A New Boundary Scheme for BGK Model

Peng Wang†, Shiqing Zhang‡
Yangtze Center of Mathematics and College of Mathematics,
Sichuan University, Chengdu 610064, People’s Republic of China

Abstract

In this paper, we proposed a new boundary condition scheme for the BGK model which has second order accuracy and can be developed to higher accuracy. Numerical tests show that the numerical solutions of the BGK model applied to the new boundary scheme have great agreement with analytical solutions. It is also found that the numerical accuracy of the present schemes is much better than that of the original extrapolation schemes proposed by Guo et al at small grid.

Key Words: fluid mechanics; BGK methods; finite difference; boundary conditions; numerical method.

2000 Mathematical Subject Classification: 74F10, 76M25, 76P05

1 Introduction

In the past 20 years, the Boltzmann-BGK method in the simulation of fluid showed great success. Compared to traditional numerical methods, the Boltzmann-BGK method that based on the mesoscopic view got macroscopic variables throughout the moment integration of distribution function \( f \). For the mesoscopic property, the Boltzmann-BGK can be easily applied to a very large scope, such as multiphase, multicomponent high-speed compressible flows and so on\([12, 14, 10]\). In simulation, the boundary condition in practice is usually given by macroscopic variables, in BGK method we actually use the distribution function. Up to now there are no universal method to get the distribution function throughout the macroscopic variables, so it’s necessary to discuss the distribution function of boundary conditions.

Virtual equilibrium method, interpolation method and non-equilibrium extrapolation method are the main boundary schemes used in BGK model nowadays. Most of the schemes based on some sort of extrapolation methods to get the distribution functions on boundary \([6, 13, 9, 8, 2]\). In this paper, we got a new boundary scheme based on...
mathematical analysis. This new boundary scheme has second order accuracy, can be easily to develop to higher order accuracy and can be implemented by different viscosity between flow node and the boundary node. In the following sections, we first give implicit-explicit scheme of BGK model, and then discuss boundary scheme, in the last, we applied this new boundary condition scheme together with the implicit-explicit scheme of BGK model to Couette flow and lid driven cavity flow to test accuracy and stability of this boundary scheme.

2 BGK method

2.1 Basic BGK model

The standard dynamics theory of mesoscopic model is described by the Boltzmann equation as follow

\[ \frac{\partial f}{\partial t} + \vec{e} \cdot \nabla f = J, \]

where \( f \) denotes the distribution function, \( \vec{e} \) denotes the molecule velocity vector, and \( J \) represents the collision term. By the model of BGK, we can easily simplify the collision term \( J \) to the following formulation

\[ \frac{\partial f}{\partial t} + \vec{e} \cdot \nabla f = \frac{1}{\tau}(f^{eq} - f), \]

where \( \tau \) denotes the relaxation time and \( f^{eq} \) denotes the local equilibrium distribution function.

By the Hermite expansion or Taylor expansion, we discrete the infinite velocity space to finite space \( \{e_0, e_2, \cdots, e_N\} \) to make the equation (2) be a set of discrete velocity equations.

\[ \frac{\partial f_i}{\partial t} + \vec{e}_i \cdot \nabla f_i = \frac{1}{\tau}(f_i^{eq} - f_i), (i = 0, 1, \cdots, N). \]

The macroscopic density \( \rho \) and velocity \( \vec{u} \) can be obtained by the moments of the distribution function

\[ \rho = \sum f_i, \quad \rho \vec{u} = \sum \vec{e}_i f_i. \]

In 1992, Qian proposed a D2Q9 model. The \( f_i^{eq} \) of D2Q9 is

\[ f_i^{eq} = \rho \omega_i [1 + \frac{\vec{e}_i \cdot \vec{u}}{c_s^2} + \frac{(\vec{e}_i \cdot \vec{u})^2}{2c_s^4} - \frac{||\vec{u}||^2}{2c_s^2}], \]

where \( \omega_i \) is a weight coefficient, \( c_s = 1/\sqrt{3} \) is the local sound speed. For D2Q9 model, the discrete speed is

\[ \vec{e}_i = c \begin{pmatrix} 0 & 1 & 0 & -1 & 0 & \sqrt{2} & -\sqrt{2} & -\sqrt{2} & \sqrt{2} \\ 0 & 0 & 1 & 0 & -1 & \sqrt{2} & \sqrt{2} & -\sqrt{2} & -\sqrt{2} \end{pmatrix} (i = 0, 1, \cdots, 8), \]
where the \( c = 1 \). The sound speed and weight coefficient is

\[
c_s = \frac{1}{\sqrt{3}}, \quad \omega_i = \begin{cases} 
4/9, & |\vec{e}_i|^2 = 0, \\
1/9, & |\vec{e}_i|^2 = \epsilon^2, \\
1/36, & |\vec{e}_i|^2 = 2\epsilon^2.
\end{cases}
\] (7)

Apply Enskog-Chapman expansion to recover the macroscopic incompressible Navier-Stokes equations without outer force

\[
\nabla \cdot \vec{u} = 0, \\
\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\frac{1}{\rho} \nabla p + \mu \Delta \vec{u},
\] (8)

where the \( \mu \) represents the kinematic viscosity. We need the discrete velocity and equilibrium distribution function satisfying the following equation:

\[
\rho = \sum_i f_i^{(eq)}, \quad \rho \vec{u} = \sum_i \vec{e}_i f_i^{(eq)}, \quad \rho u_i u_j + p \delta_{ij} = \sum_i e_{ia} e_{ib} f_i^{(eq)},
\] (9)

and

\[
\mu = \tau c_s^2.
\] (10)

In this paper, we applied an explicit-implicit scheme to test the validness of the new scheme of boundary condition.

2.2 Time and spatial discrete

For the calculation of the equations (3) of the basic BGK model, we integrate the equation (3) in both side to get

\[
\begin{cases} 
\int_t^{t+\Delta t} \frac{\partial f_i}{\partial t} + \int_t^{t+\Delta t} \vec{e}_i \cdot \nabla f_i = \int_t^{t+\Delta t} \frac{1}{\tau} (f_i^{(eq)} - f_i), \\
f(0, \vec{x}, \vec{e}) = f_0(\vec{x}, \vec{e}).
\end{cases}
\] (11)

where the \( f_0(\vec{x}, \vec{e}) \) represents the initial value. By mean value theorem of integrals, the equality (11) can be written as

\[
f_{i}^{n+1} - f_{i}^{n} + \vec{e}_i \cdot \nabla f_i(t_\xi, \vec{x}) \Delta t = \frac{\Delta t}{\tau} (f_i^{(eq)}(t_\xi, \vec{x}) - f_i(t_\xi, \vec{x})),
\] (12)

where \( t < t_\xi < t+\Delta t \), the superscript \( n \) represents the step number, i.e. \( f_i^n = f(t, \vec{x}) \), \( f_i^{n+1} = f(t + \Delta t, \vec{x}) \).

For time discrete, we calculates advection term \( \vec{e}_i \cdot \nabla f_i(t_\xi, \vec{x}) \Delta t \) as an explicit finite-difference form and the collision term \( \frac{\Delta t}{\tau} (f_i^{(eq)}(t_\xi, \vec{x}) - f_i(t_\xi, \vec{x})) \) as a implicit finite-difference form, and we got

\[
f_{i}^{n+1} - f_{i}^{n} + \Delta t \vec{e}_i \cdot \nabla f_i^n = \Delta t [\theta J_{i}^{n+1} + (1 - \theta)J_{i}^{n}],
\] (13)
where the $\theta$ represents the degree of implicity, in this paper we make it to be 0.5, and $J^n = \frac{\Delta t}{\tau}(f_i^{(eq)}(t, \bar{x}) - f_i(t, \bar{x}))$, $J^{n+1} = \frac{\Delta t}{\tau}(f_i^{(eq)}(t + \Delta t, \bar{x}) - f_i(t + \Delta t, \bar{x}))$.

Z.L Guo and T.S Zhao introduced a new distribution function to remove the implicity of the equation (13), and the new distribution function is

$$g_i = f_i + \pi \theta (f_i - f_i^{(eq)})$$  \hspace{1cm} (14)

where $\pi = \Delta t / \tau$ [7]. Applying this new distribution function to equation (13), we can delete the implicity of the collision term and got

$$f_i^n = \frac{1}{1 + \pi \theta (g_i^n + \pi \theta f_i^{(eq), n})},$$  \hspace{1cm} (15)

$$g_i^{n+1} = -\Delta t \vec{e}_i \cdot \nabla_h f_i^n + (1 - \pi + \pi \theta)f_i^n + \pi(1 - \theta)f_i^{(eq), n}.$$  \hspace{1cm} (19)

In the following part, we discuss about the spatial discrete scheme. We apply a mixed-difference scheme which combined upwind scheme with central scheme. The central difference of $\frac{\partial f_i}{\partial x_\alpha}$ is

$$(\frac{\partial f_i}{\partial x_\alpha})_c = \frac{1}{2\Delta x_\alpha} [f_i(x_\alpha + \Delta x_\alpha, \cdot) - f_i(x_\alpha - \Delta x_\alpha, \cdot)].$$  \hspace{1cm} (16)

The second-order upwind-difference scheme is

$$(\frac{\partial f_i}{\partial x_\alpha})_u = \begin{cases} \frac{1}{2\Delta x_\alpha} [3f_i(x_\alpha, \cdot) - 4f_i(x_\alpha - \Delta x_\alpha, \cdot) + f_i(x_\alpha - 2\Delta x_\alpha, \cdot)] & \text{if } e_{i\alpha} \geq 0, \\ -\frac{1}{2\Delta x_\alpha} [3f_i(x_\alpha, \cdot) - 4f_i(x_\alpha + \Delta x_\alpha, \cdot) + f_i(x_\alpha + 2\Delta x_\alpha, \cdot)] & \text{if } e_{i\alpha} < 0. \end{cases}$$  \hspace{1cm} (17)

The mixture form is

$$\frac{\partial f_i}{\partial x_\alpha} = (\zeta \frac{\partial f_i}{\partial x_\alpha})_c + (1 - \zeta)(\frac{\partial f_i}{\partial x_\alpha})_u,$$  \hspace{1cm} (18)

where $\zeta \in [0, 1]$.

By the time discrete and the space discrete, we got the entire iterative form:

$$g_i^{n+1} = -\Delta t \vec{e}_i \cdot \nabla_h f_i^n + (1 - \pi + \pi \theta)f_i^n + \pi(1 - \theta)f_i^{(eq), n},$$

$$f_i^n = \frac{1}{1 + \pi \theta (g_i^n + \pi \theta f_i^{(eq), n})},$$  \hspace{1cm} (19)

where the $\nabla_h$ represents the equation (18). By equation (14) and (1), we got

$$\rho^{n+1} = \sum g_i^{n+1}, \hspace{1cm} \bar{u}^{n+1} = \frac{1}{\rho^{n+1}} \sum \vec{e}_i g_i^{n+1}.$$  \hspace{1cm} (20)
2.3 Scheme of boundary condition

It’s well-known that the scheme of the boundary condition plays a very important role in the flow computation. It not only relates to the stability of the computation, but also relates to the accuracy of the computation. In simulation, the boundary condition is usually given by macroscopic variables, but in BGK method, we actually use the distribution function. For those reasons, we discuss the following boundary conditional scheme for the BGK model.

Based on equation (5) and (22), we can easily get the boundary conditional scheme for the given by macroscopic variables, but in BGK method, we actually use the distribution function. For this reason $f_i^{(eq)}(t, \vec{x}_p)$ was approximated by

$$f_i^{(eq)}(t, \vec{x}_p) = f_i^{(eq)}(t, \vec{x}_p) + f_i^{(neq)}(t, \vec{x}_p).$$  \hspace{1cm} (21)

where the $\vec{x}_p$ denotes the position of the physical boundary. At present work, we also decompose boundary distribution functions into equilibrium part and the non-equilibrium part. In BGK model, the equilibrium $f_i^{(eq)}(t, \vec{x}_p)$ functions can be assumed as the functional of $\vec{u}, \rho, p, T$ which are related with the time and space $\vec{x}$. For this reason $f_i^{(eq)}(t, \vec{x}_p)$ was approximated by

$$f_i^{(eq)}(t, \vec{x}_p) = f_i^{(eq)}(t, \rho(t, \vec{x}_f), \vec{u}(t, \vec{x}_p)).$$  \hspace{1cm} (22)

where the $\vec{x}_f$ denotes the flow node that next to the $\vec{x}_p$, i.e. $\vec{x}_f = \vec{x}_p + \vec{e}_i \Delta x$, and this approximation is at least third order accuracy [13]. For the $f_i^{(neq)}(t, \vec{x}_p)$ part, consider the boundary distribution function which satisfies the equation

$$\frac{\partial f_i(t, \vec{x}_p)}{\partial t} + \vec{e}_i \cdot \nabla f_i(t, \vec{x}_p) = \frac{1}{\tau_\ast} (f_i^{(eq)}(t, \vec{x}_p) - f_i(t, \vec{x}_p)), (i = 0, 1, \cdots, N).$$  \hspace{1cm} (23)

where the $\tau_\ast$ is determined by the viscosity between physical boundary and the fluid. If we think that the viscosity between physical boundary and the fluid is the same as inner flow, we have the $\tau_\ast = \tau$. In this paper, we set $\tau_\ast = \tau$. Assume the solution of equation (23) can be expanded as

$$f_i(t, \vec{x}_p) = f_i^{(eq)}(t, \vec{x}_p) + \tau_\ast f_i^{(1)}(t, \vec{x}_p) + \tau_\ast^2 f_i^{(2)}(t, \vec{x}_p) + \cdots.$$  \hspace{1cm} (24)

Substitute (24) into equation (23) and compare the for coefficient $\tau_\ast$, we have

$$f_i^{(1)}(t, \vec{x}_p) = - (\frac{\partial}{\partial t} + \vec{e}_i \cdot \nabla) f_i^{(eq)}(t, \vec{x}_p).$$  \hspace{1cm} (25)

Based on equation (24) and (22), we can easily got the $f_i^{(eq)}(t, \vec{x}_p)$ throughout the macroscopic variables. By $f_i^{(eq)}(t, \vec{x}_p)$, we can got the $f^{(1)}(t, \vec{x}_p)$ based on equation (25). We use $\tau_\ast f_i^{(1)}(t, \vec{x}_p)$ to approximate $f^{(neq)}(t, \vec{x}_p)$ part. By equation (24), the accuracy of $f_i^{(eq)}(t, \vec{x}_p) + \tau_\ast f_i^{(1)}(t, \vec{x}_p)$ to approximate $f_i(t, \vec{x}_p)$ is second order. On the boundary, we have distribution

$$f_i(t, \vec{x}_p) = f_i^{(eq)}(t, \vec{x}_p) - \tau_\ast (\frac{\partial}{\partial t} + \vec{e}_i \cdot \nabla) f_i^{(eq)}(t, \vec{x}_p).$$  \hspace{1cm} (26)
If we want to get the higher accuracy scheme, we can mix Guo’s scheme with proposed scheme, and we have

\[ f_i(t, \bar{x}_p) = f_i^{(eq)}(t, \bar{x}_p) - \tau_s(\frac{\partial}{\partial t} + \vec{e}_i \cdot \nabla) f_i^{(eq)}(t, \bar{x}_p) \]

\[ + f_i(t, \bar{x}_f) + \tau_s(\frac{\partial}{\partial t} + \vec{e}_i \cdot \nabla) f_i^{(eq)}(t, \bar{x}_f) - f_i^{(eq)}(t, \bar{x}_f), \]

(27)

To get the value of \( f^{(1)}(t, \bar{x}_p) \), we discrete the time differential operator \( \frac{\partial}{\partial t} \) as

\[ (\frac{\partial f_i^{(eq)}(t, \bar{x}_p)}{\partial t})_{BT} = \frac{1}{\Delta t} [f_i^{(eq)}(t + \Delta t, \cdot) - f_i^{(eq)}(t, \cdot)], \]

(28)

and discrete differential operator \( \nabla \) at boundary as

\[ (\frac{\partial f_i^{(eq)}(t, \bar{x}_p)}{\partial x_\alpha})_{BS} = \frac{1}{2\Delta x_\alpha} [3f_i^{(eq)}(x_\alpha, \cdot) - 4f_i^{(eq)}(x_\alpha - \Delta x_\alpha, \cdot) + f_i^{(eq)}(x_\alpha - 2\Delta x_\alpha, \cdot)]. \]

(29)

Summing up the above discussion, we have entire finite difference method for the Blotzmann-BGK model. The following part, we will apply above boundary scheme together with the implicit-explicit difference scheme to test the validness of the proposed boundary scheme.

3 Numerical Simulations

In this section, we will apply the new boundary scheme together with the implicit-explicit scheme of BGK model to Couette flow and lid driven cavity flow to test accuracy and stability of this boundary scheme.

3.1 Couette flow

The Couette plate flow is defined in the region \( 0 \leq x \leq 1, 0 \leq y \leq 1 \) under a periodic boundary condition at the entrance and exit. The bottom plate is kept stationary, and the top plate moves horizontally with a constant velocity \( u_0 \). This Couette flow has the following analytical solution

\[ \vec{u}^*(t, x, y) = \left( \frac{y}{H} + 2 \sum_{k=1}^{\infty} \frac{(-1)^k}{\lambda_k H} \exp(-\mu \lambda_k^2 t) \sin(\lambda_k y) \right) \hat{e}_x, \]

(30)

where the \( \lambda_k = k\pi/H \), \( k = 1, 2, \ldots \) and \( H = L = 1.0 \). We defined the average error as

\[ \text{AverageError} = \frac{1}{n} \sum_n \sqrt{\frac{(u_{x,n} - u_{x,n}^*)^2 + (u_{y,n} - u_{y,n}^*)^2}{(u_{x,n}^*)^2 + (u_{y,n}^*)^2}}, \]

(31)
where the $n$ denotes the number of the grid.

We set $Re = (Lu_0)/\mu = 10$, $\zeta = 0.9$ and use the grid $N_x \times N_y = 5 \times 10$, $N_x \times N_y = 10 \times 20$, $N_x \times N_y = 20 \times 40$, $N_x \times N_y = 40 \times 80$ for simulation. The proposed scheme \cite{26} is implemented to top and bottom plates, and the periodic boundary condition is implemented to the entrance and exit \cite{12}. The numerical velocity profiles at time $t = 0.5$, $t = 5$, $t = 10$, $t = 30$ together with analytical solutions are plotted in figure 1. From the figure, we can see the numerical solution greatly agreed with the analytical solution. The average error of Guo scheme and proposed scheme are plotted in figure 2. Comparing Guo’s scheme, the proposed scheme at small grid have better accuracy.

Figure 1: Numerical result which applied the Figure 2: Average error of Guo scheme and proposed boundary scheme for the couette proposed scheme for couette flow

3.2 Two dimensional lid driven square cavity flow

The lid driven square cavity flow is classical benchmark problem in numerical simulation of the fluid. In lid driven square cavity flow, the top lid of the cavity has a constant velocity toward right, and the other three boundary hold still. The geometry of the lid driven flow is very simply and the phenomena is very complicated.

In this section we apply proposed boundary scheme for the lid driven cavity flow. The width and height is chosen to be $L = 1.0$. The initial density $\rho = 1.0$, top velocity of lid is chosen to be $\vec{u} = (u_x, u_y) = (0.1, 0)$. The size of the mesh is $N_x \times N_y = 128 \times 128$, set $\Delta t = 0.1 \times \Delta y$. The streamline for $Re = 400, 1000, 3000, 5000$ were plotted in figure 3. For $Re = 400$, we can see three vortices in the figure and the center of the vortex is at $x = 0.5563, y = 0.6103$. For $Re = 1000$ it also has three vortices and the coordinates of the vortex center is $x = 0.5334, y = 0.5759$. For $Re = 3000$, we see four vortices in the picture.
and the center of the vortex is $x = 0.5224, y = 0.5581$. When $Re = 5000$, we can see there are four vortices in the figure and the center of the vortex is $x = 0.5210, y = 0.5543$. All four position of the centers of the vortex well matched the paper [12, 7].

4 Conclusion

In this paper, we discussed a new boundary scheme together with the implicit-explicit scheme for BGK model. The main point of this scheme is to decompose the distribution function on the boundary node into equilibrium and non-equilibrium parts. Based on the mathematical analysis, we use $-\tau_* f_i^{(1)}(t, \vec{x}_p)$ to approximate the non-equilibrium. We tested this new boundary scheme in Couette flow and lid driven flow. Numerical test showed that the numerical solutions of the BGK model applied to proposed boundary scheme is very agreement with the former paper [4, 13] and analytical solution and also showed second order accuracy.

The proposed scheme include the different relaxation time $\tau_*$ that depend on the dif-
different viscosity between the flow and the boundary. For this reason, we can adjust the scheme according to viscosity between boundary and inner flow. By the equation (24), we can theoretically develop this scheme to higher order accuracy. The scheme is very simply and doesn’t need any more node. In one word, comparing with the original extrapolation schemes, we have proposed a new method for the implementation of boundary conditions for BGK model which are shown to be of second order accuracy, and have better numerical stability.

References

[1] P. L. Bhatnagar, E. P. Gross, and M. Krook. A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-Component Systems. Phys. Rev., 94:511–525, May 1954.

[2] M’hamed Bouzidi, Mouaouia Firdaouss, and Pierre Lallemand. Momentum transfer of a Boltzmann-lattice fluid with boundaries. Physics of Fluids, 13(11):3452–3459, 2001.

[3] C. Cercignani. The Boltzmann Equation and Its Applications. Applied mathematical sciences. Springer-Verlag, 1988.

[4] Shiyi Chen and Gary D. Doolen. Lattice boltzmann method for fluid flows. Annual Review of Fluid Mechanics, 30(1):329–364, 1998.

[5] D.Q.Li and T.H.Qing. Physics and Partial Differential Equations. Higher Education Publishing House, Beijing, 2005.

[6] Olga Filippova and Dieter H?nel. Grid refinement for lattice-bgk models. Journal of Computational Physics, 147(1):219 – 228, 1998.

[7] Zhaoli Guo and T. S. Zhao. Explicit finite-difference lattice boltzmann method for curvilinear coordinates. Phys. Rev. E, 67:066709, Jun 2003.

[8] Renwei Mei, Li-Shi Luo, and Wei Shyy. An accurate curved boundary treatment in the lattice boltzmann method. Journal of Computational Physics, 155(2):307 – 330, 1999.

[9] Renwei Mei and Wei Shyy. On the finite difference-based lattice boltzmann method in curvilinear coordinates. Journal of Computational Physics, 143(2):426 – 448, 1998.

[10] Dewei Qi. Simulations of fluidization of cylindrical multiparticles in a three-dimensional space. International Journal of Multiphase Flow, 27(1):107 – 118, 2001.

[11] Y. H. Qian, D. D’Humires, and P. Lallemand. Lattice BGK Models for Navier-Stokes equation. EPL (Europhysics Letters), 17(6):479, 1992.
[12] Y.L.He, Y.Wang, and Q.Li. *Lattice Boltzmann method theory and applications*. Science Publishing House, Beijing, 2008.

[13] Guo Zhao-Li, Zheng Chu-Guang, and Shi Bao-Chang. Non-equilibrium extrapolation method for velocity and pressure boundary conditions in the lattice boltzmann method. *Chinese Physics*, 11(4):366, 2002.

[14] Z.L.Guo and C.G.Zheng. *Theory and Applications of Lattice Boltzmann Method*. Science Publishing House, Beijing, 2008.