

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

Qisu Zou ^{*†} and Xiaoyi He ^{‡§}

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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 new method to specify these conditions are proposed. These conditions are consistent with the boundary condition we proposed in [1] using an idea of bounce-back of non-equilibrium distribution. These conditions give excellent results for the regular LBGK models, and were shown to be second-order accurate by numerical examples. When they are used together with the improved incompressible LBGK model in [2], the simulation results recover the analytical solution of the plane Poiseuille flow driven by pressure (density) difference with machine accuracy.

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]. Besides, theoretical discussion is easier for the LBGK due to its simple form. Some recent theoretical discussions on LBGK [1, 4, 5] have enhanced our understanding of the method and the effect of boundary conditions. In [4], analytical solutions of distribution functions for plane Poiseuille flow with forcing and plane Couette flow have been obtained for the 2-D triangular and square lattice Boltzmann BGK models. It is found that the bounce-back boundary condition produces distribution functions with a first-order error compared with the analytical distribution functions. In [5], a new technique was developed to seek the analytic solution of LBGK model for some simple flow. For example, the velocity profile from the 2-D square and triangular LBGK models are shown to satisfy a second-order difference equation of the Navier-Stokes equation in the case of plane Poiseuille flow with forcing and Couette flow. The technique is generalized in [1] to include steady-state flows with both x and y velocities, which

^{*}Theoretical Division, Los Alamos National Lab, Los Alamos, NM 87545

[†]Dept. of Math., Kansas State University, Manhattan, KS 66506

[‡]Center for Nonlinear Studies, Los Alamos National Lab

[§]Theoretical Biology and Biophysics Group, Los Alamos National Lab

are assumed to be independent of x . The analysis provides a framework to analyze any velocity boundary condition. For example, the analysis explains why the velocity boundary condition for the 2-D triangular LBGK model proposed in [6] generates results of machine accuracy for plane Poiseuille flow with forcing.

In practice, however, a flow is often driven by pressure difference. In general, the pressure gradient through the flow field is not a constant and the local pressure gradient is unknown before solving the flow. Hence 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.

Since in lattice Boltzmann method, the pressure is related to the density by the isothermal equation of state as $p = c_s^2 \rho$ (c_s is the sound speed of the model), 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: the real pressure gradient obtained in the simulation for the Poiseuille flow is not a constant. It is approximately a constant only some distance away from the inlet and outlet of the channel. Besides, even away from the inlet and outlet region, the pressure gradient is different from the intended value. Maier *et al.* [8] proposed an alternative pressure or velocity flow boundary condition for the 3-D 15-velocity direction LBGK model, and their results are greatly improved over the equilibrium distribution approach. The pressure or velocity flow boundary condition in [8] is obtained through a post-streaming rule to the distribution functions based on an extrapolation. However, this pressure or velocity boundary condition is still to be improved due to some inconsistency (see discussion in Section 2). Its inaccuracy is most noticeable in the following case: when this pressure or velocity boundary condition is applied to the modified LBGK [2], which corresponds to a macroscopic momentum equation having the analytical solution of Poiseuille flow with pressure (density) gradient, the simulation results are far from the analytical results.

In this paper, we propose a general way to specify pressure or velocity on flow boundaries. The implementation is a natural extension of the wall boundary condition described in our previous paper [1]. The result shows a clear improvement to the flow boundary conditions in [8] for ordinary LBGK models. Besides, for the modified LBGK model, These flow boundary conditions produce results of machine accuracy for Poiseuille flow.

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

2.1 Governing Equation

The square lattice LBGK model (d2q9) is expressed as ([9],[10],[11]):

$$f_i(\mathbf{x} + \delta \mathbf{e}_i, t + \delta) - f_i(\mathbf{x}, t) = -\frac{1}{\tau} [f_i(\mathbf{x}, t) - f_i^{(eq)}(\mathbf{x}, t)], \quad i = 0, 1, \dots, 8, \quad (1)$$

where the equation is written in physical units. Both the time step and the lattice spacing have the value of δ in physical units. $f_i(\mathbf{x}, t)$ is the density distribution function along the direction \mathbf{e}_i at (\mathbf{x}, t) . The particle speed \mathbf{e}_i 's are given by $\mathbf{e}_i = (\cos(\pi(i-1)/2), \sin(\pi(i-1)/2), i = 1, 2, 3, 4$, and $\mathbf{e}_i = \sqrt{2}(\cos(\pi(i-4-\frac{1}{2})/2), \sin(\pi(i-4-\frac{1}{2})/2), i = 5, 6, 7, 8$. Rest particles of type 0 with $\mathbf{e}_0 = 0$ is also allowed (see Fig. 1). The right hand side represents the collision term and τ is the single relaxation time which controls the rate of approach to equilibrium. The density per node, ρ , and the macroscopic flow velocity, $\mathbf{u} = (u_x, u_y)$, are defined in terms of the particle distribution function by

$$\sum_{i=0}^8 f_i = \rho, \quad \sum_{i=1}^8 f_i \mathbf{e}_i = \rho \mathbf{u}. \quad (2)$$

The equilibrium distribution functions $f_i^{(eq)}(\mathbf{x}, t)$ depend only on local density and velocity and they can be chosen in the following form (the model d2q9 [10]):

$$\begin{aligned} f_0^{(eq)} &= \frac{4}{9}\rho[1 - \frac{3}{2}\mathbf{u} \cdot \mathbf{u}], \\ f_i^{(eq)} &= \frac{1}{9}\rho[1 + 3(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u} \cdot \mathbf{u}], \quad i = 1, 2, 3, 4 \\ f_i^{(eq)} &= \frac{1}{36}\rho[1 + 3(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u} \cdot \mathbf{u}], \quad i = 5, 6, 7, 8. \end{aligned} \quad (3)$$

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):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (4)$$

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

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha(c_s^2 \rho) + \partial_\beta(2\nu \rho S_{\alpha\beta}), \quad (5)$$

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 $p = c_s^2 \rho$, where c_s is the speed of sound with $c_s^2 = \frac{1}{3}$, and $\nu = \frac{2\tau - 1}{6}\delta$, with ν being the kinematic viscosity. The form of the error terms and the derivation of these equations can be found in [12, 13].

In this paper, 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:

$$u_x = u_0(1 - \frac{y^2}{L^2}), \quad u_y = 0, \quad \frac{\partial p}{\partial x} = -G, \quad \frac{\partial p}{\partial y} = 0, \quad (6)$$

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

$$G = 2\rho\nu u_0/L^2, \quad (7)$$

and the flow density ρ is a constant. The Reynolds number is defined as $\text{Re} = u_0(2L)/\nu$.

The Poiseuille flow is an exact solution of the steady-state incompressible Navier-Stokes equations:

$$\nabla \cdot \mathbf{u} = 0. \quad (8)$$

$$\partial_\beta(u_\alpha u_\beta) = -\partial_\alpha\left(\frac{p}{\rho_0}\right) + \nu\partial_{\beta\beta}u_\alpha, \quad (9)$$

On the other hand, the steady-state macroscopic equations of LBGK model, Eq. (1), is given by:

$$\nabla \cdot (\rho \mathbf{u}) = 0, \quad (10)$$

$$\partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha(c_s^2 \rho) + \frac{2\tau-1}{6}\delta\partial_\beta\partial_\beta(\rho u_\alpha). \quad (11)$$

These equations are different from the incompressible Navier-Stokes equations Eqs. (8,9) by terms containing the spatial derivative of ρ . These discrepancies are called compressibility error in LBE model. Thus, the Poiseuille flow given by Eq. (6) is not the exact solution of Eqs. (10, 11) when pressure (density) gradient drives the flow. That is, due to change of pressure (density) in the x -direction, u_x is not constant in the x -direction, and the velocity profile of the solution of Eqs. (10, 11) is no longer a parabolic profile. For a fixed Mach number (u_0 fixed), as $\delta \rightarrow 0$, the velocity of the LBGK simulation will not converge to the velocity in Eq. (6) because the compressibility error becomes dominating. This phenomenon is seen in the result in [8], where the error of velocity increases as the number of lattice grid increases. Besides, from $\partial_x(\rho u_x) = 0$ (suppose $u_y = 0$ in the simulation), one can see that u_x should be increasing linearly along the flow direction since ρ is decreasing linearly. This makes the comparison of u_x with the analytical velocity of Poiseuille flow somehow ambiguous.

To make a more sensible study for Poiseuille flow with pressure (density) or velocity flow boundary condition, it is better to use the improved incompressible LBGK model proposed in [2]. The model (called d2q9i) is given by Eq. (1) with the same \mathbf{e}_i and the following equilibrium distributions:

$$\begin{aligned} f_0^{(eq)} &= \frac{4}{9}[\rho - \frac{3}{2}\mathbf{v} \cdot \mathbf{v}], \\ f_i^{(eq)} &= \frac{1}{9}[\rho + 3\mathbf{e}_i \cdot \mathbf{v} + \frac{9}{2}(\mathbf{e}_i \cdot \mathbf{v})^2 - \frac{3}{2}\mathbf{v} \cdot \mathbf{v}], \quad i = 1, 2, 3, 4, \\ f_i^{(eq)} &= \frac{1}{36}[\rho + 3\mathbf{e}_i \cdot \mathbf{v} + \frac{9}{2}(\mathbf{e}_i \cdot \mathbf{v})^2 - \frac{3}{2}\mathbf{v} \cdot \mathbf{v}], \quad i = 5, 6, 7, 8, \end{aligned} \quad (12)$$

and

$$\sum_{i=0}^8 f_i = \sum_{i=0}^8 f_i^{(eq)} = \rho, \quad \sum_{i=1}^8 f_i \mathbf{e}_i = \sum_{i=1}^8 f_i^{(eq)} \mathbf{e}_i = \mathbf{v}, \quad (13)$$

where $\mathbf{v} = (v_x, v_y)$ (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 $O(\delta^2)$):

$$\nabla \cdot \mathbf{v} = 0, \quad (14)$$

$$\partial_\beta(v_\alpha v_\beta) = -\partial_\alpha(c_s^2 \rho) + \nu\partial_{\beta\beta}v_\alpha, \quad (15)$$

are exactly the steady-state incompressible Navier-Stokes equation. In the model, pressure is related to density by $c_s^2 \rho = p/\rho_0$ ($c_s^2 = 1/3$) for a flow with constant density like Poiseuille flow, and $\nu = \frac{2\tau-1}{6}\delta$.

If the flow is steady, d2q9i is superior to d2q9 to simulating incompressible flows. If the flow is unsteady, one may consider the continuity equation derived from d2q9 given by $\partial_t \rho + (\nabla \cdot \rho) \mathbf{u} + \rho \nabla \cdot \mathbf{u} = 0$. In a situation where the first two terms likely cancel each other, d2q9 may be of advantage (to approximate the continuity equation $\nabla \cdot \mathbf{u}$). If the first two terms have the same sign, then d2q9i is better.

2.2 Review of The Velocity Wall Boundary Condition

It is proved in [1, 5] that if the flow is steady and independent of x , then the solution f_i of Eq. (1) produces a velocity profile that satisfies a difference equation which is a second-order approximation of the Navier-Stokes equation. If the boundary condition is chosen correctly, then the difference equation near the boundary is consistent with the difference equation inside.

A velocity wall boundary condition is proposed in [1] 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 need to determine f_2, f_5, f_6 and ρ from Eqs. (2), which can be put into the form:

$$f_2 + f_5 + f_6 = \rho - (f_0 + f_1 + f_3 + f_4 + f_7 + f_8), \quad (16)$$

$$f_5 - f_6 = \rho u_x - (f_1 - f_3 - f_7 + f_8), \quad (17)$$

$$f_2 + f_5 + f_6 = \rho u_y + (f_4 + f_7 + f_8). \quad (18)$$

Consistency of Eqs. (16,18) gives

$$\rho = \frac{1}{1 - u_y} [f_0 + f_1 + f_3 + 2(f_4 + f_7 + f_8)]. \quad (19)$$

We assume the bounce-back 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 as

$$\begin{aligned} f_2 &= f_4 + \frac{2}{3}\rho u_y, \\ f_5 &= f_7 - \frac{1}{2}(f_1 - f_3) + \frac{1}{2}\rho u_x + \frac{1}{6}\rho u_y, \\ f_6 &= f_8 + \frac{1}{2}(f_1 - f_3) - \frac{1}{2}\rho u_x + \frac{1}{6}\rho u_y. \end{aligned} \quad (20)$$

The collision step is applied to the boundary nodes also. For non-slip boundaries, this boundary condition is reduced to that in [8].

2.3 Specification of Pressure on a Flow Boundary

Now let us turn to pressure (density) flow 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 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:

$$f_1 + f_5 + f_8 = \rho_{in} - (f_0 + f_2 + f_3 + f_4 + f_6 + f_7), \quad (21)$$

$$f_1 + f_5 + f_8 = \rho_{in} u_x + (f_3 + f_6 + f_7), \quad (22)$$

$$f_5 - f_8 = f_2 - f_4 + f_6 - f_7. \quad (23)$$

Consistency of Eqs. (21,22) gives

$$u_x = 1 - \frac{[f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)]}{\rho_{in}}. \quad (24)$$

We use bounce-back 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:

$$\begin{aligned} f_1 &= f_3 + \frac{2}{3}\rho_{in}u_x, \\ f_5 &= f_7 - \frac{1}{2}(f_2 - f_4) + \frac{1}{6}\rho_{in}u_x, \\ f_8 &= f_6 + \frac{1}{2}(f_2 - f_4) + \frac{1}{6}\rho_{in}u_x. \end{aligned} \quad (25)$$

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; ρ is specified, and $u_x = u_y = 0$. We need to determine f_1, f_2, f_5, f_6, f_8 . We use bounce-back rule for the non-equilibrium part of the particle distribution normal to the inlet and the boundary to find:

$$f_1 = f_3 + (f_1^{(eq)} - f_3^{(eq)}) = f_3, \quad f_2 = f_4 + (f_1^{(eq)} - f_3^{(eq)}) = f_4, \quad (26)$$

Using these f_1, f_2 in Eqs. (2), we find:

$$f_5 = f_7, \quad f_6 = f_8 = \frac{1}{2}[\rho_{in} - (f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_7)]. \quad (27)$$

Similar procedure can be applied to top inlet node and outlet nodes including outlet corner nodes. The case that ρ and non-zero u_y is specified at a flow boundary along y -direction can be handled in the same way.

Here, it is useful to compare our pressure boundary condition with that proposed in [8], which is given by the following post-streaming rule (an extrapolation) at inlet: after streaming, f_1, f_5, f_8 are calculated as

$$f_i(\mathbf{x}, t) = f_i^+(\mathbf{x}, t - \delta) - (f_j(\mathbf{x}, t) - f_j^+(\mathbf{x}, t - \delta)), \quad i = 1, 5, 8 \quad (28)$$

where $f_i^+(\mathbf{x}, t - \delta) \equiv f_i(\mathbf{x}, t - \delta) - \frac{1}{\tau}(f_i(\mathbf{x}, t - \delta) - f_i^{(eq)}(\mathbf{x}, t - \delta))$ is the distribution functions at previous time step after collision and before streaming, f_j is along \mathbf{e}_j with $\mathbf{e}_j = \mathbf{e}_i - 2\mathbf{e}_n$ (the inner normal $\mathbf{e}_n = \mathbf{e}_1$ in the case). Thus, for $i = 1, 5, 8$, $j = 3, 6, 7$ respectively. The density ρ is set to the specified inlet value and u_y is set to zero to compute $f_i^{(eq)}(\mathbf{x}, t)$. At the bottom, f_1, f_8 are computed using Eq. (28) and then f_2, f_5, f_6 are obtained in the treatment of wall boundary condition. Notice, however, that at the inlet, $\sum_{i=0}^8 f_i$ may not be equal to the specified density and $\sum_{i=1}^8 e_{iy} f_i$ may not be equal to zero with this post-streaming operation. This inconsistency causes some inaccuracy in simulations and leaves room for improvement.

2.4 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 case of channel flow, after streaming, f_2, f_4, f_3, f_6, f_7 are known at inlet. u_x, u_y

are specified at inlet (for the special case of Poiseuille flow, $u_y = 0$), we need to determine ρ and f_1, f_5, f_8 . This is actually equivalent to a velocity wall boundary condition. Using our velocity wall boundary condition in [1] previously described, we find:

$$\begin{aligned}\rho &= \frac{1}{1 - u_x} [f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)], \\ f_1 &= f_3 + \frac{2}{3}\rho u_x, \\ f_5 &= f_7 - \frac{1}{2}(f_2 - f_4) + \frac{1}{2}\rho u_y + \frac{1}{6}\rho u_x, \\ f_8 &= f_6 + \frac{1}{2}(f_2 - f_4) - \frac{1}{2}\rho u_y + \frac{1}{6}\rho u_x.\end{aligned}\tag{29}$$

The effect of specifying velocity at inlet is similar to specifying pressure (density) at inlet. Density difference in the flow can be 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 bounce-back on normal distributions gives:

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

expressions of x, y momenta give:

$$\begin{aligned}f_5 - f_6 + f_8 &= -(f_1 - f_3 - f_7) = f_7, \\ f_5 + f_6 - f_8 &= -(f_2 - f_4 - f_7) = f_7,\end{aligned}\tag{30}$$

which gives

$$\begin{aligned}f_5 &= f_7, \\ f_6 &= f_8 = \frac{1}{2}[\rho - (f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_7)],\end{aligned}\tag{31}$$

but there is no more equation available to determine ρ . The situation is similar to a corner wall node (the intersection of two perpendicular walls). In the situation, ρ at the inlet bottom node can be taken as the ρ of its neighboring flow node, thus the velocity inlet condition is specified.

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 ρ and unknown f_i 's.
- Given ρ and the velocity along the boundary, find the velocity normal to the boundary and unknown f_i 's.

Eq. (2) is used to determine ρ or the normal velocity and the unknown f_i 's. The formula are given in sections 2.2, 2.3, 2.4.

Again, it is useful to compare our velocity flow boundary condition with that proposed in [8], which is given by the following post-streaming rule (a zeroth-order extrapolation) at inlet: after streaming, f_1, f_5, f_8 are calculated using

$$f_i(\mathbf{x}, t) = f_i^+(\mathbf{x}, t - \delta), \quad i = 1, 5, 8\tag{32}$$

where $f_i^+(\mathbf{x}, t - \delta)$ is the distribution function at previous time step after collision. After ρ is computed using f_i 's, $f_i^{(eq)}(\mathbf{x}, t)$ can be computed using this ρ and the specified velocities u_x, u_y . In this approach, the determination of unknown f_i 's does not use the information of known f_i 's at present time. This is inconsistent with the present distribution in the flow. Suppose that initially, $f_i^{(eq)}$, $i = 0, \dots, 8$ are computed by using some density ρ_0 and the specified u_x, u_y , and one assigns $f_i = f_i^{(eq)}$, $i = 0, \dots, 8$, then collision does not change f_i , and the post-streaming rule Eq. (32) does not change f_i and ρ . Hence $f_i = f_i^{(eq)}$ for all time in the simulation. This velocity inlet condition amounts to assign the equilibrium distribution to f_i and it makes a significant error. The result is worse than that of pressure inlet condition [8].

2.5 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. It is from equations $\sum_{i=0}^8 f_i = \rho$ and $\sum_{i=1}^8 \mathbf{e}_i f_i = \mathbf{v}$ and hence some modifications are needed as follows:

- In wall boundary condition, Eq. (19) is replaced by

$$\rho = v_y - [f_0 + f_1 + f_3 + 2(f_4 + f_7 + f_8)]. \quad (33)$$

and in Eq. (20), $\rho u_x, \rho u_y$ are replaced by v_x, v_y respectively.

- In pressure flow boundary condition, Eq. (24) is replaced by

$$v_x = \rho - [f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)], \quad (34)$$

and in Eq. (25), $\rho_{in} u_x$ is replaced by v_x .

- Similar replacement in velocity flow boundary condition, Eq. (29).

3 Numerical Results and Discussion

We report and discuss the numerical results for Poiseuille flow with pressure (density) or velocity flow boundary condition. The simulation is performed on both models d2q9 and d2q9i. The main result in the simulation of d2q9i is the achievement of machine accuracy. The main result in the simulation of d2q9 is the achievement of second-order accuracy of the boundary conditions. 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 ρ_0 , and zero velocities. The steady-state is reached if

$$\frac{\sum_i \sum_j |u_x(i, j, t + \delta) - u_x(i, j, t)| + |u_y(i, j, t + \delta) - u_y(i, j, t)|}{\sum_i \sum_j |u_x(i, j, t)| + |u_y(i, j, t)|} \leq \delta \cdot Tol.$$

For model d2q9i, u_x, u_y are replaced by v_x, v_y . Tol is a tolerance usually set to 10^{-10} . On the wall, boundary condition discussed in section 2.2 is used to make non-slip boundaries.

We also define a L1 error as:

$$err_1 \equiv \frac{\sum_i \sum_j |u_x^t(i, j) - u_x(i, j)| + |u_y^t(i, j) - u_y(i, j)|}{\sum_i \sum_j |u_x^t(i, j)| + |u_y^t(i, j)|}, \quad (35)$$

where u_x^t, u_y^t is the analytical velocity.

3.1 Results of Model d2q9i

For model d2q9i, we carried out simulations with a variety of Re , nx , ny , u_0 (u_0 is the peak velocity in the channel) using the pressure or velocity flow boundary condition. The range of Re is from 0.0001 to 30.0; the range of τ 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 a pressure gradient of $G = 0.1$. The magnitude of average density ρ_0 is irrelevant for the simulation [2].

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

- The velocity field v_x 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^{-12} . For example, for $nx = 5$, $ny = 3$, $u_0 = 0.1$, $\tau = 0.56$, $Re = 10$, the relative L1 error of \mathbf{v} in the whole flow region is $0.485 \cdot 10^{-10}$.
- The density is uniform in the cross channel direction, and linear in the flow direction. The density difference $\rho(i+1, j) - \rho(i, j)$ is a constant through the flow region, its value is equal (up to machine accuracy) to the analytical value set by the constant pressure gradient.
- Velocity v_x is uniform in the x -direction, the results are the same for different nx .

If the computed velocity were plotted with the analytical velocity, there would be no difference to naked-eyes.

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. For $ny = 5$, the maximum Re is about 30. Refinement of mesh can increase the maximum Re .

When the pressure flow boundary condition is replaced by the method in [8], machine accuracy can no longer be obtained, for a simple case $nx = 17$, $ny = 9$, $u_0 = 0.03542$, $\tau = 0.67$, $Re = 5$, with a moderate pressure gradient of $G = 0.001004$, $\rho_{in} = 5.006$, $\rho_{out} = 4.994$, the relative L1 error of \mathbf{v} in the whole flow region is $0.1824 \cdot 10^{-2}$, with maximum of $|v_y|$ being $0.1364 \cdot 10^{-3}$, not very small compared to u_0 . The density difference $(\rho(i+1, j) - \rho(i, j))/\delta$ is no longer a constant, its range is from -0.002094 to -0.003872 (the analytical value is $-0.003012 = -G/c_s^2 = -3G$). The result indicates that the pressure or velocity flow boundary condition proposed in this paper is a clear improvement of that in [8].

Similar results of 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.

3.2 Results of Model d2q9

Since the ordinary LBGK model d2q9 is still widely used for simulations. It is worthwhile to do some simulations with d2q9 with our flow boundary conditions and show that they give a second-order accuracy. We use d2q9 to Poiseuille flow with pressure or velocity flow boundary condition. Since as $\delta \rightarrow 0$ the computed solution does not approach the analytical solution, we will use the result of the finest mesh as the exact solution to compute the error. Simulations with successively doubled lattice steps are carried out to observe the convergence. The example uses fixed $Re = 10$, $u_0 = 0.1$, $\rho_0 = 5$. The pressure gradient G in Eq. (6) and then pressure (density)

at inlet/outlet can be obtained as $G = 0.02$ and $\rho_{in} = 5.12, \rho_{out} = 4.88$ respectively to be used in the pressure (density) flow boundary condition. For the velocity flow boundary condition, the analytical velocities in Eq. (6) are used at inlet, and ρ_0 is specified at outlet. Thus, the results of the pressure flow boundary condition and the velocity flow boundary condition are similar but not identical. Define $lx = nx - 1, ly = ny - 1$ to represent the number of lattice steps in x - and y -directions, we use $lx = 4, 8, 16, 32, 64, 128, 256, ly = 2, 4, 8, 16, 32, 64, 128$ respectively to do the simulation. The L1 error is defined in Eq. (35) with u_x^t, u_y^t being replaced by the computed velocities of $lx = 256, ly = 128$. τ has to be changed as lx, ly are changed to keep the same Re, u_0 (values of τ are included in Table I). The convergence result is summerized in Table I. The case of $lx = 4, ly = 2$ was not shown in Table I, because the simulation is unstable for the velocity inlet condition. The ratio of two consecutive L1 errors is also shown. The ratio is approximately equal to 4, indicating a second-order accuracy. For all runs, it is also observed that

- Velocity u_x is monotonically increasing in the x -direction, the result is not sensitive to the value of lx , we usually take $lx = 2 \cdot ly$. If the pressure boundary condition in [8] is used, u_x on the centerline of the channel decreases first, then increases, and decreases again near the outlet. This behavior deviates from the macroscopic continuity equation of LBGK $\partial_x(\rho u_x) = 0$ in the case, indicating that errors are introduced by the pressure boundary condition in [8]. An example of centerline velocity u_x as a function of x is presented in Fig. 4.
- u_y is very small compared to u_0 , with maximum of $|u_y|$ being approximately of $10^{-6} \cdot u_0$ in typical cases. If the pressure boundary condition in [8] is used, maximum value of $|u_y|$ is like $10^{-3} \cdot u_0$ typically.
- The density is uniform in the cross channel direction, and linear in the flow direction. The density difference $\rho(i+1, j) - \rho(i, j)$ is almost a constant through the flow region, its value is equal to the analytical value with a fluctuation of less than 0.03 % in a worst case observed with Re= 5. If the pressure boundary condition in [8] is used, The fluctuation of density difference $\rho(i+1, j) - \rho(i, j)$ from the analytical value reaches 20 % for the same case mentioned above with Re = 5.

In the case where the density gradient is small, the computed velocity profile are close to the analytical velocity profile of Poiseuille flow. We present an example here with $nx = 9, ny = 5$, Re=0.8333, $u_0 = 0.008333$, $G = 0.001667$, $\rho_{in} = 5.01, \rho_{out} = 4.99$ with both pressure (density) flow boundary conditions in this paper and in [8]. Fig. 2 shows the velocity u_x as a function of y at $i = 5$ (the middle section of the channel), Fig. 3 shows the centerline density profile along the x direction, and Fig. 4 shows the centerline u_x along the x direction. the solid line represents the corresponding analytical solution and the symbols $\diamond, +$ represent the computed solutions with the pressure boundary conditions in this paper and in [8] respectively. Both computed velocities u_x at the mid-channel has no difference to the analytical solution to naked eyes (the relative error are of order 10^{-3} for both pressure boundary conditions). The computed centerline density with our method looks identical to the analytical solution (given as a linear function crossing ρ_{in} and ρ_{out} at inlet and outlet respectively), while the centerline density with the method in [8] has a discernible difference with the linear function especially near the inlet and outlet. The centerline u_x with our method is monotonically increasing, the behavior is consistent with the continuity equation of LBGK $\partial_x(\rho u_x) = 0$ in the case, while the centerline u_x with the method in [8] has a

behavior inconsistent with the continuity equation near the inlet and outlet. This again shows an clear improvement of our method to that in [8].

4 Flow Boundary Conditions and Preliminary Results for the 3-D 15-velocity LBGK Model

Since 3-D model is needed in practical problems, we give a discussion of the pressure or velocity flow boundary condition for the 3-D 15-velocity LBGK model (d3q15) and present a brief statement about its simulation results. The model is based on the LBGK equation Eq. (1) with $i = 0, 1, \dots, 14$, where $\mathbf{e}_i, i = 0, 1, \dots, 14$ are the column vectors of the following matrix:

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

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

$$\sum_{i=0}^{14} f_i = \rho, \quad \sum_{i=1}^{14} f_i \mathbf{e}_i = \rho \mathbf{u}. \quad (36)$$

The equilibrium can be chosen as:

$$\begin{aligned} f_0^{(eq)} &= \frac{1}{8}\rho - \frac{1}{3}\rho \mathbf{u} \cdot \mathbf{u}, \\ f_i^{(eq)} &= \frac{1}{8}\rho + \frac{1}{3}\rho \mathbf{e}_i \cdot \mathbf{u} + \frac{1}{2}\rho (\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{1}{6}\rho \mathbf{u} \cdot \mathbf{u}, \quad i = I \\ f_i^{(eq)} &= \frac{1}{64}\rho + \frac{1}{24}\rho \mathbf{e}_i \cdot \mathbf{u} + \frac{1}{16}\rho (\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{1}{48}\rho \mathbf{u} \cdot \mathbf{u}, \quad i = II \end{aligned} \quad (37)$$

Since we will use this model for 2-D simulation in this paper, it is clear to give a projection of the velocities in the xz plane as shown in Fig. 1. The y -axis is pointing into the paper, so are velocity directions 3,7,9,12,14, 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). The flow direction is still x , and the cross channel direction is z . 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 velocity wall boundary condition proposed in [1] has the following version for the model d3q15: take the case of a bottom node (wall node) as shown in Fig. 1, the wall is on xy plane. After streaming, $f_i, (i = 0, 1, 2, 3, 4, 6, 8, 9, 12, 13)$ are known, Suppose that u_x, u_y, u_z are specified on the wall, we need to determine $f_i, i = 5, 7, 10, 11, 14$ and ρ from Eqs. (36). Similar to the derivation in d2q9, ρ is determined by a consistency condition as:

$$\rho = \frac{1}{1 - u_z} [f_0 + f_1 + f_2 + f_3 + f_4 + 2(f_6 + f_8 + f_9 + f_{12} + f_{13})]. \quad (38)$$

The expression of z - momentum gives:

$$f_5 + f_7 + f_{10} + f_{11} + f_{14} = \rho u_z + (f_6 + f_8 + f_9 + f_{12} + f_{13}), \quad (39)$$

If we use bounce-back rule for the non-equilibrium part of the particle distribution $f_i, (i = 5, 7, 10, 11, 14)$ to set

$$\begin{aligned} f_i &= f_{i+1} + (f_i^{(eq)} - f_{i+1}^{(eq)}), \quad i = 5, 7, 11 \\ f_i &= f_{i-1} + (f_i^{(eq)} - f_{i-1}^{(eq)}), \quad i = 10, 14 \end{aligned} \quad (40)$$

then Eq. (39) is satisfied, and all f_i are defined. In order to get the correct x -, y -momenta, we further fix this f_5 (bounce-back of non-equilibrium f_i in the normal direction) and modify $f_7, f_{10}, f_{11}, f_{14}$ as in [8]:

$$f_i \leftarrow f_i + \frac{1}{4}e_{ix}\delta_x + \frac{1}{4}e_{iy}\delta_y, \quad i = 7, 10, 11, 14 \quad (41)$$

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

$$\begin{aligned} f_5 &= f_6 + \frac{2}{3}\rho u_z, \\ f_i &= f_j + \frac{1}{12}\rho u_z + \frac{1}{4}[e_{ix}(\rho u_x - f_1 + f_2) + e_{iy}(\rho u_y - f_3 + f_4)], \end{aligned} \quad (42)$$

where j is the index corresponding to $\mathbf{e}_j = -\mathbf{e}_i$ (e.g., $j = 8$ for $i = 7$ and $j = 9$ for $i = 10$). In the case of non-slip boundary, this boundary condition is reduced to that in [8].

The derivation of pressure (density) flow boundary condition uses a similar way as for velocity wall boundary condition. Suppose the boundary (take the case of inlet in Fig. 1) is on yz plane with specified ρ_{in} and $u_y = u_z = 0$. After streaming, we need to determine u_x and $f_i, (i = 1, 7, 9, 11, 13)$ from Eq. (36). The consistency condition gives:

$$\rho_{in}u_x = \rho_{in} - [f_0 + f_3 + f_4 + f_5 + f_6 + 2(f_2 + f_8 + f_{10} + f_{12} + f_{14})], \quad (43)$$

which determines u_x at inlet, using a similar procedure as in deriving the boundary condition, we find:

$$\begin{aligned} f_1 &= f_2 + \frac{2}{3}\rho_{in}u_x, \\ f_i &= f_j + \frac{1}{12}\rho_{in}u_x - \frac{1}{4}[e_{iy}(f_3 - f_4) + e_{iz}(f_5 - f_6)], \quad i = 7, 9, 11, 13 \end{aligned} \quad (44)$$

where j direction is opposite to i direction.

Same procedure as in d2q9 is used at the inlet bottom node (non-slip) to derive:

$$\begin{aligned} f_1 &= f_2, \quad f_5 = f_6, \\ f_7 &= f_8 - \frac{1}{2}(f_3 - f_4), \quad f_{11} = f_{12} + \frac{1}{2}(f_3 - f_4), \\ f_9 &= f_{10} = f_{13} = f_{14} \\ &= \frac{1}{4}[\rho_{in} - (f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7 + f_8 + f_{11} + f_{12})], \end{aligned} \quad (45)$$

and similar results for inlet top and outlet condition.

The pressure (density) boundary condition in [8] is specified as post-streaming rule (take the inlet as an example):

$$f_i(\mathbf{x}, t) = f_i^+(\mathbf{x}, t - \delta) - (f_j(\mathbf{x}, t) - f_j^+(\mathbf{x}, t - \delta)), \quad i = 1, 7, 9, 11, 13 \quad (46)$$

where $f_i^+(\mathbf{x}, t - \delta)$ is the distribution functions at previous time step after collision, f_j is along \mathbf{e}_j with $\mathbf{e}_j = \mathbf{e}_i - 2\mathbf{e}_n$ (the inner normal $\mathbf{e}_n = \mathbf{e}_1$ in the case). Thus, $j = 2, 14, 12, 10, 8$ for $i = 1, 7, 9, 11, 13$ respectively. Then ρ is set to ρ_{in} and u_y, u_z are set to zero to compute $f_i^{(eq)}$. Again, the density and z -momentum from f_i may not be correct, indicating some inconsistency.

The velocity flow boundary condition, which can be viewed simply a velocity wall boundary condition, can be derived similarly. But the corner node with non-slip condition needs some treatment as in the d2q9 case. The details are easy to work out and omitted here.

Simple modifications are used to derive wall boundary condition, pressure (density) or velocity flow boundary condition for the improved incompressible model d3q15i, which is the counterpart of d2q9i in 3-D case.

Simulations on plane Poiseuille flow are performed on d3q15 and d3q15i using the pressure or velocity flow boundary condition. The only difference with 2-D simulations is periodic condition is used on y -direction, and initial condition is uniform in y direction with zero velocity. It is found that the result is uniform in the y -direction and is independent of the number of nodes in y -direction. u_y is identically zero (in the order of 10^{-16} because of round-off error). The results are very similar, although not identical, to the results of d2q9, d2q9i. Again, d3q15i with our boundary condition and pressure (density) flow boundary condition gives results with machine accuracy, showing a clear improvement over the pressure boundary condition in [8].

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Table I. L1 relative error of velocities as lx, ly are doubled, $Re=10$, $u_0 = 0.1$ with our pressure or velocity flow boundary condition. Error are from comparison with the velocities of $lx = 256, ly = 128$ ($\tau = 4.34$). The symbol (-2) represents 10^{-2} . Ratio of two consecutive L1 errors is also shown.

inlet condition	lx ly τ	8 4 0.62	16 8 0.74	32 16 0.98	64 32 1.46	128 64 2.42
pressure (density)	L1 error ratio	0.1049(-2) 4.159	0.2522(-3) 4.110	0.6135(-4) 4.208	0.1458(-4) 5.003	0.2915(-5)
velocity	L1 error ratio	0.2301(-3) 4.713	0.4882(-4) 4.183	0.1167(-4) 4.207	0.2774(-5) 4.970	0.5582(-6)

6 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, 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).

Fig. 2, Velocity u_x as a function of y at $i = 5$ (the middle section of the channel) for the case $nx = 9, ny = 5$, $Re=0.8333$, $u_0 = 0.008333$, $G = 0.001667$, $\rho_{in} = 5.01, \rho_{out} = 4.99$ with pressure (density) flow boundary conditions. The solid line represents the corresponding analytical solution of Poiseuille flow. The symbols $\diamond, +$ represent the computed solutions with the pressure flow boundary conditions in this paper and in [8] respectively.

Fig. 3, Centerline density profile along the x direction for the case $nx = 9, ny = 5$, $Re=0.8333$, $u_0 = 0.008333$, $G = 0.001667$, $\rho_{in} = 5.01, \rho_{out} = 4.99$ with pressure (density) flow boundary condition. The solid line represents the corresponding analytical solution (a linear function crossing ρ_{in} and ρ_{out} at inlet and outlet respectively). The symbols $\diamond, +$ represent the computed solutions with the pressure flow boundary conditions in this paper and in [8] respectively.

Fig. 4, Centerline u_x along the x direction for the case $nx = 9, ny = 5$, $Re=0.8333$, $u_0 = 0.008333$, $G = 0.001667$, $\rho_{in} = 5.01, \rho_{out} = 4.99$ with pressure (density) flow boundary condition. The solid line represent the analytical solution of Poiseuille flow. The symbols $\diamond, +$ represent the computed solutions with the pressure flow boundary conditions in this paper and in [8] respectively.







