Improved treatment of the open boundary in the method of lattice Boltzmann equation

Dazhi Yu, Renwei Mei and Wei Shyy
Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, FL 32611-6250 USA

Abstract: The method of lattice Boltzmann equation (LBE) is a kinetic-based approach for fluid flow computations. In LBE, the distribution functions on various boundaries are often derived approximately. In this paper, the pressure interaction between an inlet boundary and the interior of the flow field is analysed when the bounce-back condition is specified at the inlet. It is shown that this treatment reflects most of the pressure waves back into the flow field and results in a poor convergence towards the steady state or a noisy flow field. An improved open boundary condition is developed to reduce the inlet interaction. Test results show that the new treatment greatly reduces the interaction and improves the computational stability and the quality of the flow field.

Keywords: lattice Boltzmann equation; boundary condition; inlet; bounce-back.


Biographical notes: Dazhi Yu received his PhD in Aerospace from University of Florida. He is now a Postdoctoral Research Associate in Aerospace Department at Texas A&M University. His research interests include lattice Boltzmann method, parallel computation, and turbulence.

Renwei Mei is Professor of the Department of Mechanical and Aerospace Engineering at University of Florida. His research areas include particle dispersion and collision in turbulence, boiling heat transfer and two-phase flow, lattice Boltzmann method, and desalination. He is interested in applying computational methods and applied mathematics to solve practical thermal fluid problem.

Wei Shyy is currently Professor and Chairman of the Department of Mechanical and Aerospace Engineering at University of Florida (UF). He is the author or a coauthor of three books dealing with computational and modelling techniques involving fluid flow, interfacial dynamics, and moving boundary problems. He has written papers dealing with computational and modelling issues related to fluid dynamics, heat/mass transfer, combustion, material processing, parallel computing, biological flight and aerodynamics, design optimisation, micro-scale and biofluid dynamics.
1 INTRODUCTION

1.1 General description of the method

Since the last two decades or so, there has been a rapid progress in developing the method of the lattice Boltzmann equation (LBE) as an alternative, computational technique for solving a variety of complex fluid dynamic systems [1–16]. Adopting the macroscopic method for computational fluid dynamics (CFD), macroscopic variables of interest, such as velocity \( \mathbf{u} \) and pressure \( p \), are usually obtained by solving the Navier-Stokes (NS) equations (e.g., see [17,18]). In the LBE approach, one solves the kinetic equation for the particle velocity distribution function \( f(\mathbf{x},\mathbf{\xi},t) \), where \( \mathbf{\xi} \) is the particle velocity vector, \( \mathbf{x} \) is the spatial position vector, and \( t \) is the time. The macroscopic quantities (such as mass density \( \rho \) and momentum density \( \rho \mathbf{u} \)) can then be obtained by evaluating the hydrodynamic moments of the distribution function \( f \). Lattice gas automata, the predecessor of LBE, were first proposed by Frisch et al. [19]. The theoretical foundation of LBE was established in the subsequent papers, notably in McNamara and Zanetti [20], Higuera and Jimenez [21], Koelman [22] and Qian et al. [23].

A popular kinetic model adopted in the literature is the single relaxation time approximation, the so-called BGK model [24]:

\[
\frac{\partial f}{\partial t} + \mathbf{\xi} \cdot \nabla f = -\frac{1}{\lambda} (f - f^{(eq)})
\]

where \( f^{(eq)} \) is the equilibrium distribution function (the Maxwell-Boltzmann distribution function), and \( \lambda \) is the relaxation time.

To solve for \( f \) numerically, equation (1) is first discretised in the velocity space using a finite set of velocities \( \{\mathbf{\xi}_\alpha\} \) without affecting the conservation laws [15, 24,25],

\[
\frac{\partial f_{a}}{\partial t} + \mathbf{\xi}_a \cdot \nabla f_{a} = -\frac{1}{\lambda} (f_{a} - f_{a}^{(eq)})
\]

In the above equation, \( f_{a}(\mathbf{x},t) \equiv f(\mathbf{x},\mathbf{\xi}_a,t) \) is the distribution function associated with the \( \alpha \)-th discrete velocity \( \mathbf{\xi}_a \) and \( f_{a}^{(eq)} \) is the corresponding equilibrium distribution function. The 9-bit square lattice model, which is often referred to as the D2Q9 model (Figure 1), has been successfully used for simulating 2-D flows. In the D2Q9 model, we use \( e_{\alpha} \) to denote the discrete velocity set and we have

\[
\begin{align*}
e_0 &= 0, \\
e_{\alpha} &= c(\cos((a - 1)p/4), \sin((a - 1)p/4)) \\
for \alpha &= 1, 3, 5, 7, \\
e_{\alpha} &= \sqrt{2} c(\cos((a - 1)p/4), \sin((a - 1)p/4)) \\
for \alpha &= 2, 4, 6, 8
\end{align*}
\]

where \( c = \delta x/\delta t, \delta x \) and \( \delta t \) are the lattice constant and the time step size, respectively. The equilibrium distribution for D2Q9 model is of the following form [23]

\[
f_{a}^{(eq)} = w_{\alpha} \left[ \rho + \frac{3}{c^2} e_{\alpha} \cdot u + \frac{9}{2c^4} (e_{\alpha} \cdot u)^2 - \frac{3}{2c^2} u \cdot u \right]
\]

where \( w_{\alpha} \) is the weighting factor given by

\[
w_{\alpha} = \begin{cases} 
4/9, & \alpha = 0 \\
1/9, & \alpha = 1, 3, 5, 7 \\
1/36, & \alpha = 2, 4, 6, 8.
\end{cases}
\]

With the discretised velocity space, the density and
momentum fluxes can be evaluated as

$$\rho = \sum_{k=0}^{8} f_{\alpha} = \sum_{k=0}^{8} f_{\alpha}^{(eq)}$$  \hspace{1cm} (6)$$

and

$$\rho u = \sum_{k=1}^{8} e_{\alpha} f_{\alpha} = \sum_{k=1}^{8} e_{\alpha} f_{\alpha}^{(eq)}$$  \hspace{1cm} (7)$$

The speed of sound in this model is $c_s = c/\sqrt{3}$ and the equation of state is that of an ideal gas,

$$p = \rho c_s^2$$  \hspace{1cm} (8)$$

Equation (2) can be further discretised in space and time. The completely discretised form of equation (1), with the time step $\delta t$ and space step $e_{\alpha} \delta t$, is:

$$f_{\alpha}(x_i + e_{\alpha} \delta t, t + \delta t) - f_{\alpha}(x_i, t) = -\frac{1}{\tau} [f_{\alpha}(x_i, t) - f_{\alpha}^{(eq)}(x_i, t)]$$  \hspace{1cm} (9)$$

where $\tau = \lambda/\delta t$, and $x_i$ is a point in the discretised physical space. The above equation is the discrete lattice Boltzmann equation [20,21,26] with BGK approximation [24]. Equation (9) is usually solved in the following two steps where $\sim$ represents the post-collision state.

The viscosity in the NS equation derived from equation (9) is

$$\nu = (\tau - 1/2)e_s^2 \delta t$$  \hspace{1cm} (10)$$

This modification of the viscosity formally makes the LBGK scheme a second-order method for solving incompressible flows [25,27]. The positivity of the viscosity requires that $\tau > 1/2$.

It is noted that the collision step is completely local and the streaming step takes very little computational effort. Equation (9) is explicit, easy to implement, and straightforward to parallelise.

1.2 Issues in the boundary condition treatment

Like in any other fluid flow computations, the numerical boundary condition is a very important issue in the LBE method. Two classes of boundaries are often encountered in computational fluid dynamics: open boundaries and the solid wall. The open boundaries typically include lines (or planes) of symmetry, periodic cross-sections, infinity, and inlet and outlet. At these boundaries, velocity or pressure is usually specified in the macroscopic description of fluid flow. Unlike solving the NS equations where the macroscopic variables, their derivatives, or a well established constraint (such as the mass continuity for pressure distributions) can often be explicitly specified at boundary [28], in the LBE method, these conditions need to be converted into distribution function $f$.
back on the link scheme [29], one typically requires that the known velocity profile \( u(x_I) \) be specified at \( x_A + \frac{1}{2}e_\alpha dt \) with \( \Omega = 0.5 \), where \( \Omega \) is the fraction of a link in the fluid region intersected by inlet boundary,

\[
\Omega = \frac{|x_B - x_I|}{|x_B - x_A|} 0 \leq \Omega \leq 1 \quad (11)
\]

The standard bounce-back scheme for \( \tilde{f}_\alpha(x_A) \) at the inlet \( x_A \) gives:

\[
\tilde{f}_\alpha(x_A) = \tilde{f}_\alpha(x_A + e_\alpha \delta t) + 2w_\alpha \rho(x_A + \frac{1}{2}e_\alpha dt) \frac{3}{c^2} e_\alpha \cdot u(x) \quad (12)
\]

for \( \alpha = 1, 2, 8 \) and \( \bar{\alpha} = 5, 6, 4 \). We note that \( \tilde{f}_\alpha(x_A) \) in equation (12) depends on \( \tilde{f}_\alpha(x_A + e_\alpha \delta t) \) and \( \rho(x_A + 1/2e_\alpha \delta t) \). Thus, it creates a mechanism for the pressure waves to propagate along the \( e_\alpha \) direction through \( \tilde{f}_\alpha(x_A + e_\alpha \delta t) \) and to reflect back to the interior of computational domain along the \( e_\bar{\alpha} \) direction through \( \tilde{f}_\bar{\alpha}(x_A) \).

3 CONCLUSIONS

Computations based on the bounce-back based inlet condition and interpolation-based superposition condition are performed for various cases. Bounce-back based inlet condition results in slower convergence towards steady or dynamically steady state and causes stronger interaction between the inlet and interior field. Such interaction may affect the long-term behaviour of the solution, especially at higher \( Re \). The interpolation-based superposition scheme can reduce the impact of the boundary-interior interaction on the unsteady development of the flow field, improves the convergence rate, improves the computational stability, and improves the quality of the overall solution.

ACKNOWLEDGEMENTS

The work reported in this paper has been partially supported by NASA Langley Research Center, with David Rudy as the project monitor. The authors thank Dr. Li-Shi Luo for many helpful discussions. The work reported in this paper has been partially supported by NASA Langley Research Center, with David Rudy as the project monitor. The authors thank Dr. Li-Shi Luo for many helpful discussions.

REFERENCES


