

Analysis and boundary condition of the lattice Boltzmann BGK model with two velocity components

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Abstract

In this paper, we study the two dimensional lattice Boltzmann BGK model (LBGK) by analytically solving a simple flow in a 2 -D channel. The flow is driven by the movement of upper boundary with vertical injection fluid at the porous boundaries. The velocity profile is shown to satisfy a second-order finite-difference form of the simplified incompressible Navier-Stokes equation. With the analysis, different boundary conditions can be studied theoretically. A momentum exchange principle is also revealed at the boundaries. A general boundary condition for any given velocity boundary is proposed based on the analysis.

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1 Introduction

The lattice Boltzmann equation (LBE) method has become a promising tool for simulation of transport phenomena in recent years. Great success has been achieved in applying LBE for various flow problems such as hydrodynamics [1, 2, 3, 4], flow through porous media [5, 6, 7], magnetohydrodynamics [8, 9, 10], multiphase flow [5, 6, 11, 12, 13, 14], reaction-diffusion equation [15], and particle suspensions [16]. Compared to its precursor, the lattice gas automata (LGA), LBE method is more computationally efficient using current parallel computers, and some artifacts like non-Galilean invariance in LGA can be eliminated in LBE. Careful qualitative comparisons of LBE with traditional computational fluid dynamics methods showed that the method is accurate, and capable of simulating complex phenomena [3, 4, 17, 18, 19].

Although it has been proved [20, 21, 22, 18] that the LBE recovers the Navier-Stokes equation with a second-order of accuracy in space and time in the interior of flow domain, the real hydrodynamic boundary conditions have not been well studied. The no-slip condition on the wall is one of the examples. The classical model for the non-moving wall boundary condition in LBE is the so-called bounce-back rule borrowed from the LGA method. Under the bounce-back rule, all the particles colliding with walls bounce back to the flow domain in the same direction. Theoretical discussion and computational experience indicate that the bounce-back rule actually gives a zero velocity half way between the bounce back row and the first row in the flow and it introduces an error of first-order in lattice spacing for LGA and LBE [23, 24, 18]. To solve this problem, various boundary conditions [25, 26] have been proposed to replace the bounce-back rule and progress has been made. In [25], a boundary condition for the triangular (FHP) LBGK model was proposed for any given velocity boundary, the boundary condition generated results of machine accuracy for plane Poiseuille flow. In [26], a non-slip boundary condition and prescribed pressure or velocity inlet condition for the 3-D 15-velocity direction LBGK model were proposed and results of good accuracy for various flows are achieved. However, due to the lack of the fundamental physical reasoning and the lack of mathematical analysis, these schemes have not revealed the general nature of boundary conditions.

Recently we have developed [27] a new technique to analytically solve the LBGK equation for 2-D Poiseuille flow and Couette flow. This technique provides us a useful tool to analyze the error generated by various boundary conditions. In this study, we will extend our effort to include a flow with velocities in both directions. In addition, a general boundary condition for any given velocity straight boundary is proposed.

2 Governing Equation

In this study, we will only use the square lattice LBGK model. The procedure can be easily extended to the triangular lattice model, for which study is easier due to the smaller number of velocity directions than that of the square model.

The model is expressed as:

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

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 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. 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, $\mathbf{u} = (u, v)$, 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 [21]):

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

Assume the flow is steady and

$$\frac{\partial u}{\partial x} = 0, \quad \frac{\partial v}{\partial x} = 0, \quad \rho = \text{const}, \quad (4)$$

then $f_i(\mathbf{x}, t)$ is only a function of y . This happens when the flow is driven by boundaries moving in the x -direction with injection in the y -direction from the porous boundaries (see Fig. 1). From Eq. (1) we have

$$\begin{aligned} f_0^j &= \frac{4\rho}{9}[1 - 1.5(u_j^2 + v_j^2)] \\ f_1^j &= \frac{\rho}{9}[1 + 3u_j + 3u_j^2 - 1.5v_j^2] \\ f_2^j &= \frac{\rho}{9\tau}[1 + 3v_{j-1} + 3v_{j-1}^2 - 1.5u_{j-1}^2] + (1 - \frac{1}{\tau}) f_2^{j-1} \\ f_3^j &= \frac{\rho}{9}[1 - 3u_j + 3u_j^2 - 1.5v_j^2] \\ f_4^j &= \frac{\rho}{9\tau}[1 - 3v_{j+1} + 3v_{j+1}^2 - 1.5u_{j+1}^2] + (1 - \frac{1}{\tau}) f_4^{j+1} \\ f_5^j &= \frac{\rho}{36\tau}[1 + 3u_{j-1} + 3v_{j-1} + 3u_{j-1}^2 + 3v_{j-1}^2 + 9u_{j-1}v_{j-1}] + (1 - \frac{1}{\tau}) f_5^{j-1} \\ f_6^j &= \frac{\rho}{36\tau}[1 - 3u_{j-1} + 3v_{j-1} + 3u_{j-1}^2 + 3v_{j-1}^2 - 9u_{j-1}v_{j-1}] + (1 - \frac{1}{\tau}) f_6^{j-1} \\ f_7^j &= \frac{\rho}{36\tau}[1 - 3u_{j+1} - 3v_{j+1} + 3u_{j+1}^2 + 3v_{j+1}^2 + 9u_{j+1}v_{j+1}] + (1 - \frac{1}{\tau}) f_7^{j+1} \\ f_8^j &= \frac{\rho}{36\tau}[1 + 3u_{j+1} - 3v_{j+1} + 3u_{j+1}^2 + 3v_{j+1}^2 - 9u_{j+1}v_{j+1}] + (1 - \frac{1}{\tau}) f_8^{j+1}, \end{aligned} \quad (5)$$

where f_i^j stands for the density distribution along the direction \mathbf{e}_i at $y = j\delta$.

According to Eqs. (2, 6), the x -momentum can be expressed as

$$\begin{aligned}
\rho u_j &= f_1^j - f_3^j + f_5^j - f_6^j - f_7^j + f_8^j \\
&= \frac{2\rho}{3}u_j + \frac{\rho}{6\tau}[u_{j-1} + u_{j+1}] + \frac{\rho}{2\tau}[u_{j-1}v_{j-1} - u_{j+1}v_{j+1}] \\
&\quad + (1 - \frac{1}{\tau})[f_5^{j-1} - f_6^{j-1} - f_7^{j+1} + f_8^{j+1}] \\
&= \frac{2\rho}{3}u_j + \frac{\rho}{6\tau}[u_{j-1} + u_{j+1}] + \frac{\rho}{2\tau}[u_{j-1}v_{j-1} - u_{j+1}v_{j+1}] \\
&\quad + (1 - \frac{1}{\tau})[\rho u_{j-1} + \rho u_{j+1} - (f_1^{j-1} - f_3^{j-1} - f_7^{j-1} + f_8^{j-1}) \\
&\quad - (f_1^{j+1} - f_3^{j+1} + f_5^{j+1} - f_6^{j+1})] \\
&= \frac{2\rho}{3}u_j + \frac{\rho}{6\tau}[u_{j-1} + u_{j+1}] + \frac{\rho}{2\tau}[u_{j-1}v_{j-1} - u_{j+1}v_{j+1}] \\
&\quad + \frac{1}{3}(1 - \frac{1}{\tau})[\rho u_{j-1} + \rho u_{j+1} - \rho u_j].
\end{aligned} \tag{6}$$

which further gives us

$$\frac{u_{j+1}v_{j+1} - u_{j-1}v_{j-1}}{2\delta} = \nu \frac{u_{j+1} + u_{j-1} - 2u_j}{\delta^2}, \tag{7}$$

where $\nu = (2\tau - 1)\delta/6$ is the kinematic viscosity of the fluid [18]. The above equation is exactly the second-order finite-difference form of the simplified incompressible Navier-Stokes equation under the assumption Eq. (4) and constant pressure:

$$\frac{\partial(uv)}{\partial y} = \nu \frac{\partial^2 u}{\partial y^2} \tag{8}$$

In the y -direction, it is easy to prove that

$$v_j = \text{const.} \tag{9}$$

This result is obvious for an incompressible flow under the assumption Eq.(4).

3 Boundary Condition

The derivation of Eq. (6) is for the interior of the flow. The same procedure can be used to derive the relationship of velocities near the wall. For example, at $j = 1$ (near the bottom of the flow region), we have

$$\begin{aligned}
\rho u_1 &= f_1^1 - f_3^1 + f_5^1 - f_6^1 - f_7^1 + f_8^1 \\
&= \frac{2\rho}{3}u_1 + \frac{\rho}{6\tau}[u_0 + u_2] + \frac{\rho}{2\tau}[u_0v_0 - u_2v_2] + (1 - \frac{1}{\tau})[f_5^0 - f_6^0 - f_7^2 + f_8^2] \\
&= \frac{2\rho}{3}u_1 + \frac{\rho}{6\tau}[u_0 + u_2] + \frac{\rho}{2\tau}[u_0v_0 - u_2v_2] \\
&\quad + (1 - \frac{1}{\tau})[\rho \tilde{u}_0 + \rho u_2 - (f_1^0 - f_3^0 - f_7^0 + f_8^0) - (f_1^2 - f_3^2 + f_5^2 - f_6^2)] \\
&= \frac{2\rho}{3}u_1 + \frac{\rho}{6\tau}[u_0 + u_2] + \frac{\rho}{2\tau}[u_0v_0 - u_2v_2] + \frac{1}{3}(1 - \frac{1}{\tau})[\rho u_0 + \rho u_2 - \rho u_1] + \\
&\quad (1 - \frac{1}{\tau})\rho[\tilde{u}_0 - u_0],
\end{aligned} \tag{10}$$

where $\tilde{u}_0 \equiv (f_1^0 - f_3^0 + f_5^0 - f_6^0 - f_7^0 + f_8^0)/\rho$. In the above derivation, it is assumed that equilibrium distributions at the boundary are calculated by using u_0, v_0 . Eq. (10) further gives

$$\frac{u_2 v_2 - u_0 v_0}{2\delta} = \nu \frac{u_2 + u_0 - 2u_1}{\delta^2} + \frac{\tau - 1}{\delta} [\tilde{u}_0 - u_0]. \quad (11)$$

Notice that \tilde{u}_0 may not be equal to u_0 for a specific boundary condition. Therefore, for any $\tau \neq 1$ and $\tilde{u}_0 \neq u_0$, the velocity no longer satisfies the second-order difference equation Eq. (7) at the fluid layer closest to the wall. Nevertheless, if we carefully choose a boundary condition to force $\tilde{u}_0 = u_0$, the velocities will satisfy the same second-order difference equation as an approximation of the Navier-Stokes equation.

Similarly, near the top of the region, we have an equation:

$$\frac{u_n v_n - u_{n-2} v_{n-2}}{2\delta} = \nu \frac{u_n + u_{n-2} - 2u_{n-1}}{\delta^2} + \frac{\tau - 1}{\delta} [\tilde{u}_n - u_n], \quad (12)$$

where $\tilde{u}_n \equiv (f_1^n - f_3^n + f_5^n - f_6^n - f_7^n + f_8^n)/\rho$. Again, the velocities will satisfy the same second-order difference equation if $\tilde{u}_n = u_n$.

The above restriction to \tilde{u}_0 (as well as \tilde{u}_n) has a profound physical meaning. If we analyze the momentum exchange between a wall and its nearest fluid layer, we have (note that the streaming step is applied to the f_i after relaxation)

$$\begin{aligned} \Delta M &= f_5^1 - f_6^1 - (f_8^0 - f_7^0) \\ &= (1 - \frac{1}{\tau})[f_5^0 - f_6^0] + \frac{\rho}{6\tau}(u_0 + 3u_0 v_0) - (f_8^0 - f_7^0) \\ &= f_5^1 - f_6^1 - (1 - \frac{1}{\tau})[f_8^1 - f_7^1] - \frac{\rho}{6\tau}(u_1 - 3u_1 v_1). \end{aligned}$$

Addition of the last two equations gives

$$\begin{aligned} 2\Delta M &= \Delta M + (1 - \frac{1}{\tau})[f_5^0 - f_6^0 - (f_8^1 - f_7^1)] - \frac{\rho}{6\tau}(u_1 - u_0) + \frac{\rho}{2\tau}(u_1 v_1 + u_0 v_0) \\ &= (2 - \frac{1}{\tau})\Delta M - \frac{1}{6}(2 - \frac{1}{\tau})(u_1 - u_0) + \frac{\rho}{2\tau}(u_1 v_1 + u_0 v_0) + \\ &\quad (1 - \frac{1}{\tau})\rho(\tilde{u}_0 - u_0), \end{aligned} \quad (13)$$

or

$$\Delta M = -\rho\nu \frac{u_1 - u_0}{\delta} + \frac{\rho}{2}(u_1 v_1 + u_0 v_0) + (\tau - 1)\rho(\tilde{u}_0 - u_0). \quad (14)$$

where $(u_1 - u_0)/\delta \approx \partial u/\partial y$ near the wall. If $\tilde{u}_0 = u_0$, this is the statement that the momentum exchange calculated from the exchange of f_i 's is equal to the momentum exchange carried by vertical velocity plus the viscous force. This is a momentum exchange principle. Obviously, for any $\tau \neq 1$, if a specific boundary conditions gives $\tilde{u}_0 \neq u_0$, it gives the wrong momentum exchange between a wall and its nearest fluid neighbor. In other words, in order to guarantee the correct momentum exchange, one must choose a boundary condition in which $\tilde{u}_0 = u_0$ is satisfied.

The same conclusion can be drawn for boundary condition in the vertical direction. Although we have shown in the last section that $v_j = \text{const}$ in the interior of flow domain,

this constant does not necessarily equal to the vertical velocity at boundaries. For instance, at $j = 1$, we have

$$\begin{aligned}\rho v_1 &= f_2^1 - f_4^1 + f_5^1 + f_6^1 - f_7^1 - f_8^1 \\ &= \frac{\rho}{2\tau}[v_0 + v_2] + \frac{\rho}{2\tau}[v_0^2 - v_2^2] + (1 - \frac{1}{\tau})\rho[\tilde{v}_0 + v_2 - v_1]\end{aligned}$$

or

$$(2\tau - 1)(v_0 - v_1) + (v_0^2 - v_1^2) + 2(\tau - 1)(\tilde{v}_0 - v_0) = 0, \quad (15)$$

where $\tilde{v}_0 \equiv (f_2^0 - f_4^0 + f_5^0 + f_6^0 - f_7^0 - f_8^0)/\rho$. Obviously for any $\tau \neq 1$, the mass conservation is satisfied near the boundary ($v_1 = v_0$) if and only if $\tilde{v}_0 - v_0 = 0$.

Based on the analysis given above, we propose a boundary condition for a straight boundary with given velocity u_0, v_0 for the square lattice. We will illustrate this at the bottom boundary ($j = 0$) as an example. After streaming, $f_0^0, f_1^0, f_3^0, f_4^0, f_7^0, f_8^0$ are known, and f_2^0, f_5^0, f_6^0 , hence ρ , need to be defined.

- Step 1: Calculation of the density ρ .

The restrictions on the boundary velocity and density discussed above state that

$$\rho = f_0^0 + f_1^0 + f_2^0 + f_3^0 + f_4^0 + f_5^0 + f_6^0 + f_7^0 + f_8^0, \quad (16)$$

$$\rho u_0 = f_1^0 - f_3^0 + f_5^0 - f_6^0 - f_7^0 + f_8^0, \quad (17)$$

$$\rho v_0 = f_2^0 - f_4^0 + f_5^0 + f_6^0 - f_7^0 - f_8^0, \quad (18)$$

Comparison of Eqs. (16, 18) gives ρ as:

$$\rho = \frac{1}{1 - v_0}[f_0^0 + f_1^0 + f_3^0 + 2(f_4^0 + f_7^0 + f_8^0)]. \quad (19)$$

- Step 2: Equilibrium part of the unknown distributions.

From the given boundary velocity and the density calculated in step 1, we can calculate the equilibrium part of the distributions f_2^0, f_5^0, f_6^0 by using Eq. (4).

- Step 3: Non-equilibrium part of the unknown distributions.

Substitution of $f_i = f_i^{0(eq)} + f_i^{0'}$, $i = 1, \dots, 8$ into Eqs. (17, 18) gives

$$f_5^{0'} - f_6^{0'} = -(f_1^{0'} - f_3^{0'} - f_7^{0'} + f_8^{0'}), \quad (20)$$

$$f_5^{0'} + f_6^{0'} = -(f_2^{0'} - f_4^{0'} - f_7^{0'} - f_8^{0'}), \quad (21)$$

where $f_i^{0'}$ is the non-equilibrium distribution part of f_i^0 .

Furthermore, 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, $f_2^{0'} = f_4^{0'}$). Under this condition, the other two undefined non-equilibrium distributions can be uniquely determined

$$f_5^{0'} = f_7^{0'} - 0.5(f_1^{0'} - f_3^{0'}), \quad (22)$$

$$f_6^{0'} = f_8^{0'} + 0.5(f_1^{0'} - f_3^{0'}). \quad (23)$$

The introduction of non-equilibrium part is only for the purpose of discussion of the method, the non-equilibrium part need not be calculated explicitly. In summary, the final form of the unknown distributions from steps 2,3 can be determined as

$$f_2^0 = f_4^0 + \frac{2\rho v_0}{3}, \quad (24)$$

$$f_5^0 = f_7^0 - 0.5(f_1^0 - f_3^0) + \frac{\rho u_0}{2} + \frac{\rho v_0}{6}, \quad (25)$$

$$f_6^0 = f_8^0 + 0.5(f_1^0 - f_3^0) - \frac{\rho u_0}{2} + \frac{\rho v_0}{6}. \quad (26)$$

Once all the after-streaming distributions at the boundary are determined, the collision step can be easily applied to all nodes including the boundary nodes.

The above procedures have specified a new boundary condition for any given velocity straight boundary. This boundary condition produces the velocity profile of the exact solution for the plane Poiseuille flow with forcing [27]. For the special flow with Eq. (4), this boundary condition yields the correct velocity profile as the solution of the difference equation Eqs. (7, 11, 12) under the condition $\tilde{u}_0 = u_0$, and $\tilde{u}_n = u_n$ (the formula of the velocity profile is given in the following section).

4 Velocity Profile

The governing equation for the velocity profile Eq. (7) can be solved under different tangent velocities at upper and bottom boundaries. For simplicity, we assume $v_j = v_0 = \text{const}$, and u_0 and u_n are given. Eq. (7) can be written as

$$(2 - R)u_{j+1} - 4u_j + (2 + R)u_{j-1} = 0, \quad (27)$$

where $R \equiv v_0\delta/\nu$. Assuming a solution of the form

$$u_j = \lambda^j, \quad (28)$$

we have a quadratic equation for λ :

$$(2 - R)\lambda^2 - 4\lambda + (2 + R) = 0, \quad (29)$$

which has two solutions:

$$\lambda_0 = 1, \quad \lambda_1 = \frac{2 + R}{2 - R}. \quad (30)$$

The general solution of Eq. (27) is:

$$u_j = a\lambda_1^j + b, \quad j = 1, \dots, n - 1, \quad (31)$$

where a, b are some constants. The corresponding difference equations near bottom and top boundaries, Eqs. (11, 12), are used to determine a, b . These two equations can be written in the following way:

$$(2 - R)u_2 - 4u_1 + (2 + R)u_0 + \epsilon_0 = 0, \quad \text{where } \epsilon_0 \equiv \frac{12(\tau - 1)}{2\tau - 1}(\tilde{u}_0 - u_0), \quad (32)$$

$$(2 - R)u_n - 4u_{n-1} + (2 + R)u_{n-2} + \epsilon_n = 0, \quad \text{where } \epsilon_n \equiv \frac{12(\tau - 1)}{2\tau - 1}(\tilde{u}_n - u_n), \quad (33)$$

Substituting the general solution in Eq. (31) into Eqs. (32, 33) yields a linear system of equations for a, b , and solving them finally gives the solution:

$$u_j = \frac{\lambda_1^j - 1}{\lambda_1^n - 1} u_n + \frac{\lambda_1^n - \lambda_1^j}{\lambda_1^n - 1} u_0 + \frac{\lambda_1^n - \lambda_1^j}{\lambda_1^n - 1} \frac{\epsilon_0}{2 + R} + \frac{\lambda_1^j - 1}{\lambda_1^n - 1} \frac{\epsilon_n}{2 - R}. \quad (34)$$

The last two term represents the error introduced at the boundaries if $\tilde{u}_0 \neq u_0$ or $\tilde{u}_n \neq u_n$. For the boundary condition introduced in Section 3, $\tilde{u}_0 = u_0, \tilde{u}_n = u_n$, hence $\epsilon_0 = \epsilon_n = 0$.

In the special case of $\tilde{u}_0 = u_0 = 0$ and $\tilde{u}_n = u_n = U$, the solution becomes:

$$\frac{u_j}{U} = \frac{\lambda_1^j - 1}{\lambda_1^n - 1}. \quad (35)$$

It is easy to prove that this solution is a second-order approximation of the analytical solution

$$\frac{u}{U} = \frac{e^{\text{Re } y/L} - 1}{e^{\text{Re}} - 1}, \quad (36)$$

where Re is the Reynolds number defined as $\text{Re} = v_0 L / \nu$ with L being the width of the flow region.

5 Discussion

It is shown in the paper that the flow velocity from the 2D LBGK simulation in the injected porous boundary case satisfies a second-order difference formula as an approximation of the Navier-Stokes equation. This gives us a better understanding of the LBGK method. The velocity formula near boundaries are consistent with the velocity formula inside the flow domain if the boundary condition is such that the distribution functions at the boundary give the correct boundary velocity and thereafter the momentum exchange principle is satisfied. A boundary condition for any given velocity boundary for the 2D square lattice LBGK model can be proposed based on the analysis in this paper. This boundary condition can be easily extended to the 3D 15-velocity direction model.

For the triangular lattice, the boundary condition proposed by Nobel *et al.* [25] gives the correct boundary velocity. It uses three equations: $\sum_{i=0}^6 f_i = \rho$, and $\sum_{i=1}^6 f_i \mathbf{e}_i = \rho \mathbf{u}$ at a boundary node to determine three unknowns: ρ and two f_i 's which are not defined after the streaming step (for example, f_2, f_3 at the bottom boundary). The technique does not have an immediate extension to the square lattice because the number of unknowns on the boundary in the square lattice is larger than the number of restricting equations. For the 3D 15-velocity direction lattice, Maier *et al.* [26] proposed a boundary condition for solid boundary (can be easily extended to the case with boundaries with tangential velocities). First, the bounce-back is used to find the unknown f_i 's, hence the normal velocity is zero and the density and tangent velocity at the wall node can be calculated, then the f_i 's, which are on the directions pointing into the flow and have a non-zero projection on the wall, will be adjusted to correct the tangent velocity while keeping the normal velocity and density unchanged. In the case where the normal velocity is zero, the boundary condition

proposed in this paper is reduced to that proposed by Maier *et al.*. In the case where the normal velocity is non-zero, the boundary condition in this paper can be extended to the 3D 15-velocity direction lattice. In the present discussion, analysis of the velocity profile is also given and the analysis provides a framework to study any boundary condition theoretically.

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References

- [1] S. Succi, R. Benzi and F. Higuera, “The lattice Boltzmann equation: a new tool for computational fluid dynamics,” *Physica D* **47**, 219, (1991).
- [2] S. Chen, Z. Wang, X. Shan and G.D. Doolen, “Lattice Boltzmann computational fluid dynamics in three dimensions,” *J. Stat. Phys.* **68**, 379 (1992).
- [3] G. McNamara and B. Alder, “Lattice Boltzmann simulation of high Reynolds number fluid flow in two dimensions,” *Microscopic Simulations of Complex Hydrodynamic Phenomena*, edited by M. Mareschal and B.L. Holien, (Plenum, New York, 1992).
- [4] D.O. Martinez W.H. Matthaeus, S. Chen and D.C. Montgomery, “Comparison of spectral method and lattice Boltzmann simulations of two-dimensional hydrodynamics,” *Phys. Fluids*, **6** (3), 1285 (1994).
- [5] A.K. Genstensen, PhD thesis, Massachusetts Institute of Technology, 1992.
- [6] A.K. Genstensen and D.H. Rothman, “Microscopic modeling of immiscible fluids in three dimensions by a lattice-Boltzmann method,” *Europhys. Lett.* **18**(2), 157 (1992).
- [7] D.W. Grunau PhD Thesis, Colorado State University, 1993.
- [8] S. Chen, H. Chen, D.O. Martinez and W.H. Matthaeus, “Lattice Boltzmann model for simulation of magnetohydrodynamics,” *Phys. Rev. Lett.*, **67**, 3776 (1991).
- [9] S. Succi, M. Vergassola and R. Benzi, “Recent advances in the theory of the lattice Boltzmann equation,” *Phys. Rev. A*, **43**, 4521 (1991).
- [10] D.O. Martinez, S. Chen and W.H. Matthaeus, “Lattice Boltzmann magnetohydrodynamics,” *Phys. Plasmas*, **1** (6), 1994.
- [11] D. Grunau, S. Chen and K. Eggert, “A lattice-Boltzmann model for multiphase fluid flows,” *Phys. Fluids A* **5**, 2557 (1993).
- [12] X. Shan and H. Chen, “Lattice Boltzmann model for simulating flows with multiple phases and components,” *Phys. Rev. E* **47** (3), 1815 (1993).
- [13] X. Shan and H. Chen, “Simulation of nonideal gases and liquid-gas phase transitions by the lattice Boltzmann equation,” *Phys. Rev. E* **49** (4), 49 (1994).
- [14] D. Rothman and S. Zaleski, “Lattice-gas models of phase separation: interfaces, phase transitions, and multiphase flow,” *Rev. Modern Phys.*, **66**, 1417 (1994).
- [15] S. Ponce-Dawson, S. Chen, and G.D. Doolen, “Lattice Boltzmann computations for reaction-diffusion equations,” *J. Chem. Phys.* **98**, 1514 (1993).
- [16] A.J.C. Ladd, “Numerical simulations of particulate suspensions via a discretized Boltzmann equation. Part 1. Theoretical foundation”, *J. Fluid Mech.* **271**, 285 (1994).

- [17] M.B. Reider and J.D. Sterling, “Accuracy of Discrete-Velocity BGK Models for the Simulation of the Incompressible Navier-Stokes Equations”, to appear in *Computers and Fluids* (1994).
- [18] S. Hou, Q. Zou, S. Chen, G. D. Doolen, and A. C. Cogley, “Simulation of cavity flow by the lattice Boltzmann method,” *J. Comp. Phys.* **118**, 329 (1995).
- [19] S. Hou, Q. Zou, S. Chen, G. D. Doolen, and A. C. Cogley, “A lattice Boltzmann simulation for 3D cavity flow”, preprint, 1995.
- [20] H. Chen, S. Chen, and W. H. Matthaeus, “Recovery of Navier-Stokes equations using a lattice-gas Boltzmann method,” *Phys. Rev. A* **45**, 5771 (1992).
- [21] Y. Qian, D. d’Humières and P. Lallemand, “Recovery of Navier-Stokes equations using a lattice-gas Boltzmann method,” *Europhys. Lett.* **17** (6), 479 (1992).
- [22] Y. H. Qian and S. A. Orszag, “Lattice BGK models for Navier-Stokes equation,” *Europhys. Lett.* **21** (3), 255 (1993).
- [23] R. Cornubert, D. d’Humières and D. Levermore, “A Knudsen layer theory for lattice gases,” compressible regimes,” *Physica D* **47** (6), 241 (1991).
- [24] I. Ginzbourg and P.M. Adler, “Boundary flow condition analysis for the three-dimensional lattice Boltzmann model,” *J. Phys. II, France* **4**, 191 (1994).
- [25] D.R. Noble, S. Chen, J.G. Georgiadis, R.O. Buckius, “A consistent hydrodynamic boundary condition for the lattice Boltzmann method,” *Phys. Fluids* **7**, 203 (1995).
- [26] R. S. Maier, R. S. Bernard and D. W. Grunau, “Boundary conditions for the lattice Boltzmann method”, preprint (1995).
- [27] X. He, L.S. Luo and M. Dembo, “Analytic solutions of simple flows and hydrodynamic boundary conditions of the lattice Boltzmann BGK equation”, preprint (1995).

7 Figure Caption

Schematic plot of flow driven by the movement of upper boundary with vertical injection fluid at the porous boundaries. Also included is a 9-bit square lattice used in this paper.

