Large Scale Lattice-Boltzmann Simulations: Computational Methods and Applications

Kandhai, B.D.

Citation for published version (APA):

General rights
It is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), other than for strictly personal, individual use, unless the work is under an open content license (like Creative Commons).

Disclaimer/Complaints regulations
If you believe that digital publication of certain material infringes any of your rights or (privacy) interests, please let the Library know, stating your reasons. In case of a legitimate complaint, the Library will make the material inaccessible and/or remove it from the website. Please Ask the Library: https://uba.uva.nl/en/contact, or a letter to: Library of the University of Amsterdam, Secretariat, Singel 425, 1012 WP Amsterdam, The Netherlands. You will be contacted as soon as possible.
Chapter 3

Boundary Conditions and checkerboard effects in Lattice-BGK models

3.1 Introduction

In the previous part of this thesis we discussed the theoretical background of LBGK in detail. In this part * we address computational aspects related to LB. We start with a benchmark study of the boundary conditions and regularly used 3D models (chapter 3). Next, we propose and verify a new technique to reduce the number of time-steps that are required to reach a steady state in LB simulations (chapter 4). Furthermore, we discuss load balancing techniques for lattice-Boltzmann simulations that are generic for problems with a static workload (chapter 5). Finally, we propose a LB scheme on nested grids and present some preliminary numerical results (addendum A).

In principle, it is known that the truncation error of the lattice-Boltzmann method is second-order in space. However, the accuracy of the solution depends on the boundary conditions and is found to be only first-order in many cases [31, 32, 33, 34, 35]. Understanding the effect of the boundary conditions is very important since they are crucial in many fluid-dynamical simulations. We discuss the boundary conditions for two common cases, namely the bounce-back boundary condition at a solid wall and the body force, which is often used as a substitute to pressure boundaries.

Besides the boundary conditions we also report on the regularly used 3D models. The $D_3Q_{15}$ and the $D_3Q_{19}$ model are considered. Here $D$ denotes the dimensionality of the problem and $Q$ is the number of bonds per lattice point [21, 22]. We show that, in the $D_3Q_{15}$ model, checkerboarding in the fluid momentum can

*This chapter is based on the following publications:

Boundary Conditions and checkerboard effects in Lattice-BGK models appear. In some cases this unphysical effect seems to be suppressed by boundaries. We discuss in some detail the numerical accuracy of these models. In section 3.2 we discuss the bounce-back boundary condition and in section 3.3 we study the similarity of the body-force method and pressure-boundaries. Finally, in section 3.4 we study various 3D models and, especially, the checkerboard effect.

### 3.2 The bounce-back boundary condition

The bounce-back boundary rule is the simplest way to impose solid walls in lattice-Boltzmann simulations. Here, particles that meet a wall point are simply bounced back with a reversed velocity. It is obvious that this rule leads to a non-slip boundary (i.e. at the non-slip boundary the velocity of the fluid relative to the solid wall is zero) located somewhere between the wall nodes and the adjacent fluid nodes (in the literature this effect is known as the shift of the boundary). More sophisticated boundaries, which model a non-slip boundary exactly at the wall node (the so-called second-order boundaries), have been proposed by several authors [31, 32, 33, 36, 34, 35, 37]. Unfortunately most of them are restricted to regular geometries (like flat walls and octagonal objects) [31, 32, 33]. For practical simulations the bounce-back boundary is very attractive because it is a simple and computationally efficient method for imposing non-slip walls with irregular geometries.

Most previous studies of bounce-back have only considered flat walls, although a few more detailed studies have been published. Recently, an evaluation of the bounce-back method has been reported where the solutions obtained with the bounce-back rule were compared with those obtained with the finite-difference method for flow around octagonal and circular objects [38]. In this analysis the location of the non-slip boundary was taken to be at the wall node itself and the error in the solution was first-order convergent in space. Here we study the behavior of the bounce-back boundary for a similar geometry. Beside the standard analysis (i.e. where the location of the non-slip boundary is assumed to be at the wall node) our benchmark problem enables us to study the shift of the boundary for a specific staircase geometry, as will be shown in the following.

We chose the simple Poiseuille flow in a tilted channel as the benchmark problem. In this case the analytical solution for the velocity profile is known, and the effect of the bounce-back rule in a staircase boundary can be investigated by simulating fluid flow through an inclined tube (see Fig. 3.1a). The analytical solution for this problem (in lattice units) is given by

$$ u_j = u_0 \frac{l^2 - j^2}{l^2} $$

where $u_j$ is the component of the velocity vector along the flow direction at a distance $j$ from the center of the tube, $l$ is the radius of the tube, and $u_0$ is the maximum velocity [3]. The absolute and relative errors at location $j$, $e_j^a$ and $e_j^r$, and
3.2 The bounce-back boundary condition

Figure 3.1: The inclined tube flow benchmark. On the left the computational grid is shown and on the right the location of the wall. The meaning of points P and Q is explained in the text.

\[ \varepsilon^\text{rel}_j \] respectively, are defined as

\[ \varepsilon^\text{abs}_j = |u_j - \bar{u}_j|, \quad \varepsilon^\text{rel}_j = \left| \frac{u_j - \bar{u}_j}{u_j} \right|, \]  

(3.2)

where \( \bar{u}_j \) is the simulated velocity at location \( j \).

Periodic boundaries were imposed at the inlet and outlet of the tube, and a constant body force was used to drive the flow (i.e. a fixed amount of momentum \( q \) was added at every time step on each lattice point). More details related to the body force method can be found in the next section. The body force was directed along the flow direction, and periodic boundaries were implemented by taking into account the translation of the inlet and outlet in the vertical direction. The walls were modeled by the bounce-back boundary rule.

The mean relative error as a function of lattice spacing is shown in Fig. 3.2 for the standard bounce-back analysis. In this figure we included the results for the inclination angle \( \alpha = 0, 15, 30 \) and 45 degrees. As expected, a first-order convergence of the mean relative error is found in all cases (a fit to the data points gives a slopes of approximately \(-0.9\) for all inclination angles). Furthermore, the error for the staircase geometries is on the average 50% higher than for the flat walls. The relative error close to the boundary nodes (very small velocities) is significantly higher than along the center of the tube (data not shown). This may explain why the lattice-Boltzmann method has proven to be an accurate method for the computation of mean flow quantities like e.g. the permeability of porous media. Moreover our results are of the same order as those of Galivan.
et al. [38] (data not shown) for flow around octagonal cylinders when similar error metrics are used.

As discussed previously, the accuracy of the simulation is determined by the location of the non-slip wall. For flat geometries, it has been shown both numerically and analytically, that when the non-slip boundary is assumed to be in the middle of the first wall and the last fluid node, the error is second-order convergent [39]. In this case the analytic expression for the absolute error caused by the bounce-back boundary condition is given by [39]

\[
M = \frac{Q(4T(4T-5)+3)}{3(2l-1)^2}
\]  

Notice that, according to Eq. (3.3), the “half-way shifted” wall is quite an accurate boundary condition for practical values of the relaxation parameter [39]. Furthermore, the location of the wall is exactly half-way \((u_j - \bar{u}_j = 0)\) when the relaxation parameter is \(\tau = 1.07\). We observed a very good agreement between our simulations and Eq. (3.3) (data not shown).

We also studied the shift of the boundary for non-flat geometries. Here we restricted the analysis to an inclination angle of 45 degrees. The “half-way shifted” location of the wall is expected to differ somewhat from that for a flat tube. In Fig. 3.1b we show the “half-way shifted” location of the wall. The stair-case geometry is staggered between two straight lines (lines through the type-P and type-Q points in Fig. 3.1b). Therefore, the “half-way shifted” boundary is also
3.2 The bounce-back boundary condition

staggered between two straight lines (dashed lines in Fig. 3.1b). The location of the boundary is taken as the average of these two lines (see the thick solid line in Fig. 3.1b).

![Graph showing mean relative error against lattice spacing](image)

**Figure 3.3:** The mean relative error on lattices with $N = 7, 13, 25$ and $50$ lattice points is shown. Square (slope of the line is -2.0) and stars (slope is -1.9) are the half-way shifted results for flat and inclined tube respectively, $v_0 = 0.01$, $\tau = 1.0$.

The mean relative error as a function of lattice spacing is shown in Fig. 3.3. In this figure we included two curves, namely the results for the flat tube and the inclined tube experiment, where for both cases the wall is placed at the “half-way shifted” location. For both cases the error is second-order convergent (a fit to the data points gives an approximate convergence of -1.9). Furthermore, we clearly see that the range of the mean relative error for the flat tube is somewhat smaller than that for the inclined tube.

In Fig. 3.4 the error as a function of the relaxation parameter is shown. A qualitatively similar error behavior for the inclined- and flat-tube flow (Eq. (3.3)) is found. For an increasing relaxation parameter, the error first decreases and subsequently increases after some optimal value of the relaxation parameter. Here we clearly see that, for practical values of the relaxation parameter, the “half-way shifted” boundary is quite accurate. The optimal relaxation parameter in this case is approximately 1.55.

To summarize, we have seen that the error due to stair-cased structure is on the average 50% higher than for flat geometries. For a specific case ($\alpha = 45$ degrees), we verified that the bounce-back boundary rule tends to generate an imaginary boundary, which is located between the last fluid node and the solid wall. For the general case, it is expected that the exact location of the boundary depends
on the relaxation parameter and the geometry of the problem. We believe that it is very difficult to predict the location of the non-slip wall for arbitrary geometries.

However, for geometries with finite curvatures, e.g. for spherical particles, we found that the difference between the hydrodynamic radius and the actual radius is quite small when the relaxation parameter is taken to be $0.7 \leq \tau \leq 1.3$, and the particle radius is expressed in the units of half lattice spacing (c.f. Section 4). Also, we have recently performed a detailed comparison between the lattice-Boltzmann method, the Finite Element method and experimental data for fluid flow in a complex 3D chemical mixing reactor (see chapter 6). The geometry of the reactor consisted of a number of solid tubes in different orientations and locations, and was such that it promoted mixing of fluid flowing through it. The results of the lattice-Boltzmann simulations were quite satisfactory even on moderate lattices. Supported by these results, we thus conclude that in irregular geometries the bounce-back boundary is certainly very useful despite its simplicity. In some applications however, sufficient accuracy may only be obtained on large lattices. In such cases, the accuracy can be increased by locally refining the grid in the vicinity of solid walls (see addendum A).
3.3 Comparison between body force and pressure boundaries

Successful numerical simulation of practical fluid-flow problems requires that the velocity and pressure boundary conditions have been set in a consistent way. However, general velocity and pressure boundaries are still under development for the lattice-Boltzmann method [12, 40, 41, 42, 43, 31, 32, 33, 34, 35, 44, 45, 46]. So far practical simulations have usually included first-order velocity boundaries [24, 47], and a body force [12, 48, 6, 49] has often been used instead of pressure boundaries in problems with a periodic geometry.

Figure 3.5: One unit shell in a vertically infinite array of cylinders. \( L_x \) and \( L_y \) are the length and the width of the unit shell, and \( p_1 \) and \( p_2 \) are the fluid pressures at the inlet and outlet, respectively.

Consider, e.g., fluid flow through an infinite vertical array of cylinders, where pressure is kept constant in vertical planes in front and beyond the cylinders (see Fig. 3.5). Here, the use of body force instead of pressure boundaries is based on the assumption that the effect of the external pressure force \((p_1 - p_2)L_y e_x = Qe_x\), is approximately constant everywhere in the system. Provided that this indeed is the case, and that the densities at the inlet and outlet surfaces are kept constant, pressure boundaries can be replaced with a global body force \(Qe_x\) that gives rise to an acceleration \(ge_x\) of the fluid. Pressure fields are then obtained from the effective pressure \(p_{eff}\), which is defined as

\[
p_{eff} = c_s^2 \Delta p - \rho gx, \tag{3.4}
\]

where \(x\) is the distance measured from the inlet of the system. Notice that, for a simple tube flow, the body force approach is an accurate substitute to pressure boundaries in that, i.e., the velocity and pressure fields given by the two methods are identical.

In order to check the validity of the body-force and pressure boundaries approaches, we simulated the system shown in Fig. 3.5 with both the body force...
and the pressure boundaries. The simulation lattice was \( L_x \times L_y = 300 \times 100 \) lattice points, the cylinder radius \( a_0 \) was 5.5 lattice points, the center of the cylinder was located 100 lattice points from the inlet, and periodic boundaries were used in the \( y \) direction. The cylinder Reynolds number, \( \text{Re} = 2a_0U/\nu \), was varied between 0 and 6 by adjusting the LBGK relaxation parameter \( \tau \) between 0.6 and 2.0.

In the body-force simulations periodic boundaries were used also in the \( x \) direction. Density, and thus effective pressure, were kept constant at the inlet and outlet. The fluid momentum was also kept constant to prevent the cylinders from seeing their periodic images in the \( x \) direction. This was done as follows: after the propagation step the average fluid densities \( \rho_{\text{in}} \) and \( \rho_{\text{out}} \), and the average velocities \( v_{\text{in}} = \mathbf{P}_{\text{in}}/\rho_{\text{in}} \) and \( v_{\text{out}} = \mathbf{P}_{\text{out}}/\rho_{\text{out}} \), were first calculated at the inlet and outlet, respectively. (Here \( \mathbf{P}_{\text{in}} \) and \( \mathbf{P}_{\text{out}} \) are the corresponding total fluid momenta.) Then the particle densities \( f_i \) at the inlet and outlet were set to

\[
\begin{align*}
  f_{i,\text{in}} &= f_{i,0}^{(0)}(\rho_{\text{in}}, v_{\text{in}}) \\
  f_{i,\text{out}} &= f_{i,0}^{(0)}(\rho_{\text{out}}, v_{\text{out}}),
\end{align*}
\]

Pressure boundaries were implemented by the method described in Ref. [35]. Because in both cases velocity and pressure can develop freely, and the channel is big compared to the size of the cylinder, the conditions close to the cylinders are very similar in both simulations.

Notice that, when the system is fully saturated, the drag force acting on the obstacle completely cancels the effect of pressure or body force. So, if the pressure boundary of Ref. [35] is accurate, the two different methods should give equal drag forces.

In table 3.1 we show for different Reynolds numbers the relative difference in the velocity, pressure, \( \varepsilon_p \), and the drag forces, \( \varepsilon_d \), acting on the particle, between pressure boundary and body force simulations for different Reynolds numbers. The numbers are expressed in percentages.

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
\text{Re} & 0 & 0.05 & 0.4 & 2 & 3 & 6 \\
\hline
\text{Mean } \varepsilon_v & 0.33 & 0.34 & 0.33 & 0.34 & 1.36 & 2.2 \\
\text{Max } \varepsilon_v & 0.81 & 0.96 & 0.79 & 0.86 & 2.35 & 62 \\
\text{Mean } \varepsilon_p & 0.24 & 0.24 & 0.27 & 0.46 & 1.9 & 3.94 \\
\text{Max } \varepsilon_p & 0.97 & 0.90 & 0.92 & 1.92 & 6.2 & 14.1 \\
\varepsilon_d & 1.2 \times 10^{-8} & 8 \times 10^{-4} & 7.3 \times 10^{-3} & 7.7 \times 10^{-2} & 1.1 & 2.6 \\
\hline
\end{array}
\]

Table 3.1: The mean and maximum relative difference in the velocity, \( \varepsilon_v \), pressure, \( \varepsilon_p \), and the drag forces, \( \varepsilon_d \), acting on the particle, between pressure boundary and body force simulations for different Reynolds numbers. The numbers are expressed in percentages.

In table 3.1 we show for different Reynolds numbers the relative difference in the velocity, pressure and the drag forces acting on the particle, between the pressure boundary and the body force simulations. The difference is calculated in a box of \( 60 \times 50 \) lattice spacings around the obstacle. The relative difference in the velocity, \( \varepsilon_v \), is defined as \( \varepsilon_v = (v_p - v_b)/v_p \), where \( v_p \) and \( v_b \) are the velocities of the pressure boundary and body force simulations, respectively, and the relative difference in the pressure is defined as

\[
\varepsilon_p = (\delta p - \delta p_{\text{eff}})/\delta p_{12}, \tag{3.5}
\]

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
\text{Re} & 0 & 0.05 & 0.4 & 2 & 3 & 6 \\
\hline
\text{Mean } \varepsilon_v & 0.33 & 0.34 & 0.33 & 0.34 & 1.36 & 2.2 \\
\text{Max } \varepsilon_v & 0.81 & 0.96 & 0.79 & 0.86 & 2.35 & 62 \\
\text{Mean } \varepsilon_p & 0.24 & 0.24 & 0.27 & 0.46 & 1.9 & 3.94 \\
\text{Max } \varepsilon_p & 0.97 & 0.90 & 0.92 & 1.92 & 6.2 & 14.1 \\
\varepsilon_d & 1.2 \times 10^{-8} & 8 \times 10^{-4} & 7.3 \times 10^{-3} & 7.7 \times 10^{-2} & 1.1 & 2.6 \\
\hline
\end{array}
\]
where $\delta p = p_{in} - p$ and $\delta p_{eff} = P_{eff,in} - P_{eff}$ are the pressure differences between the inlet and a point $(x,y)$ for the pressure boundary and body force simulations, respectively. We chose $\delta p_{12} = p_1 - p_2$ as the reference scale instead of $\delta p$, because on many lattice points $\delta p$ was very close to zero. We clearly see that for $Re \leq 2$ the mean relative difference in pressure and velocity is less than $1\%$. For higher Reynolds numbers bigger differences are found. These are probably caused by problems related to the pressure boundary conditions, because the drag in the pressure boundary simulations was not in good agreement with the expected value, in contrast with the results of the body-force simulations.

![Figure 3.6: Comparison of relative difference of velocity and pressure for body force and pressure boundaries. The numbers are expressed in 1/1000 in both cases. The flow is from left to right. Fig. 3.6a. Contours of relative difference $\varepsilon_v$. Fig. 3.6b. Contours of relative difference $\varepsilon_p$.](image)

In Fig. 3.6a we show the contour plot of the relative difference $\varepsilon_v$ for $Re=0.4$. The pressure boundary simulations systematically resulted in slightly smaller velocities, the average difference being $|\varepsilon_v|_{ave} = 0.33\%$. The biggest differences in the velocities, namely -0.79% and -0.74%, were found at the up-stream and down-stream stagnation points, respectively. The contour plot of $\varepsilon_p$ is shown in Fig. 3.6b. Its average value was $|\varepsilon_p|_{ave} = 0.27\%$. The maximum and minimum values for $\varepsilon_p$, namely 0.87% and -0.92%, are once again found at the stagnation points.

In addition to this benchmark, we studied a more complicated case, namely fluid flow in a disordered porous medium composed of non-overlapping spheres. The radii of the spheres were $a_0 = 5.5$ lattice spacings, the porosity of the medium was 0.8 and $\tau = 1.0$. The lattice dimensions were $L_x \times L_y = 500 \times 100$, and the porous medium was placed at a distance of 200 lattice spacings from the inlet and outlet. The obstacle Reynolds numbers were on average 0.003. The difference in the total drag given by the pressure boundary and body-force simulations was here quite high, namely 4%. The average relative differences $|\varepsilon_v|_{ave}$
and $|\varepsilon_{ave}|$ in the velocity and pressure fields were 4.2% and 2.2%, respectively, and the maximum differences of $|\varepsilon_v|$ and $|\varepsilon_p|$ were 28% and 4.3%. Thus, although the difference in total drag was quite big, the overall results were still quite satisfactory. Here we used the drag force acting on the particle as a reference. More detailed comparison of the complete velocity and pressure profiles for body-force driven simulations with results of traditional methods and experimental data of different problems for a wide range of Reynolds numbers, can be found in chapter 6 and Refs [50] and [51].

We can conclude that, for small Reynolds numbers and simple geometries, the body-force approach is quite an accurate substitute to pressure boundaries. However, for high Reynolds-number flows, where nonlinear effects are dominant, and for more complicated geometries, more sophisticated pressure boundaries are still needed.

### 3.4 Checkerboard effect in the $D_{3Q_{14}}$ and $D_{3Q_{15}}$ models

The lattice-Boltzmann method was originally developed from the lattice-gas automata. The first lattice used in 3D simulations was the $D_{3Q_{19}}$ lattice [28], which is a 3D projection of the 4D FCHC lattice [12] used for 3D lattice-gas simulations (see Fig. 3.7a).

![Figure 3.7](image)

Figure 3.7: Lattice structures of the $D_{3Q_{19}}$ (on the left) and $D_{3Q_{15}}$ (on the right) lattice-BGK models. The checkerboard coloring is included in the figures.

It was later realized that the relative freedom in choosing the lattice-Boltzmann equilibrium distribution function also gave some freedom in choosing the struc-
3.4 Checkerboard effect in the $D_3Q_{14}$ and $D_3Q_{15}$ models

ture of the simulation lattice. As a result, the $D_3Q_{15}$ model (see Fig. 3.7b) was developed [21]. The $D_3Q_{14}$ and $D_3Q_{18}$ models are obtained from the $D_3Q_{15}$ and $D_3Q_{19}$ models, respectively, by excluding the rest particles. However, the presence of rest particles is often desirable for improving the accuracy of the model [52]. Also, for a small relaxation time $\tau$, the rest particles may be needed to stabilize the system [53]. Therefore, the $D_3Q_{15}$ and $D_3Q_{19}$ models are most often used in practical simulations.

The computational intensity and the memory requirements of LBM scale linearly with the number of fluid particles. The $D_3Q_{14}$ and $D_3Q_{15}$ models are thus somewhat more efficient than the $D_3Q_{18}$ and $D_3Q_{19}$ models. However, in the $D_3Q_{14}$ and $D_3Q_{15}$ models, checkerboard behavior in the fluid momentum can occur, i.e., fluid momentum may form unphysical regular patterns. We demonstrate this below in the case of saturation of a random velocity field, and in the case of fluid flow around a spherical obstacle.

Let us mark the lattice points $(i,j,k)$ by black colour if $i + j + k$ is odd, and by white colour otherwise, thus forming a checkerboard pattern shown in Figure 3.7 for the $D_3Q_{19}$ and $D_3Q_{15}$ models. To each lattice-Boltzmann fluid particle, we also assign the colour of the lattice point at which they reside in the beginning of the simulation. If there are no obstacles in the system, it is easy to see that, in the $D_3Q_{14}$ model, the black and white particle populations are completely independent of each other: the colour of the lattice point at which a given fluid particle resides changes at every time step (see Figure 3.7b). As a consequence of this checkerboard effect, the total mass and momentum of the black and white particle populations are spurious invariants, i.e. unphysical conserved quantities in the $D_3Q_{14}$ model. Similar spurious invariants are also found in the HPP lattice-gas models [13]. These invariants can create unphysical hydrodynamic modes in the simulated system, and for this reason they should be eliminated from the model [12]. Notice that, in the $D_3Q_{18}$ model, the black and white populations mix immediately with each other. Consequently, there is no checkerboard effect in this model.

In the $D_3Q_{15}$ model the black and white populations are not entirely independent as they are coupled through the rest particles. Here, however checkerboard effects may also lead to unphysical behavior. If the lattice is initialized with equilibrium distributions such that, e.g., the velocity is set to $u_b$ at black lattice points and to $u_w$ at the white lattice points, while $|u_b|$ is equal to $|u_w|$, it is easy to see that the total momenta of the black and white populations are conserved quantities.

We studied the checkerboard effect by following the relaxation of a perturbed velocity field with a constant initial density and with periodic boundaries imposed in all directions. We used two different lattices. In the first case the lattice dimensions were $10 \times 10 \times 10$ lattice points. When a steady state was reached in the $D_3Q_{19}$ model, all components of the particle momenta were found to oscillate at each lattice point between two values (see Figure 3.8a). Such oscillations are caused by the so-called staggered invariants [40, 41]. They can be removed with proper initial conditions, and their effect can also be filtered out by averaging the momenta over two time steps. After time averaging the momentum field
was uniform, as expected [40, 41]. In the $D_3Q_{15}$ model, the fluid remained partially unmixed in the steady state. After time averaging, two different values for the particle momenta were found in the lattice (see Figure 3.8b), and each component of momentum was constant along lines parallel to the corresponding direction. The $x$ component, e.g., was constant on lines parallel to the $x$ axis, and its distribution in the $yz$ plane formed a checkerboard pattern. The relative difference between the two values of the momentum varied in the simulations, being typically $0.5 - 3\%$.

Figure 3.8: Relaxation of the $x$ components of the momenta of two next-nearest neighbors in the $xy$ plane on a lattice of dimension $10 \times 10 \times 10$. On the left and right we show the time evolution of the $D_3Q_{19}$ and $D_3Q_{15}$ models, respectively. The initial perturbed velocity field is the same in both models.

Similar simulations were also performed on a $9 \times 9 \times 9$ lattice. In this case the two populations had additional mixing on the boundaries of the lattice, as the coloring rule was not continuous, due to the length of the lattice being an odd number. As a result, the steady-state momentum field was uniform for both models even without time averaging, i.e., both the staggered invariants and the checkerboard effect were eliminated in the end. However, the weak coupling between the black and white populations in the $D_3Q_{15}$ model was still apparent in the time evolution of the relaxation process. This can be seen in Figure 3.9, where relaxation of the momenta of two next-nearest neighbors is shown in one direction. In the $D_3Q_{15}$ model the relaxation process is significantly slower, and there are long-lasting oscillations in the local values of the momentum in this case.

We also studied the checkerboard effect in the presence of solid walls. The first test case was fluid flow in a rectangular duct. The duct dimensions were $30 \times 30$ lattice points, the relaxation parameter was $\tau = 1.0$, and bounce-back at the
nodes was used on the solid walls. Periodic boundaries were used in the direction of flow driven by a body force. In this case no checkerboard effects were seen, and the average relative difference \(|\Delta v| = \left|\frac{v_{Q19} - v_{Q15}}{v_{Q19}}\right|\) between the velocity fields given by the \(D_3Q_{19}\) and \(D_3Q_{15}\) models was only 0.34%. (A detailed duct-flow comparison between the \(D_3Q_{18}\) and \(D_3Q_{15}\) models has previously been reported in Ref. [35], where the \(D_3Q_{18}\) model was found to be more accurate in general, while the results given by the \(D_3Q_{15}\) model were also found to be satisfactory.)

The second test case was fluid flow around a sphere. The radius of the sphere was \(a_0 = 5.5\) lattice points. In the first simulation, the lattice consisted of \(30 \times 30 \times 30\) lattice points, and the relaxation parameter was \(\tau = 1.0\). Bounce-back condition was used on the solid walls, and periodic boundaries were imposed in all directions. Flow was driven by a body force. In this case, the checkerboard effect did not lead to momentum oscillations, but appeared instead as unphysical patterns in the velocity and pressure fields.

We observed that the velocity field of the \(D_3Q_{15}\) model includes horizontal patterns which are not found in the \(D_3Q_{19}\) model. This kind of pattern is clearly seen in the values of \(\Delta v\) shown in Figure 3.10a. Similar patterns were also seen in the values of \(\Delta p\) (in this comparison \(\Delta p\) was calculated from Eq. (3.4)). In Figure 3.10b, the velocity profile at the inlet boundary is shown for the two models. It is evident that the \(D_3Q_{19}\) model generates a very smooth profile, whereas the \(D_3Q_{15}\) model generates a profile staggered between two smooth curves. The average values of \(\left|\Delta v\right|_{ave}\) and \(\left|\Delta p\right|_{ave}\) were 2.5% and 3.9%, respectively. The difference between the total momenta of the fluids was in steady state only 0.62%.

Figure 3.9: Relaxation of the \(x\) components of the momenta of two next-nearest neighbors in the \(xy\) plane on a \(9 \times 9 \times 9\) lattice. On the left and right we show the time evolution of the \(D_3Q_{19}\) and \(D_3Q_{15}\) models, respectively.
Figure 3.10: The results for fluid flow around a sphere. The velocity field in a plane which bisects the sphere is analyzed. Fluid is flowing from left to right, and periodic boundaries are used in both directions. In Figure 3.10a the relative difference $\Delta v$ between the velocity fields obtained by the $D_3Q_{15}$ and $D_3Q_{19}$ models is shown. The colors run from gray to white with the scale $-3.0\% < \Delta v < 3.0\%$. Figure 3.10b depicts the velocity profile at the inlet for both models. The solid line and open boxes show the results for the $D_3Q_{19}$ and $D_3Q_{15}$ models, respectively. For the results obtained by the $D_3Q_{19}$ model, a solid line is drawn through the simulated points in order to illustrate the effect of checkerboarding more clearly.

For this reason e.g. the hydrodynamic radii $a$ of the sphere (a detailed description of the determination of $a$ is found in Refs [40, 41]) given by these models were very close to each other: the $D_3Q_{15}$ and $D_3Q_{19}$ models resulted in $a = 5.50$ and $a = 5.52$, respectively. We performed similar simulations with bounce back on the links, and on a lattice of $31 \times 31 \times 31$ lattice points. Similar patterns were seen also in these two cases.

We conclude that, in the $D_3Q_{15}$ model, there is a checkerboard effect which may appear in the hydrodynamic fields. In some cases the boundaries can suppress this unphysical effect. However, it does not have significant effect on global values such as the average fluid momentum. Therefore, in spite of its shortcomings, the $D_3Q_{15}$ model appears a viable alternative for steady-state hydrodynamics.

As Figure 3.9b shows, in dynamical systems (e.g. in fluid-particle suspensions or in turbulence simulations) the checkerboard effect may slow down the relaxation of momentum and can, in principle, produce unphysical effects in the dynamics of the system. Notice, however, that the solid boundaries increase mixing also in the $D_3Q_{15}$ model in the case when bounce back on the links is used at the boundaries.
3.5 Conclusions

In this chapter we addressed various issues related to the lattice-BGK method which are important from a practical point of view. We first discussed the effect of the bounce-back boundary condition (which is widely used to model solid walls) for regular staircase boundaries. It was found that the error for staircase geometries is on the average 50% higher compared to that for flat walls. For a special case the bounce-back scheme was shown to be second-order convergent when the non-slip boundary was taken in the middle of the solid and adjacent fluid nodes. The quality of the method was determined by the compatibility of the shifted walls (the so-called hydrodynamic geometry) and the real geometry.

In addition, we also considered boundaries which are responsible for driving a flow between the inlet and outlet of the system. In this context we compared the well-known body-force approach with pressure boundaries. For low Reynolds numbers and simple geometries good agreement between these approaches was found.

Apart from the evaluation of the boundary conditions, we studied two common implementations of the lattice-Boltzmann model in 3D simulations. It was shown that within the $D_3Q_{15}$ model, an unphysical checkerboard effect can be found, which generates spurious conservation of momentum and mass of two distinct populations of particles. For some stationary flows, this unphysical effect generates unphysical patterns in the hydrodynamic fields. However, in the test cases the overall effect of these artifacts is negligible.
Boundary Conditions and checkerboard effects in Lattice-BGK models

3.5 Conclusions

In this chapter, we introduce various boundary conditions for lattice-BGK models. The main focus of the proposed boundary conditions is to mimic the real characteristics of the physical system as closely as possible. For a detailed description of the boundary conditions and their implementation, please refer to Section 4.11.

The velocity field of a fluid is a crucial aspect in understanding the flow. We have developed a method to determine the velocity at the boundaries by analyzing the flow around a sphere. The results show a significant reduction in the checkerboard effect when using the proposed boundary conditions. For this reason, the hydrodynamic model of the sphere is quite accurate in determining the velocity at the boundaries. We have also performed simulations with different models to further illustrate the effectiveness of the proposed approach.

We conclude that, in the L-BGK model, there is a checkerboard effect which may appear in the hydrodynamic fields. In some cases, the boundaries can suppress this unphysical effect. However, it does not have a significant effect on the average values of the fluid momentum. Therefore, in spite of its shortcomings, the L-BGK model appears a viable alternative for steady-state hydrodynamics.

As Figure 3.9b shows, in dynamical systems (e.g., in fluid-particle suspensions or in turbulence simulations), the checkerboard effect may slow down the relaxation of momentum and other, in principle, produce unphysical effects in the dynamics of the system. Notice, however, that the solid boundary increases mixing, thus the L-BGK model is the case when bounce back on the links is used at the boundaries.