On pressure and velocity flow boundary conditions and bounceback for the lattice Boltzmann BGK model

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Abstract

Pressure (density) and velocity boundary conditions inside a flow domain are studied for 2-D and 3-D lattice Boltzmann BGK models (LBGK) and a new method to specify these conditions are proposed. These conditions are constructed in consistency of the wall boundary condition based on an idea of bounceback of non-equilibrium distribution. When these conditions are used together with the improved incompressible LBGK model [1], the simulation results recover the analytical solution of the plane Poiseuille flow driven by pressure (density) difference with machine accuracy. Since the half-way wall bounceback boundary condition is very easy to implement and was shown theoretically to give second-order accuracy for 2-D Poiseuille flow with forcing, it is used with pressure (density) inlet/outlet conditions proposed in this paper and in [2] to study the 2-D Poiseuille flow and the 3-D square duct flow. The numerical results are approximately second-order accurate. The magnitude of the error of the half-way wall bounceback is comparable with that using some other published boundary conditions. Besides, the bounceback condition has a much better stability behavior than that of other boundary conditions.

1 Introduction

The lattice Boltzmann equation (LBE) method has achieved great success for simulation of transport phenomena in recent years. Among different LBE methods, the lattice Boltzmann BGK model is considered more robust [3]. Some recent theoretical discussions on LBGK [4, 5] have enhanced our understanding of the method and the effect of boundary conditions. They explains why the velocity boundary condition for the 2-D triangular LBGK model proposed in [4] generates results of machine accuracy for plane Poiseuille flow with forcing, and the bounceback or equilibrium scheme generate an first-order error to the velocity. Moreover, the bounceback scheme with the wall located half-way between a flow node and a bounceback node (it will be called “half-way

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wall bounceback” thereafter) is shown theoretically to produce results of second-order accuracy for the simple flows considered.

The above mentioned results with Poiseuille flows are obtained with external forcing to drive the flow. In practice, however, a flow is often driven by pressure difference, and the pressure gradient in many cases cannot be replaced by an external force in LBGK computations. In this situation, boundary conditions usually need be implemented by giving prescribed pressure or velocity on some “flow boundaries”, which are not solid walls or interfaces of two distinct fluids. Instead, they are imaginary boundaries inside a flow domain (e.g. inlet and outlet in a pipe flow). Their existence is purely for the convenience of study. The implementation of these boundary conditions in LBGK is very important but it has not yet been well studied.

In lattice Boltzmann method, a specification of pressure difference amounts to a specification of density difference. Early works (see, for example, [7]) to implement pressure (density) flow boundary condition is simply to assign the equilibrium distribution computed with the specified density and some velocity (maybe zero) to the distribution function. This method introduces significant errors. Skordos [8] proposed to add a term to the equilibrium distribution to improve it, the scheme requires the gradient of density and velocities at boundaries. Inamuro et al. [9] and Maier et al. [10] proposed new boundary conditions for lattice Boltzmann simulations. In their simulation of Poiseuille flow with pressure (density) gradient, the pressure boundary condition was treated in different way compared to their wall boundary condition. Chen et al. [2] also proposed a way to specify general boundary conditions including flow boundary conditions.

In this paper, we propose a way to specify pressure or velocity on flow boundaries. They are treated as one type of general boundary conditions, which are based on an idea of bounceback of non-equilibrium part with modifications. When applied to the modified LBGK model, These boundary conditions produce results of machine accuracy for 2-D Poiseuille flow with pressure (density) or velocity inlet/outlet conditions. It is also noticed that although all the proposed new boundary conditions ([2,4,5,10]) including the boundary conditions in this paper yield improved accuracy compared to the bounceback boundary condition, they are difficult to implement for general geometries, because there is a need to distinguish distribution functions according to their orientation to the wall. Besides, there are additional works or different treatments at corner nodes. On the other hand, the complete bounceback scheme does not distinguish distribution functions and is very easy to implement in a parallel way, which was considered as one of the advantages of LGA or LBE method. In this paper, the half-way wall bounceback boundary condition with two flow boundary conditions are applied to the 2-D Poiseuille flow and a 3-D square duct flow using the d2q9i and d3q15i lattice Boltzmann models respectively. The results are approximately second-order accurate. The error is comparable with that using some published boundary conditions. Moreover, the half-way wall bounceback boundary condition for stationary walls is much more stable than the boundary conditions in [2,4,5,10] and in this paper. Thus, we recommend to use the half-way wall bounceback boundary condition for stationary walls and use the boundary conditions proposed in this paper or in [2,10] only for flow boundary conditions.

2 Governing Equation

The square lattice LBGK model (d2q9) is expressed as ([11],[12],[13]):

\[ f_i(x + \delta e_i, t + \delta) - f_i(x, t) = -\frac{1}{\tau}[f_i(x, t) - f_i^{(eq)}(x, t)], \quad i = 0, 1, ..., 8, \]  

(1)
where the equation is written in physical units. Both the time step and the lattice spacing have the value of \( \delta \) in physical units. \( f_i(x, t) \) is the density distribution function along the direction \( e_i \) at \((x, t)\). The particle speed \( e_i \)'s are given by \( e_i = (\cos(\pi(i - 1)/2), \sin(\pi(i - 1)/2), i = 1, 2, 3, 4, \) and \( e_i = \sqrt{2}(\cos(\pi(i - 4 - 1/2)/2), \sin(\pi(i - 4 - 1/2)/2), i = 5, 6, 7, 8. \) Rest particles of type 0 with \( e_0 = 0 \) is also allowed (see Fig. 1). The right hand side represents the collision term and \( \tau \) is the single relaxation time which controls the rate of approach to equilibrium. The density per node, \( \rho \), and the macroscopic flow velocity, \( u = (u_x, u_y) \), are defined in terms of the particle distribution function by

\[
\sum_{i=0}^{8} f_i = \rho, \quad \sum_{i=1}^{8} f_i e_i = \rho u. \tag{2}
\]

The equilibrium distribution functions \( f_i^{(eq)}(x, t) \) depend only on local density and velocity and they can be chosen in the following form (the model d2q9 [12]):

\[
f_i^{(eq)} = t_i \rho [1 + 3(e_i \cdot u) + \frac{9}{2}(e_i \cdot u)^2 - \frac{3}{2}u \cdot u], \quad t_0 = \frac{4}{9}, \quad t_i = \frac{1}{9}, \quad i = 1: 4; \quad t_i = \frac{1}{36}, \quad i = 5: 8. \tag{3}
\]

A Chapman-Enskog procedure can be applied to Eq. (1) to derive the macroscopic equations of the model. They are given by: the continuity equation (with an error term \( O(\delta^2) \) being omitted):

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \tag{4}
\]

and the momentum equation (with terms of \( O(\delta^2) \) and \( O(\delta u^3) \) being omitted):

\[
\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha(c^2_s \rho) + \partial_\beta(2\nu \rho S_{\alpha\beta}), \tag{5}
\]

where the Einstein summation convention is used. \( S_{\alpha\beta} = \frac{1}{2}[(\partial_\alpha u_\beta + \partial_\beta u_\alpha) \) is the strain-rate tensor. The pressure is given by \( p = c^2_s \rho \), where \( c_s \) is the speed of sound with \( c^2_s = \frac{1}{3} \), and \( \nu = \frac{2\tau - 1}{6}\delta \), with \( \nu \) being the the kinematic viscosity. The form of the error terms and the derivation of these equations can be found in [14, 15].

For 2-D case, we will take the Poiseuille flow as an example to study the pressure (density) or velocity inlet/outlet condition. The analytical solution of Poiseuille flow in a channel with width \( 2L \) for the Navier-Stokes equation is given by:

\[
u \frac{\partial^2 u_x}{\partial y^2}, \quad u_y = 0, \quad \frac{\partial p}{\partial x} = -G, \quad \frac{\partial p}{\partial y} = 0, \tag{6}
\]

where the pressure gradient \( G \) is a constant related to the centerline velocity \( u_0 \) by

\[
G = 2\rho \nu u_0/L^2, \tag{7}
\]

and the flow density \( \rho \) is a constant. The Reynolds number is defined as \( Re = u_0(2L)/\nu \).

The Poiseuille flow is an exact solution of the steady-state incompressible Navier-Stokes equations with constant density \( \rho_0 \):

\[
\nabla \cdot u = 0, \tag{8}
\]

\[
\partial_\beta(u_\alpha u_\beta) = -\partial_\alpha(\frac{p}{\rho_0}) + \nu \partial_\beta \partial_\alpha u_\alpha, \tag{9}
\]

\[
\nabla \cdot u = 0.
\]

\[
\partial_\beta(u_\alpha u_\beta) = -\partial_\alpha(\frac{p}{\rho_0}) + \nu \partial_\beta \partial_\alpha u_\alpha,
\]

\[
\nabla \cdot u = 0.
\]
On the other hand, the steady-state macroscopic equations of the LBGK model are different from the incompressible Navier-Stokes equations Eqs. (8,9) by terms containing the spatial derivative of \( \rho \). These discrepancies are called compressibility error in LBE model. Thus, when pressure (density) gradient drives the flow, \( u_x \) in a LBGK simulation increases in the \( x \)–direction, the velocity profile from the simulation is no longer a parabolic profile. For a fixed Mach number (\( u_0 \) fixed), as \( \delta \to 0 \), the velocity of the LBGK simulation will not converge to the velocity in Eq. (6) because the compressibility error becomes dominant. This makes the comparison of \( u_x \) with the analytical velocity of Poiseuille flow somehow ambiguous.

To make a more accurate study for Poiseuille flow with pressure (density) or velocity flow boundary condition, it is better to use the improved incompressible LBGK model proposed in [1]. The model (called d2q9i) is given by Eq. (1) with the same \( e_i \) and the following equilibrium distributions:

\[
    f_i^{(eq)} = t_i[\rho + 3e_i \cdot v + \frac{9}{2}(e_i \cdot v)^2 - \frac{3}{2}v \cdot v], \quad t_0 = \frac{4}{9}, \quad t_i = \frac{1}{9}, \quad i = 1:4; \quad t_i = \frac{1}{36}, \quad i = 5:8. \tag{10}
\]

and

\[
    \sum_{i=0}^{8} f_i = \sum_{i=0}^{8} f_i^{(eq)} = \rho, \quad \sum_{i=1}^{8} f_i e_i = \sum_{i=1}^{8} f_i^{(eq)} e_i = v, \tag{11}
\]

where \( v = (v_x, v_y) \) (like the momentum in the ordinary LBGK model) is used to represent the flow velocity. The macroscopic equations of d2q9i in the steady-state case (apart from error terms of \( O(\delta^2) \)):

\[
    \nabla \cdot v = 0, \tag{12}
\]

\[
    \partial_\beta(v_\alpha v_\beta) = -\partial_\alpha(c_s^2 \rho) + \nu \partial_\beta v_\alpha, \tag{13}
\]

are exactly the steady-state incompressible Navier-Stokes equation with constant density \( \rho_0 \). In this model d2q9i, pressure is related to the calculated density by \( c_s^2 \rho = p/\rho_0 \) (\( c_s^2 = 1/3 \)), and \( \nu = \frac{2\tau - 1}{6} \). The quantity \( p/\rho_0 \) will be called the effective pressure. Although the macroscopic equations of d2q9i in the steady-state case has an error of \( O(\delta^2) \) to the steady-state Navier-Stokes equation, for some special flows like the Poiseuille flow, it is possible that this error disappears with suitable boundary conditions.

### 3 Pressure or Velocity Flow Boundary Condition of the 2-D Square Lattice LBGK Model

In this section a new boundary condition is proposed based on an idea of bounceback on non-equilibrium part as follows: take the case of a bottom node in Fig. 1, the boundary is aligned with \( x \)–direction with \( f_4, f_7, f_8 \) pointing into the wall. After streaming, \( f_0, f_1, f_3, f_4, f_7, f_8 \) are known. Suppose that \( u_x, u_y \) are specified on the wall, we want to use Eqs. (4) to determine \( f_2, f_5, f_6 \) and \( \rho \) (originated in [3]), which can be put into the form:

\[
    f_2 + f_5 + f_6 = \rho - (f_0 + f_1 + f_3 + f_4 + f_7 + f_8), \tag{14}
\]

\[
    f_5 - f_6 = \rho u_x - (f_1 - f_3 - f_7 + f_8), \tag{15}
\]

\[
    f_2 + f_5 + f_6 = \rho u_y + (f_4 + f_7 + f_8). \tag{16}
\]
Consistency of Eqs. (14,16) gives
\[ \rho = \frac{1}{1 - uy} [f_0 + f_1 + f_3 + 2(f_4 + f_7 + f_8)]. \] \hspace{1cm} (17)

We assume the bounceback rule is still correct for the non-equilibrium part of the particle distribution normal to the boundary (in this case, \( f_2 - f_2^{(eq)} = f_4 - f_4^{(eq)} \)). With \( f_2 \) known, \( f_5, f_6 \) can be found, thus
\begin{align*}
    f_2 &= f_4 + \frac{2}{3} \rho uy, \\
    f_5 &= f_7 - \frac{1}{2} (f_1 - f_3) + \frac{1}{2} \rho u_x + \frac{1}{6} \rho uy, \\
    f_6 &= f_8 + \frac{1}{2} (f_1 - f_3) - \frac{1}{2} \rho u_x + \frac{1}{6} \rho uy.
\end{align*} \hspace{1cm} (18)

The collision step is applied to the boundary nodes also. For non-slip boundaries, this boundary condition is reduced to that in [10]. A detailed discussion of implementation of boundary conditions on stationary walls in 3D case was given in [10].

3.1 Specification of Pressure on a Flow Boundary

Now let us turn to the pressure (density) flow boundary condition. In [9, 10], the pressure (density) boundary condition was treated in different way compared to the wall boundary condition. Chen et al. [2] use an extrapolation scheme on an additional layer beyond a boundary to determine the incoming \( f_i \)'s before the streaming step, their treatment of pressure boundary condition is consistent with the wall boundary condition. In this paper, we treat pressure (density) flow boundary condition the same way as the velocity wall boundary condition. Its derivation is based on Eq. (2) as for velocity wall boundary condition. Suppose a flow boundary (take the inlet in Fig. 1 as example) is along the \( y \)-direction, and the pressure (density) is to be specified on it. Suppose that \( u_y \) is also specified (e.g. \( u_y = 0 \) at the inlet in a channel flow). After streaming, \( f_2, f_3, f_4, f_6, f_7 \) are known, \( \rho = \rho_{in}, u_y = 0 \) are specified at inlet. We need to determine \( u_x \) and \( f_1, f_5, f_8 \) from Eq. (2) as following:
\begin{align*}
    f_1 + f_5 + f_8 &= \rho_{in} - (f_0 + f_2 + f_3 + f_4 + f_6 + f_7), \\
    f_1 + f_5 + f_8 &= \rho_{in} u_x + (f_3 + f_6 + f_7), \\
    f_5 - f_8 &= -f_2 + f_4 - f_6 + f_7.
\end{align*} \hspace{1cm} (19, 20, 21)

Consistency of Eqs. (19, 20, 21) gives
\[ u_x = 1 - \frac{[f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)]}{\rho_{in}}. \] \hspace{1cm} (22)

We use bounceback rule for the non-equilibrium part of the particle distribution normal to the inlet to find \( f_1 - f_1^{(eq)} = f_3 - f_3^{(eq)} \). With \( f_1 \) known, \( f_5, f_8 \) are obtained by the remaining two equations:
\begin{align*}
    f_1 &= f_3 + \frac{2}{3} \rho_{in} u_x, \\
    f_5 &= f_7 - \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho_{in} u_x, \\
    f_8 &= f_6 + \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho_{in} u_x.
\end{align*} \hspace{1cm} (23)
The corner node at inlet needs some special treatment. Take the bottom node at inlet as an example, after streaming, $f_3, f_4, f_7$ are known; $\rho$ is specified, and $u_x = u_y = 0$. We need to determine $f_1, f_2, f_5, f_6, f_8$. We use bounceback rule for the non-equilibrium part of the particle distribution normal to the inlet and the boundary to find:

$$f_1 = f_3 + (f_{1}^{(eq)} - f_{3}^{(eq)}) = f_3, \quad f_2 = f_4 + (f_{2}^{(eq)} - f_{4}^{(eq)}) = f_4,$$

(24)

Using these $f_1, f_2$ in Eqs. (20,21), we find:

$$f_5 = f_7, \quad f_6 = f_8 = \frac{1}{2} [\rho_{in} - (f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_7)].$$

(25)

Similar procedure can be applied to top inlet node and outlet nodes including outlet corner nodes.

### 3.2 Specification of Velocity on a Flow Boundary

In some calculations, velocities $u_x, u_y$ are specified at a flow boundary (take the inlet in Fig. 1 as example). In the flow region of the inlet or outlet, this is actually equivalent to a velocity wall boundary condition and can be handled in the same way as given at the beginning of the section. The effect of specifying velocity at inlet is similar to specifying pressure (density) at inlet. Density difference in the flow can be automatically generated by the velocity inlet condition.

At the inlet bottom (non-slip boundary), special treatment is needed. After streaming, $f_1, f_2, f_5, f_6, f_8$ need to be determined. Using bounceback on normal distributions gives:

$$f_1 = f_3, \quad f_2 = f_4.$$

Expressions of $x, y$ momenta give:

$$f_5 - f_6 + f_8 = -(f_1 - f_3 - f_7) = f_7,$$

$$f_5 + f_6 - f_8 = -(f_2 - f_4 - f_7) = f_7,$$

(26)

or

$$f_5 = f_7,$$

$$f_6 = f_8 = \frac{1}{2} [\rho - (f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_7)].$$

(27)

but there is no more equation available to determine $\rho$. The situation is similar to a corner wall node (the intersection of two perpendicular walls). In this situation, since $\rho$ is expected to be constant at the inlet, $\rho$ at the inlet bottom node can be taken as the $\rho$ of its neighboring flow node, thus the velocity inlet condition is specified. It is noted that this treatment is only for a special study to produce the analytical solution with model d2q9i. In practice, however, the half-way wall bounceback is recommended as boundary conditions for stationary walls and there is no need for special treatment at corner nodes. This will be discussed in section 4.

From the discussion given above, we can unify boundary conditions (on a wall boundary or in a flow boundary) in 2-D simulation on a straight boundary as:

- Given $u_x, u_y$, find $\rho$ and unknown $f_i$’s.
• Given $\rho$ and the velocity along the boundary, find the velocity normal to the boundary and unknown $f_i$’s.

The above discussion is for flat flow boundaries aligned with a plane spanned by two particle velocities of type I. It is not the purpose of this paper to derive a flow boundary condition in a general geometry. If a flow boundary has a complicated geometry or if it is not aligned with lattice directions, schemes based on extrapolations like the ones in [2, 10] can be used. However, as pointed out in [10], on a convex edge or at a convex corner, there are too few unknown $f_i$’s, if the available $f_i$’s are used, then any choice of the unknown $f_i$’s may not make the velocity correct. There have not been analytical or numerical studies on the order of accuracy for these situations. Thus the order of accuracy is not clear for these cases. Hence, the equilibrium scheme can be considered as well. The equilibrium scheme at boundaries gives second-order accuracy if $\tau = 1$ but only first-order when $\tau \neq 1$ [8, 16].

3.3 Boundary Conditions for the Modified Incompressible Model d2q9i

The velocity wall boundary condition and flow boundary conditions for d2q9i are similar to that of d2q9. The derivation is based on equations $\sum_{i=0}^{8} f_i = \rho$ and $\sum_{i=1}^{8} e_i f_i = v$ and hence some modifications are needed as follows:

• In wall boundary condition, Eq. (17) is replaced by

$$ \rho = v_y + [f_0 + f_1 + f_3 + 2(f_4 + f_7 + f_8)], $$

and in Eq. (18), $\rho u_x, \rho u_y$ are replaced by $v_x, v_y$ respectively.

• In pressure flow boundary condition, Eq. (22) is replaced by

$$ v_x = \rho_{in} - [f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)], $$

and in Eq. (23), $\rho_{in} u_x$ is replaced by $v_x$.

3.4 Numerical Results of Model d2q9i

We report and discuss the numerical results for Poiseuille flow with our wall and flow boundary conditions. The simulation is performed on the model d2q9i. The main result in the simulation is the achievement of machine accuracy. The width of the channel is assumed to be $2L = 2$. We use $nx, ny$ lattice nodes on the $x$- and $y$-directions, thus, $\delta = 2/(ny - 1)$. The initial condition is to assign $f_i = f_i^{(eq)}$ computed using a constant density $\rho_0$, and zero velocities. The steady-state is reached if

$$ \sum_{i} \sum_{j} |v_x(i, j, t + \delta) - v_x(i, j, t)| + |v_y(i, j, t + \delta) - v_y(i, j, t)| \leq \delta \cdot Tol. $$

$Tol$ is a tolerance set to $10^{-12}$ in this section.

We also define a maximum relative error of velocity $(v_x, v_y)$ as in [16]:

$$ err_m \equiv \max \frac{\sqrt{(u_x^t - v_x)^2 + (u_y^t - v_y)^2}}{u_0}, $$

7
where $u_t^x, u_t^y$ is the analytical velocity, and $u_0$ is the peak velocity, the maximum is throughout the flow.

For model d2q9i, we carried out simulations with a variety of Re, $nx, ny, u_0$ using the pressure or velocity flow boundary condition. All simulations in this paper use double-precision. The range of Re is from 0.0001 to 30.0; the range of $\tau$ is from 0.56 to 20.0 and the range of $u_0$ is from 0.001 to 0.4; the largest density difference simulated (not the limit) is $\rho_{in} = 5.6, \rho_{out} = 4.4$ with $nx = 5, ny = 3$ corresponding to an effective pressure gradient of $G' = 0.1$, where $G'$ is defined as $G' = -\frac{1}{\rho_0} \frac{dp}{dx}$. The magnitude of average density $\rho_0$ is 5, but it is irrelevant for the simulation [1].

For all cases where the simulation is stable, the steady-state velocity and density show:

- The velocity field $v_x$ is uniform in the $x$-direction, it is accurate up to machine accuracy compared to the analytical solution in Eq. (6), $v_y$ is very small with maximum of $|v_y|$ in the whole region being in the order of $10^{-13}$. For example, for $nx = 5, ny = 3, u_0 = 0.1, \tau = 0.56, Re = 10$, the maximum relative error of velocity is $0.1816 \cdot 10^{-11}$, while the maximum relative error of density is $0.3553 \cdot 10^{-15}$, and the maximum magnitude of $v_y$ is $0.5551 \cdot 10^{-15}$. The results for other cases are similar to this example.

- The density is uniform in the cross channel direction, and linear in the flow direction. the computed value and the analytical value of the density gradient differ only at the 14th digit.

It is also noticed that with pressure (density) gradient to drive Poiseuille flow, the maximum Reynolds number which makes the simulation stable is far less than that with external forcing, which is also reported in [2].

Similar results with machine accuracy are obtained by specifying the analytical velocity profile given in Eq. (6) at inlet and pressure (density) at outlet by using the flow boundary conditions in this paper. In the case, there is a uniform pressure (density) difference in the region. The value of the density difference depends on $u_0$ and the outlet density.

The accurate results in the model d2q9i give us confidence about the flow boundary conditions proposed.

### 4 On Half-way Wall Bounceback Boundary Condition

#### 4.1 Reconsider Bounceback

The bounceback rule with wall placed at the bounceback nodes gives an first-order error to velocity, both at the boundary and throughout the flow. This has been showed analytically [5] for some simple flows and computationally [15] for 2D cavity flows. The same can be said for the flows studied in this paper based on numerical results. There have been efforts to replace the bounceback boundary condition with new boundary conditions for LBE simulation. Various boundary conditions [2, 6, 8, 9, 10, 16] including the one in this paper are proposed. While these boundary conditions indeed improve the accuracy for some simple flows over the bounceback scheme, extra works are still needed to apply them to a general situation. First, for example, at a concave edge [10], the boundary conditions in [6, 8, 9, 10, 16] and in this paper do not give a natural way to determine the density, and since there are more unknowns at a node than in a plane wall node, some additional assumptions are needed to apply the boundary condition. Second, all the boundary conditions in [2, 6, 8, 9, 10, 16] including the one in this paper require different treatments on $f_i$’s depending on their orientation to the wall, the implementation of
these boundary conditions is formidable for complicated geometry like that in a porous media or for a situation where a wall is not aligned with any of the \( f_i \)'s direction. On the other hand, the “complete” bounceback scheme which assigns each \( f_i \) the value of the \( f_j \) of its opposite direction with no relaxation on the bounceback nodes is very easy and convenient to apply, the treatment is independent on the direction of \( f_i \)’s, which is one of the major advantages of LGA or LBE method. Several theoretical studies have shown that if the wall is placed at the half way between the bounceback row and the first flow row (“half-way wall bounceback”), the scheme gives a second-order accuracy [4, 5, 17, 18] for some simple flows including an inclined channel flow and a plane stagnation flow. For example, if the d2q9 model with the half-way wall bounceback is used to simulate the 2-D Poiseuille flow with forcing, the error of the velocity (it is the same for any node) is given by

\[
\frac{u^t_j - u_j}{\delta^2} = -\frac{u_0[4\tau(4\tau - 5) + 3]}{3}\delta^2
\]  

(32)

where \( u^t_j, u_j \) is the analytical and computed \( x \)-velocity respectively, \( u_0 \) is the center velocity. For a fixed \( \tau \), the error is second-order in the lattice spacing \( \delta \). Of course, large value of \( \tau \) will give large errors, which are reported in some papers [3, 9], giving an impressed vision how bad the bounceback boundary condition was. However, for practical purposes, there is no need to take large value of \( \tau \) in a simulation. Besides, the Chapman-Enskog procedure does not work right when \( \tau \) is large. For \( \tau \) between 0.5 and 1.25, the magnitude of the error given in (32) is less than or equal to \( 1.1 u_0 \delta^2 \). Thus, it is worthwhile to consider this boundary condition in more general situations especially in 3-D flows and some results are reported in section 4.2, 4.3 and section 5.

4.2 Results of Model d2q9i

To reduce the effect of compressibility error, the model d2q9i is used. Simulations with model d2q9 were also carried out, the results have very similar behavior for order of convergence but the magnitude of error in d2q9 is greater. We use d2q9i to simulate Poiseuille flow with pressure or velocity flow boundary condition. For the half-way wall bounceback, if there are \( ny \) nodes on the \( y \)-direction, then the first and last nodes are the bounceback nodes with the wall being located half-way between the bounceback node and the first flow node, there are \( ly = ny - 2 \) lattice steps across the channel and the lattice spacing is \( \delta = 2/(ny - 2) = 2/ly \) (in the case of the boundary condition in [2] \( \delta = 2/(ny - 1) = 2/ly \)). The length of the channel is set to twice as the width. At the inlet/outlet, the bounceback is also used at the nodes on the bounceback rows, thus, there is no additional treatment for the corner nodes at the inlet/outlet.

Two inlet/outlet (I/O) conditions with the half-way wall bounceback were tested:

1. I/O No. 1: the flow boundary condition given in this paper.

2. I/O No. 2: the flow boundary condition proposed in [2]. It assumes an additional layer of nodes beyond the boundary flow nodes and uses an extrapolation formula to derive the incoming \( f_i \)’s of the additional layer before streaming.

The I/O and boundary condition in [2] were also used to compare result with the the half-way wall bounceback.

For the study of accuracy, we fix \( \tau \) and the Reynolds number (which affects stability) and halve \( \delta \) each time and calculated the error in the result. Simulations with different Re and \( \tau \leq 1.3 \) are performed. Three examples with pressure specified at inlet and outlet are reported
on Table I, The example uses three sets of parameters: (1) \( \tau = 0.6, \ Re = 10 \), (2) \( \tau = 0.8, \ Re = 10 \), and (3) \( \tau = 1.1, \ Re = 1 \) (Re is restricted so that \( u_0 \) for the smallest number of lattice nodes is still small), and \( \rho_0 = 5 \). The quantity \( Tol \) in Eq. (30) is set to \( 10^{-8} \). As \( \delta \) halves, \( u_0 \) also halves, so does the Mach number, the same way as in the study of duct flow in [10]. As \( \delta \) changes, \( \nu \) and the effective pressure gradient \( G' \) and then pressure (density) at inlet/outlet also changes. \( lx, ly \) are used to represent the number of lattice steps in \( x \)- and \( y \)-directions, we use \( lx = 8, 16, 32, 64, 128, ly = 4, 8, 16, 32, 64 \) respectively to do the simulation.

The convergence result is summarized in Table I. The ratio of two consecutive maximum relative errors is also shown. The order of convergence from a least-square fitting (a linear least-squares fitting to logarithms of error and \( \delta \)) is shown in the last column.

For the cases of I/O Nos. 1, 2 with the half-way wall bounceback, the maximum relative velocity errors are very close, the ratio is approximately equal to 4, indicating a second-order accuracy. The magnitude of errors in the half-way wall bounceback is close to (sometimes smaller than) the result using I/O and boundary condition in [2]. For the cases of the half-way wall bounceback, it is also observed that

- Velocity \( v_x \) is generally uniform in the \( x \)-direction.
- \( v_y \) is small compared to \( u_0 \), with maximum of \( |v_y| \) being less than \( 0.011u_0 \) in all cases. As \( ly \) increases, the maximum of \( |v_y|/u_0 \) decreases. I/O No. 2 gives much smaller max \( |v_y| \) than I/O No. 1.
- The density is approximately uniform in the cross channel direction, and linear in the flow direction. The maximum relative density error is much less than the maximum relative velocity error and it decreases much faster than the maximum relative velocity error as \( ly \) increases. The density gradient \( (\rho(i+1,j) - \rho(i,j))/\delta \) is approximately equal to the analytical value. No. 2 gives almost the exact density distribution.

Of course, the achievement of second-order accuracy for Poiseuille flow does not necessarily mean a second-order accuracy for any flow, in next section, a 3-D duct flow will be studied.

### 4.3 Stability Issue

Another important issue is the stability related to boundary conditions. It is found that the combination of bounceback without collision on stationary walls with equilibrium distribution at flow boundaries gives the best behavior on stability. Once any boundary condition or flow boundary condition in any of the schemes in [2, 4, 4, 10, 10] or in this paper is used, the maximum Re number is reduced dramatically. For example, in the simulation of Poiseuille flow with bounceback at the wall and equilibrium scheme with velocity inlet and density outlet conditions (in the case, if density are prescribed at both inlet and outlet, the velocity is significantly smaller than the intended value for high Re flows) and with \( lx = 16, ly = 8, u_0 = 0.1 \), the maximum Re is 500. The maximum Re reduces to 63, 56 respectively for density inlet/outlet condition No. 1, No. 2 with bounceback boundary condition on the walls. The maximum Re further reduces to 42, 12 respectively for density inlet/outlet condition and boundary conditions in this paper and in [2]. It is also noted that when the parameter are close to the region of instability, the simulation may have unusual large errors. On this account, the half-way wall bounceback is safer.
5 Flow Boundary Conditions and Results for the 3-D 15-velocity LBGK Model

Since 3-D model is needed in practical problems, this section will discuss the pressure or velocity flow boundary condition for the 3-D 15-velocity LBGK model d3q15 and an incompressible model d3q15i similar to d2q9i and present some simulation results. The model d3q15 is based on the LBGK equation Eq. (1) with \( i = 0, 1, \cdots, 14 \), where \( \mathbf{e}_i, i = 0, 1, \cdots, 14 \) are the column vectors of the following matrix:

\[
E = \begin{bmatrix}
0 & 1 & -1 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
0 & 0 & 0 & 1 & -1 & 0 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 \\
0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & -1 & -1 & 1
\end{bmatrix}
\]

and \( \mathbf{e}_i, i = 1, \cdots, 6 \) are classified as type I, \( \mathbf{e}_i, i = 7, \cdots, 14 \) are classified as type II. The density per node, \( \rho \), and the macroscopic flow velocity, \( \mathbf{u} = (u_x, u_y, u_z) \), are defined in terms of the particle distribution function by

\[
\sum_{i=0}^{14} f_i = \rho, \quad \sum_{i=1}^{14} f_i \mathbf{e}_i = \rho \mathbf{u}.
\]  

(33)

The equilibrium can be chosen as:

\[
f_{0}^{(eq)} = \frac{1}{8} \rho - \frac{1}{3} \rho \mathbf{u} \cdot \mathbf{u},
\]

\[
f_{i}^{(eq)} = \frac{1}{8} \rho + \frac{1}{3} \rho \mathbf{e}_i \cdot \mathbf{u} + \frac{1}{2} \rho (\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{1}{6} \rho \mathbf{u} \cdot \mathbf{u}, \quad i \in I
\]

\[
f_{i}^{(eq)} = \frac{1}{64} \rho + \frac{1}{24} \rho \mathbf{e}_i \cdot \mathbf{u} + \frac{1}{16} \rho (\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{1}{48} \rho \mathbf{u} \cdot \mathbf{u}, \quad i \in II
\]

(34)

The model d3q15i is constructed from these formulas in a similar way as in d2q9i.

The flow to be studied in the 3-D case is the square duct flow with \( x^- \) direction being the flow direction. It is clear to give a projection of the velocities in the \( xz \) plane as shown in Fig. 1. The macroscopic equations of the model is the same as Eqs. (4,5) with \( c_s^2 = 3/8 \), and \( \nu = (2 \tau - 1) \delta/6 \).

The pressure flow boundary condition proposed in 3.1 has the following version for the model d3q15i: take the case of an inlet node as shown in Fig. 1, the inlet is on \( yz \) plane. After streaming, \( f_i, i = 0, 2, 3, 4, 5, 6, 8, 10, 12, 14 \) are known. Suppose that \( \rho_{in}, u_y = u_z = 0 \) are specified on the inlet, we need to determine \( f_i, i = 1, 7, 9, 11, 13 \) and \( u_x \) from Eqs. (33). Similar to the derivation in d2q9, \( u_x \) is determined by a consistency condition as:

\[
\rho_{in} u_x = \rho_{in} - [f_0 + f_3 + f_4 + f_5 + f_6 + 2(f_2 + f_8 + f_{10} + f_{12} + f_{14})],
\]

(35)

The expression of \( x^- \) momentum gives:

\[
f_1 + f_7 + f_9 + f_{11} + f_{13} = \rho_{in} u_x + (f_2 + f_8 + f_{10} + f_{12} + f_{14}),
\]

(36)

If we use bounceback rule for the non-equilibrium part of the particle distribution \( f_i, (i = 1, 7, 9, 11, 13) \) to set

\[
f_i = f_{i+1} + (f_{i}^{(eq)} - f_{i+1}^{(eq)}),
\]

(37)
then Eq. (36) is satisfied, and all $f_i$ are defined. In order to get the correct $y-, z-$momenta, we further fix this $f_1$ (bounceback of non-equilibrium $f_i$ in the normal direction) and modify $f_7, f_9, f_{11}, f_{13}$ as in [10]:

$$f_i \leftarrow f_i + \frac{1}{4} e_{iy} \delta_y + \frac{1}{4} e_{iz} \delta_z. \quad i = 7, 9, 11, 13$$

(38)

This modification leaves $x-$momentum unchanged but adds $\delta_y, \delta_z$ to the $y-, z-$momenta respectively. A suitable choice of $\delta_y$ and $\delta_z$ then gives the correct $y-, z-$momenta. Finally, we find:

$$f_1 = f_2 + \frac{2}{3} \rho_{in} u_x,$$

$$f_i = f_{i+1} + \frac{1}{12} \rho_{in} u_x - \frac{1}{4} [e_{iy}(f_3 - f_4) + e_{iz}(f_5 - f_6)], \quad i = 7, 9, 11, 13$$

(39)

There is no special treatment at the wall of the inlet/outlet if bounceback is used there. Modification of the flow boundary condition for $d_{3q15i}$ is similar to $d_{2q9i}$.

The velocity flow boundary condition can be derived similarly.

Simulations on 3-D square duct flow are performed on $d_{3q15i}$ and on $d_{3q15}$ using the pressure flow boundary condition. Only the result of $d_{3q15i}$ is reported, the result of $d_{3q15}$ is similar but the errors are greater. The analytical solution of a flow in an infinitely long rectangular duct $-a \leq y \leq a, -b \leq z \leq b$, with $x$ being the flow direction is given by [19]

$$u_x(y, z) = \frac{16a^2}{\mu \pi^3} \left( -\frac{dp}{dx} \right) \sum_{i=1,3,5,\ldots}^{\infty} (-1)^{(i-1)/2} \left[ 1 - \frac{\cosh(i \pi z/2a)}{\cosh(i \pi b/2a)} \right] \cos(i \pi y/2a),$$

(40)

We use $a = b = 2$ in the simulations. Results of the following boundary conditions are reported:

1. I/O No. 1 (the I/O condition discussed above) with the half-way wall bounceback at walls;
2. I/O No. 2 (the I/O condition in [2]) with the half-way wall bounceback at walls;
3. I/O and boundary conditions in [2];
4. I/O and boundary conditions in [10];
5. I/O No. 2 with the original bounceback, which is the bounceback at wall nodes without collision (only for the middle example).

The I/O No. 1 with solid boundary condition in [10] is also tried, the result on velocity is very close to that in case (4) and is not reported. Again, we fix $\tau$ and the Reynolds number, halve $\delta$ each time. Simulations with different $Re$ and $\tau \leq 1.3$ are performed. Three examples are reported on Table II: (1) $\tau = 0.6, Re = 10$, (2) $\tau = 0.8, Re = 5$, (3) $\tau = 1.1, Re = 0.2$, and all use $\rho_0 = 5$. The quantity $Tol$ in the 3-D version of Eq. (30) is set as $10^{-8}$. Define $lx, ly, lz$ to represent the number of lattice steps in $x-$ and $y-, z-$directions respectively, we use $lx = 8, 16, 32, 64, ly = lz = 4, 8, 16, 32$ respectively to do the simulation. The maximum relative error is defined similar to Eq. (31). From Table II, we can see that the results of the half-way wall bounceback give an accuracy close to second-order, so do the boundary conditions in [2, 10]. Besides, the errors with the half-way wall bounceback are comparable with that using the I/O and boundary conditions in [2, 10]. On the other hand, the original bounceback introduces an error of first-order throughout the flow (L1 error has a similar first-order behavior). Thus, the half-way wall bounceback has an essentially different behavior than the original bounceback. The calculated density has smaller errors than that of the velocity, and the density is less uniform across a section in the duct than in 2-D case.
It is noted that the orders of convergence in the case of 3-D duct flow with all boundary conditions considered are not as good as in 2-D Poiseuille flows. For example, the ratios of errors at the highest resolution are not very close to 4 in some cases (the order of convergence may be close to 2 in the cases because of an irregular large error ratio at a coarser resolution). It looks that in 3-D duct flow, the four edges pose additional difficulties to boundary conditions. Even with forcing, the density is not uniform in a cross section for the half-way wall bounceback or for boundary conditions in [2, 10]. Nevertheless, the order of convergence for 3-D duct flow is still close to 2. The half-way wall bounceback has a weaker convergence when $\tau > 1$ while the boundary condition in [2] performs better as $\tau > 1$ but worse as $\tau < 1$. On the consideration of simplicity in implementation and superior stability behavior of the half-way wall bounceback, we think that it deserves a serious consideration in a LBGK simulation.

We would like to point out that a second-order accuracy of the half-way wall bounceback in the flows considered does not imply a second-order accuracy for any flows. The statement can be applied to other boundary conditions as well. One is encouraged to do some tests on a simplified flow of the type of flows to be simulated.

6 Discussions

The major results in this paper are: first, flow boundary conditions can be treated in a similar way as wall boundary conditions, and a new way to specify flow boundary conditions based on bounceback of non-equilibrium part is proposed. For the test problem of Poiseuille flow with pressure or velocity inlet/outlet conditions, the new method recovers the analytic solution within machine accuracy. Second, we reconsider the the half-way wall bounceback boundary condition for stationary walls. It is very easy to implement. If being applied with flow boundary condition in this paper or in [2], it is approximately of second-order accuracy for the 2-D and 3-D channel flows with $\tau$ being less than or close to one. The magnitude of the error is comparable with that using some published boundary conditions. Hence, the the half-way wall bounceback is recommended for stationary walls. For flow boundary conditions in simulations of small to moderate Re numbers, one may consider the schemes in this paper or in [2]. For the cases considered, these flow boundary conditions give very close results in velocity. The scheme in [2] gives a better density distribution but a weaker stability behavior. One can also use the equilibrium distribution scheme if $\tau = 1$ can be used. However, for simulations of large Re flows, one may have to use the equilibrium flow boundary condition with velocity inlet condition and with $\tau$ close to 0.5. In that situation, the accuracy is only first-order.

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Table I. maximum relative errors for the 2-D Poiseuille flow with pressure being specified at inlet and outlet for three cases: (1) Re=10, \( \tau = 0.6 \), (2) Re=10, \( \tau = 0.8 \), (3) Re=1, \( \tau = 1.1 \). The results of two pressure flow boundary conditions I/O Nos. 1,2 with the half-way wall bounceback (HWWBB) and the result of the I/O and boundary conditions in [2] are given. In each box, the upper figure is the error, and the lower figure is the ratio of two consecutive errors. The last column shows the order of convergence using the least-squares fitting. The symbol (-2) represents \( 10^{-2} \).

| Re = 10 | I/O No. | HWWBB | ly | lx | u₀ | 8  | 16  | 32  | 64  | 128 | order |
|----------|---------|-------|-----|----|----|-----|-----|-----|-----|-----|-------|
| \( \tau = 0.6 \) | 1/0 | | 4.021 | | 0.6031(-1) | 0.4167(-1) | 0.2084(-1) | 0.1042(-1) | 0.5208(-2) | | |
| I/O No. 2 | HWWBB | | 4.001 | | 0.5917(-1) | 0.1479(-1) | 0.3699(-2) | 0.9265(-2) | 0.2352(-3) | 1.995 |
| I/O, B.C. | unstable | | | | | | | | | |
| Re = 10 | I/O No. 1 | HWWBB | 3.938 | | 0.3276(-1) | 0.8319(-2) | 0.2054(-2) | 0.5111(-3) | 0.1276(-3) | 2.003 |
| \( \tau = 0.8 \) | I/O No. 2 | HWWBB | 4.000 | | 0.3250(-1) | 0.8125(-1) | 0.2032(-2) | 0.5085(-3) | 0.1283(-3) | 1.997 |
| I/O, B.C. | unstable | | | | | | | | | |
| Re = 10 | I/O No. 1 | HWWBB | 4.011 | | 0.5550(-1) | 0.1441(-1) | 0.3617(-2) | 0.9021(-3) | 0.2249(-3) | 1.989 |
| \( \tau = 1.1 \) | I/O No. 2 | HWWBB | 4.001 | | 0.5750(-1) | 0.1437(-1) | 0.3594(-2) | 0.8984(-3) | 0.2246(-3) | 2.000 |
| I/O, B.C. | unstable | | | | | | | | | |

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Table II. Maximum relative errors for the 3-D square duct flow with pressure being specified at inlet and outlet for three cases: (1) Re=10, \( \tau = 0.6 \), (2) Re=5, \( \tau = 0.8 \), (3) Re=0.2, \( \tau = 1.1 \). The results of two pressure flow boundary conditions I/O Nos. 1, 2 with the half-way wall bounceback (HWWBB), the results of the I/O and boundary conditions in [2,10] are also given. The result of I/O in [2] with original bounceback is given for the second case. In each box, the upper figure is the error, and the lower figure is the ratio of two consecutive errors. The last column shows the order of convergence using the least-squares fitting.

| Re = 10 \( \tau = 0.6 \) | lx \( \times 10^4 \) | ly, lz \( \times 10^4 \) | 8 | 16 | 32 | 64 | order |
|-------------------------|-----------------|-----------------|----|----|----|----|-------|
| \( u_0 \) | 0.8333(-1) | 0.4167(-1) | 0.2083(-1) | 0.1042(-1) | | |
| I/O No. 1 \ HWWBB | 0.4028 | 0.1054 | 0.2742(-1) | 0.7289(-2) | 3.822 | 3.844 | 3.762 | 1.931 |
| I/O No. 2 \ HWWBB | unstable | | | | | | | |
| I/O, B.C. in [2] \ HWWBB | unstable | | | | | | | |
| I/O, B.C. in [10] | 0.2210 | 0.5565(-1) | 0.1293(-1) | 0.3132(-2) | 3.971 | 4.304 | 4.128 | 2.053 |

| Re = 5 \( \tau = 0.8 \) | lx \( \times 10^4 \) | ly, lz \( \times 10^4 \) | 8 | 16 | 32 | 64 | order |
|-------------------------|-----------------|-----------------|----|----|----|----|-------|
| \( u_0 \) | 0.1250 | 0.6250(-1) | 0.3125(-1) | 0.1563(-1) | | |
| I/O No. 1 \ HWWBB | 0.1382 | 0.3980(-1) | 0.9805(-2) | 0.2388(-2) | 3.472 | 4.059 | 4.106 | 1.959 |
| I/O No. 2 \ HWWBB | 0.1371 | 0.3659(-1) | 0.9243(-2) | 0.2310(-2) | 3.747 | 3.959 | 4.001 | 1.966 |
| I/O, B.C. in [2] \ HWWBB | 0.3397 | 0.9563(-1) | 0.2117(-1) | 0.5741(-2) | 3.552 | 4.517 | 3.688 | 1.984 |
| I/O, B.C. in [10] \ HWWBB | 0.8567(-1) | 0.1543(-1) | 0.4502(-1) | 0.1278(-2) | 5.552 | 3.427 | 3.523 | 1.998 |
| I/O No. 2 \ HWWBB | 0.6539 | 0.3345 | 0.1536 | 0.7935(-1) | 1.955 | 2.178 | 1.936 | 1.025 |
| I/O No. 2 \ bounceback | | | | | | | | |

| Re = 0.2 \( \tau = 1.1 \) | lx \( \times 10^4 \) | ly, lz \( \times 10^4 \) | 8 | 16 | 32 | 64 | order |
|------------------------|-----------------|-----------------|----|----|----|----|-------|
| \( u_0 \) | 0.1000(-1) | 0.5000(-2) | 0.2500(-2) | 0.1250(-2) | | |
| I/O No. 1 \ HWWBB | 0.2091 | 0.6537(-1) | 0.1817(-1) | 0.4807(-2) | 3.199 | 3.598 | 3.780 | 1.818 |
| I/O No. 2 \ HWWBB | 0.2114 | 0.6448(-1) | 0.1787(-1) | 0.4737(-2) | 3.279 | 3.608 | 3.772 | 1.829 |
| I/O, B.C. in [2] \ HWWBB | 0.3109 | 0.7740(-1) | 0.1966(-1) | 0.4904(-2) | 4.017 | 3.937 | 4.009 | 1.994 |
| I/O, B.C. in [10] \ HWWBB | 0.2070 | 0.4973(-1) | 0.1277(-1) | 0.3341(-2) | 4.162 | 3.894 | 3.822 | 1.982 |
8 Figure Caption

Fig. 1, Schematic plot of velocity directions of the 2-D (d2q9) model and projection of 3-D (d3q15) model in a channel. In the 3-D model, the $y-$axis is pointing into the paper, so are velocity directions 3,7,9,12,14 (they are in parentheses if shown), while the velocity directions 4,8,10,11,13 are pointing out. Velocity directions 3,4 have a projection at the center and are not shown in the figure.
