The average error associated with each set is shown for BBL, BBC1 and BBC2 boundary conditions.

<table>
<thead>
<tr>
<th>( T )</th>
<th>200</th>
<th>2000</th>
<th>20000</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n )</td>
<td>1</td>
<td>10</td>
<td>100</td>
</tr>
<tr>
<td>( \tau )</td>
<td>1</td>
<td>0.55</td>
<td>0.505</td>
</tr>
<tr>
<td>( \frac{\tilde{C}}{C} )</td>
<td>1</td>
<td>1/100</td>
<td>1/1000</td>
</tr>
<tr>
<td>( \frac{\tilde{M}}{M} )</td>
<td>1</td>
<td>1/10</td>
<td>1/100</td>
</tr>
<tr>
<td>( \frac{\tilde{E}}{E} )</td>
<td>1</td>
<td>1/10</td>
<td>1/100</td>
</tr>
<tr>
<td>( \frac{\varepsilon M'}{\varepsilon M} )</td>
<td>1</td>
<td>1/100</td>
<td>1/1000</td>
</tr>
<tr>
<td>( E_{av}, \text{BBL} )</td>
<td>instable</td>
<td>0.120</td>
<td>0.027</td>
</tr>
<tr>
<td>( E_{av}, \text{BBC1} )</td>
<td>0.0627</td>
<td>0.0352</td>
<td>0.0253</td>
</tr>
<tr>
<td>( E_{av}, \text{BBC2} )</td>
<td>0.0615</td>
<td>0.0102</td>
<td>instable</td>
</tr>
</tbody>
</table>

Samples of BBC1 obtained velocity profiles during the systolic cycle are shown in Fig. 6.2 for \( M = 0.5 \), compared to the analytical Womersley solutions. Although \( M \) is relatively high, the agreement with the analytical solution is still better than those obtained by a 10 times smaller Mach number with BBL shown in Fig. 6.1 (a). The last three rows in Table 6.3 list the average error associated with the three wall boundary conditions.

The combined influence of the boundary conditions and the Mach \( \times \) Knudsen numbers is shown in Fig. 6.3 in which the three boundary conditions are tested at a fixed Mach number \( (M = 0.05) \). From this figure it is apparently clear that it would be necessary to use a curved boundary condition at the same Mach number. In Fig. 6.4 we show the computational time as a function of the Mach number, which assures a first order behaviour, as predicted above.

From this set of simulations, we conclude that it would be faster, more stable and more accurate to use a curved boundary condition than the simple bounce-back. In addition, we have noticed that the first order BBC, which interpolates data up to the first fluid node is more stable than the second order interpolation scheme, BBC2, which interpolates data using two neighbouring fluid nodes. This may be attributed to effects from interpolation in a region of large velocity gradients in the case of BBC2. It is worth noting that the error behaviour as a function of the sampling period \( T \) has been studied in the previous chapter (see also Artoli et al., 2003e), showing error enhancement as the number of sampling points representing the period increases and behaves as first order in time instead of second order due to the compressibility effect of the D3Q19 model.

In summary, to obtain better accuracy, it would be more accurate to still use the
6.2 Simulations

Figure 6.2: Velocity profiles at $M = 0.50$ using the BBC1 boundary condition with overall average error of about 0.07, still less than the BBL results at a 10 times lower Mach number. The system is instable with the BBL at this Mach number.

Figure 6.3: Average error behaviour as a function of Mach and Knudsen numbers, for the systolic tube flow using the BBL, BBC and BBC2 boundary conditions. bounce-back on the links at lower Mach numbers than to use more sophisticated boundary conditions. For faster convergence, curved boundary conditions are pre-
Table 6.3: Simulation parameters used to enhance the spatial resolution. The mean relative error, Eav, is listed for each case.

<table>
<thead>
<tr>
<th>$D$</th>
<th>21</th>
<th>65</th>
<th>105</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$</td>
<td>1</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>$T$</td>
<td>40</td>
<td>360</td>
<td>1000</td>
</tr>
<tr>
<td>$\frac{G}{G'}$</td>
<td>1</td>
<td>1/27</td>
<td>1/125</td>
</tr>
<tr>
<td>$\frac{M}{M'}$</td>
<td>1</td>
<td>1/3</td>
<td>1/5</td>
</tr>
<tr>
<td>$\delta_t$</td>
<td>1</td>
<td>1/9</td>
<td>1/25</td>
</tr>
<tr>
<td>Eav, BBL</td>
<td>0.2412</td>
<td>0.1189</td>
<td>0.0262</td>
</tr>
<tr>
<td>Eav, BBC</td>
<td>0.2301</td>
<td>0.0557</td>
<td>0.0262</td>
</tr>
<tr>
<td>Eav, BBC2</td>
<td>stable</td>
<td>0.0560</td>
<td>0.0266</td>
</tr>
</tbody>
</table>

Table 6.4: Temporal Local Relative Error, $E_v(T)$ for BBL and BBC boundary conditions with $D = 65$ lattice nodes.

<table>
<thead>
<tr>
<th>Time</th>
<th>0</th>
<th>10T</th>
<th>20T</th>
<th>30T</th>
<th>40T</th>
<th>50T</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_v(T)$, BBL</td>
<td>0.9950</td>
<td>0.2520</td>
<td>0.0698</td>
<td>0.0279</td>
<td>0.0200</td>
<td>0.0200</td>
</tr>
<tr>
<td>$E_v(T)$, BBC</td>
<td>0.9950</td>
<td>0.2769</td>
<td>0.0615</td>
<td>0.0280</td>
<td>0.0200</td>
<td>0.0197</td>
</tr>
<tr>
<td>$E_v(T)$, BBC2</td>
<td>0.9950</td>
<td>0.2747</td>
<td>0.2520</td>
<td>0.0866</td>
<td>0.0350</td>
<td>0.0560</td>
</tr>
</tbody>
</table>

Table 6.5: Mean, variance and mean deviation of the Relative error for BBL, BBC boundary conditions with $D = 65$ lattice nodes.

<table>
<thead>
<tr>
<th>Boundary condition</th>
<th>Mean error (Eav)</th>
<th>Variance</th>
<th>Mean deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>BBL</td>
<td>0.1189</td>
<td>0.0013</td>
<td>0.0219</td>
</tr>
<tr>
<td>BBC</td>
<td>0.0557</td>
<td>0.0027</td>
<td>0.0352</td>
</tr>
<tr>
<td>BBC2</td>
<td>0.0560</td>
<td>0.0027</td>
<td>0.0350</td>
</tr>
</tbody>
</table>

ferred than the bounce-back rule if the boundary is static.

**Accuracy and Performance with the Fixed $\tau$ Method**

In order to reduce simulation time, it is necessary to have a large time-step in a coarse grid at a high Mach number. To attain that, we use the fixed $\tau$ method to perform a set of simulations in which the period is set to a minimum possible value that leads to a stable solution on the coarsest grid. Then the corresponding values for the pressure gradient and the relaxation parameter are set to yield the desired Womersley and Reynolds numbers. The convergence behaviour is studied by grid refinement in both $\delta_x$ and $\delta_t$, as explained in Table 6.1. The simulation parameters are listed in Table 6.3 together with obtained average errors associated with the three used boundary conditions. As this method results in reducing $\delta_x$, $\delta_t$ and the pressure gradient,
both accuracy and performance are significantly enhanced, since all parameters influencing the error are under control. As is shown in Fig. 6.5, at least second order convergence behaviour is guaranteed with this method. Moreover, with this method, solutions with periods smaller than the fixed $D$ method are stable and therefore the simulation time is less, but it scales as $n^2$.

The convergence behaviour as a function of time for this method is shown in Fig. 6.6, which shows the difference between the analytical and obtained velocity profiles at different simulation times. From this figure, we observe that the method converges to a reasonable accuracy after 40 complete periods, similar to the fixed $D$ method, but with a major computational gain, since the length of the period is smaller (i.e. $\delta_t$ is larger). This figure also illustrates that the error localises near to the walls, where large gradients exist, and does not enhance noticeably near to the walls on the same grid. Table 6.4 lists the error dependence as a function of simulation times for BBL, BBC1 and BBC2 boundary conditions for a tube with $D = 65$ lattice nodes, with its mean, variance and mean deviations tabulated in Table 6.5. The error is reasonably comparable to that obtained by using the fixed $D$ method. In conclusion, this method is computationally more feasible than the fixed $D$ method and is recommended to use while keeping $D$ and $T$ to their minimum values that returns stable solutions.
6.2.3 Convergence Behaviour

Convergence of the lattice Boltzmann method to steady state is significantly affected by two local processes; initialisation and boundary conditions. In this section, we focus on the influence of these processes on the convergence behaviour.

Convergence and Walls Boundary Conditions

As mentioned above, boundary conditions need to be defined at walls, inlets and outlets. For the walls, two categories of boundary conditions can be recognised; bounce-backs and curved boundaries. The bounce-back rule is a very efficient boundary condition since it only involves a single memory swapping process for each relevant distribution on each node on the surface of the simulated object. For all curved boundaries, the exact position of the walls is determined at least once if the boundary is fixed and needs to be computed dynamically for moving boundaries. On its own this is more costly than using the bounce-back rule. In addition, using curved boundary conditions involves first or second order interpolation or extrapolation for velocity, distribution functions or density or a combination of some or all of them. As demonstrated above, use of a curved boundary condition enhances the accuracy but is computationally more intensive compared to the simple bounce-back at the same Mach number. To gain the accuracy of a curved boundary condition and a performance similar to the bounce-back, an accelerating technique recently introduced by the author (Artoli et al., 2003a) may be applied, as will be described in the next chapter.

Inlet and Outlet Conditions

For lattice Boltzmann simulations, a number of inlet and outlet conditions are available. The most commonly used are periodic boundary conditions, in which distributions leaving the simulation box at the outlet are re-injected at the inlets and vice-versa. Periodic boundary conditions involve only memory swapping operations which count as at least 10 times the cross section of the simulation box per time-step. Although they are fast, and accurate, they can only be used for periodic geometry. For non-periodic geometry, inlets and outlets need to be treated differently in the following manner:

- Velocity and pressure: assign one and compute the other (Zao and He, 1997), assign both (only for inlets) extrapolate or no flux normal to the walls (only for outlets).

- Unknown distributions: compute explicitly, set to their equilibrium, copy from nearest neighbours, interpolate or extrapolate.

For the first item, if the velocity or the pressure are computed one from the other, at least 15 additions and two multiplications are needed per node on the boundary and
6.2 Simulations

Figure 6.5: Convergence behaviour obtained by reducing the grid spacing \( n \) times, time-step \( n^2 \) times and increasing the period \( n^2 \) times, for the BBL, BBC and BBC2 boundary conditions as a function of grid points representing the diameter of the tube. The relaxation parameter is kept constant and the body force is reduced \( n^3 \) times to return the same Reynolds and Womersley parameters at \( Re = 1250 \) and \( \alpha = 16 \).

therefore is at least 15 times more expensive than periodic boundary conditions. Extrapolation and no-flux schemes are far better in terms of accuracy and performance than computing velocity or pressure from one another, but they are only suitable for the outlets. A reasonable choice for time-dependent flow in irregular geometry is then to assign pressure and compute velocity at the inlet, no-flux at the outlets and set the unknown distributions to their equilibrium values. If the outlets are far enough from inflow, copying from upstream would be the most efficient outlet condition.

Initial Conditions

Time dependent flow involves large density fluctuations. Although it increases compressibility errors, this reduces the initialisation influence on convergence behaviour. However, the way in which the simulation box is initialised has little effect on the final flow fields. Since the Boltzmann equation assumes that the system is not far from equilibrium, a correct and reasonable initialisation technique is to set each distribution to its equilibrium with a small perturbation. We have adopted this initialisation process in all our simulations. It is noted that more sophisticated initialisation techniques such as second order interpolations from the boundaries may be useful but
Figure 6.6: Local deviations from Analytical solutions, $\delta E$, computed for the velocity field at $t = 20T$ (top Curve), $30T, 40T$ and $50T$ (bottom curve). The diameter of the tube is represented by 65 nodes and the period is $T = 360$ sampling points. The average errors are tabulated in Table 6.3.

they complicate the standard lattice BGK scheme.

6.3 Summary

We have shown that the lattice Boltzmann BGK method is an accurate and efficient method as a solver for time-dependent flows. Different methods for performing time dependent flows at fixed simulation parameters are tested in terms of accuracy and performance. An aortic pressure is used as an inlet condition to drive the flow in a 3d rigid tube and the Womersley solution is recovered to an acceptable accuracy. Different grid refinement techniques to study error analysis and convergence behaviour are discussed. The influence of walls, inlet and outlet boundary conditions on accuracy and performance is studied in details as a function of Mach and Knudsen numbers. It is found that the bounce-back on the links could be more efficient if used at low Mach numbers when the Mach number annealing technique is used, as will be demonstrated in the next chapter.