

A Dynamic Method for Boundary Conditions in Lattice Boltzmann method

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Abstract

It has been confirmed that implementation of the no-slip boundary conditions for the lattice-Boltzmann method play an important role in the overall accuracy of the numerical solutions as well as the stability of the solution procedure. We in this paper propose a new algorithm, i.e. the method of the dynamic boundary condition for no-slip boundary condition. The distribution functions on the wall along each of the links across the physical boundary are assumed to be composed of equilibrium and nonequilibrium parts which inherit the idea of Guo's extrapolation method. In the proposed algorithm, we apply a dynamic equation to reflect the computational slip velocity error occurred on the actual wall boundary to the correction; the calculated slip velocity error dynamically corrects the fictitious velocity on the wall nodes which are subsequently employed to the computation of equilibrium distribution functions on the wall nodes. Along with the dynamic self-correcting process, the calculation efficiently approaches the steady state. Numerical results show that the dynamic boundary method is featured with high accuracy and simplicity.

Nomenclature

δt :	time step size
δx :	lattice spacing unit
ν :	kinetic viscosity;
ρ :	fluid density
τ :	relaxation time
\mathbf{e}_α :	discrete velocity vector
c_s :	speed of sound
f_α :	partical mass distribution function
$f_\alpha^{(eq)}$:	equilibrium distribution function
Re :	Reynolds number
\mathbf{u} :	fluid velocity
R :	gas constant
T :	temperature
ω_α :	weighting factor

1. Introduction

Lattice-Boltzmann method (LBM) has been an alternative, promising fluid dynamic computational platform. In the development of LBM, there are still several problems open to further improvement. The implementation of the no-slip boundary condition has been confirmed that plays an important role in the overall accuracy of the numerical solutions as well as the stability of the solution procedure. There are various approximate methods for the treatment of no-slip boundary condition. Among them, the most representative methods are bounce-back method [1], Yu's method [2, 3] and Guo's method [4]. The present study is devoted to no-slip boundary condition with the implementation of dynamic boundary treatment, and tests have been given along with the mentioned three methods for 2-D channel Poiseuille flow, oscillating Couette flow and lid-driven cavity flow.

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2. Lattice-Boltzmann Method

We employed the incompressible D2Q9 (9-bit two-dimensional) BGK model in present study for simplicity proposed by He et al [5]. The evolution equation is

$$f_\alpha(\mathbf{X} + \mathbf{e}_\alpha \delta t, t + \delta t) - f_\alpha(\mathbf{X}, t) = -\frac{1}{\tau} [f_\alpha(\mathbf{X}, t) - f_\alpha^{eq}(\mathbf{X}, t)] \quad (1)$$

In above equation, τ is the dimensionless collision relaxation time, \mathbf{X} is the coordinate of lattice node, f_α and f_α^{eq} are the particle mass distribution function and equilibrium distribution function along the α_{th} link, respectively. f_α^{eq} is given by:

$$f_\alpha^{eq} = \omega_\alpha \left[\rho + \rho_0 \left(\frac{1}{c_s^2} \mathbf{e}_\alpha \cdot \mathbf{u} + \frac{1}{2c_s^4} (\mathbf{e}_\alpha \cdot \mathbf{u})^2 - \frac{1}{2c_s^2} (\mathbf{u} \cdot \mathbf{u}) \right) \right] \quad (2)$$

where, \mathbf{u} is fluid velocity, ρ is the fluid density, c_s is the sound speed and \mathbf{e}_α is the discrete velocity vector, which on D2Q9 square lattice space is

$$\begin{cases} (0,0) & \alpha=0 \\ (\cos[(\alpha-1)\pi/2], \sin[(\alpha-1)\pi/2])c & \alpha=1,2,3,4 \\ (\cos[(\alpha-5)\pi/2+\pi/4], \sin[(\alpha-5)\pi/2+\pi/4])\sqrt{2}c & \alpha=5,6,7,8 \end{cases} \quad (3)$$

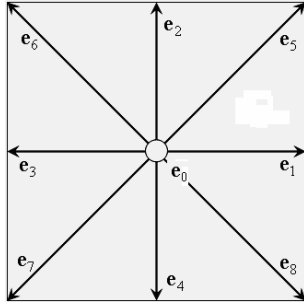


Fig.1 Discrete velocity vector of D2Q9 lattice

Here $c = \delta x / \delta t$, δx and δt are the lattice spacing unit and the time step size, respectively. Figure 1 shows the discrete velocities of the D2Q9 lattice. ω_α is the weighting factor:

$$w_\alpha = \begin{cases} 4/9 & \alpha=0 \\ 1/9 & \alpha=1,2,3,4 \\ 1/36 & \alpha=5,6,7,8 \end{cases} \quad (4)$$

The density and mass flux can be evaluated as:

$$\rho = \sum_{\alpha=0}^8 f_\alpha = \sum_{\alpha=0}^8 f_\alpha^{eq} \quad (5)$$

$$\rho \mathbf{u} = \sum_{\alpha=0}^8 \mathbf{e}_\alpha f_\alpha = \sum_{\alpha=0}^8 \mathbf{e}_\alpha f_\alpha^{eq} \quad (6)$$

In the computation, Eq. (1) can be solved by two steps, collision step and streaming step.

Collision step:

$$\tilde{f}_\alpha(\mathbf{X}, t) = f_\alpha(\mathbf{X}, t) - \frac{1}{\tau} [f_\alpha(\mathbf{X}, t) - f_\alpha^{eq}(\mathbf{X}, t)] \quad (7)$$

Streaming step:

$$f_\alpha(\mathbf{X} + \mathbf{e}_\alpha \delta t, t + \delta t) = \tilde{f}_\alpha(\mathbf{X}, t) \quad (8)$$

where \sim denotes the post-collision state of the distribution function. It is noted that the collision step is local and the streaming step involves no computation.

3. Dynamic Boundary Condition

In general, to finish the streaming step, the distribution functions at the boundaries need to be specified after the collision step during evolution of the computation. Similarly to Guo's extrapolation method, we decomposed the distribution function at a wall node along the links across the physical boundary into its equilibrium and nonequilibrium parts. While the non-equilibrium part is approximated using a first-order extrapolation based on the nonequilibrium part of the distribution function on the neighboring fluid nodes, the equilibrium part is approximated by employing a dynamic equation to auto-correct the fictitious velocity on the solid nodes.

Refer to Fig. 2. In order to obtain $\tilde{f}_{\alpha,s}$, the distribution function on node "S" along α_{th} link, we split it as,

$$\tilde{f}_{\alpha,s} = f_{\alpha,s}^{eq} + \tilde{f}_{\alpha,s}^{ne} \quad (9)$$

The equilibrium part is calculated by

$$f_{\alpha,s}^{eq} = \omega_\alpha \left[\rho_s + \rho_0 \left(\frac{1}{c_s^2} \mathbf{e}_\alpha \cdot \mathbf{u}_s + \frac{1}{2c_s^4} (\mathbf{e}_\alpha \cdot \mathbf{u}_s)^2 - \frac{1}{2c_s^2} (\mathbf{u}_s \cdot \mathbf{u}_s) \right) \right] \quad (10)$$

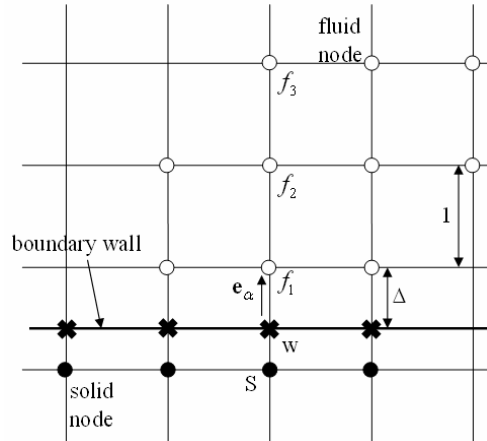


Fig.2 Layout of the lattices near the boundary

The nonequilibrium part is proposed to use

$$\tilde{f}_{\alpha,s}^{ne} = \beta \tilde{f}_{\alpha,f_1}^{ne} + (1 - \beta) \tilde{f}_{\alpha,f_2}^{ne} \quad (11)$$

where ρ_s is approximated to be equal to ρ_{f_1} , β is a parameter to be determined, and \mathbf{u}_s is solid node fictitious velocity value need to be chosen, here, it is

given from the dynamic equation:

$$\frac{du_s}{dt} = r(\bar{u}_w - u_w^o) \quad (12)$$

where \bar{u}_w is the desired wall velocity specified on the boundary wall node “W”. u_w^o is the calculated present wall velocity. Equation 12 can be written in a discrete form as follows.

$$u_s^n = u_s^o + r\delta t(\bar{u}_w - u_w^o) \quad (13)$$

Here, $\delta t=1$, the factor r is the relaxation factor, which of large value can accelerate the convergence of computation. So if u_w^o is larger than the desired wall velocity, \bar{u}_w , then the solid node velocity u_s^o is decreased, as should be reasonable.

Now the present wall velocity can be computed by using an extrapolation method with the given velocity at “ f_1 ”, “ f_2 ” and “ f_3 ”. Δ is the fraction of an intersected link in the fluid region. We use one among the following three extrapolations depending on the availability of u_{f3} and u_{f2} .

$$\left\{ \begin{array}{l} \text{0th-order:} \\ u_w^o = u_{f1} \\ \text{linear extrapolation:} \\ u_w^o = (1+\Delta)u_{f1} - \Delta u_{f2} \\ \text{quadratic extrapolation:} \\ u_w^o = \frac{1}{2}(1+\Delta)(2+\Delta)u_{f1} - \Delta(2+\Delta)u_{f2} + \frac{1}{2}\Delta(1+\Delta)u_{f3} \end{array} \right. \quad (14)$$

4. Computational Assessment

For assessment of the proposed dynamic method in implement of no-slip boundary condition, we applied the present method to several flow problems. 2-D Poiseuille flow and oscillating Couette flow are tested to check the spatial, temporal accuracy as well as stability. The cavity flow is calculated to test the ability to handle geometric singularity. The results are compared with those obtained by using other three boundary methods.

4.1 2-D Poiseuille flow

The lattice system for 2-D Poiseuille flow is specified as shown in Fig. 3. For the upstream boundary condition, we applied parabolic profile given by Eq. (15) which is corresponding to the exact solution of the fully-developed channel flow. The bounce-back scheme was applied for this velocity boundary. The normal coordinate y has its origin at the bottom wall and its discrete value is given by $y_j = j-1+\Delta$. y_c is the

value of y at the channel center, ny the grid number of LBM calculation domain height, $H = ny - 1 + 2\Delta$ the grid number of fluid domain height, the length of channel $L = 4ny + 1$. The maximum velocity u_{\max} is fixed at $u_{\max} = 0.01$. For the downstream boundary, we applied no-flux condition to implement the constant average-density along the normal y direction and the full-developed-flow properties.

$$u_{in}(y) = u_{exact}(y) = 4u_{\max}y(y_c - y)/(ny - 1 + 2\Delta)^2 \quad (15)$$

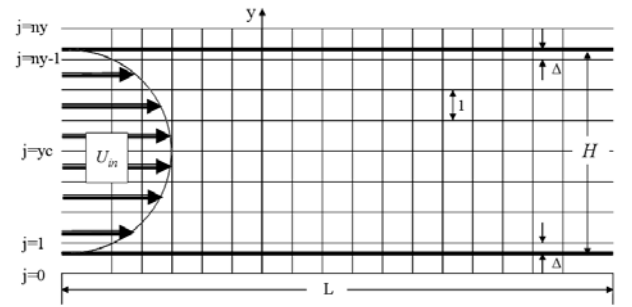


Fig.3 Lattice system for 2-D Poiseuille flow

Implementation of the boundary conditions on the solid walls, which is the main issue of this study, is given by the proposed dynamic method and other three methods, bounce-back scheme, Yu’s method and Guo’s method. For dynamic method the particular parameters are given $r = 0.1$, $\beta = 0$, quadratic extrapolation is employ to calculate the wall velocity. To assess the computational error of the LBM solution, the numerical value of the slip wall velocity on the solid wall is computed. Because the true wall velocity in the Poiseuille flow is zero, then the value of wall slip velocity u_w provides a measure of the accuracy by applying different boundary methods. Here, the numerical wall slip velocity is calculated by using the 2nd-order extrapolation scheme at the central station $i = L/2$.

$$u_w = \frac{1}{2}(1+\Delta)(2+\Delta)u(i,1) - \Delta(2+\Delta)u(i,1) + \frac{1}{2}\Delta(1+\Delta)u(i,3) \quad (16)$$

The normalized slip velocity is then given by $U_w = u_w / u(y_c)$. Figure 4 is the normalized wall slip velocity with respect to different grid number H along y direction by applying four different boundary treatments. The normalized slip velocity calculated by present method is much smaller than those by other schemes. Actually, the slip velocity value got by applying present method is on the order of 10^{-15} . This is on the same order of random machine error. So we suppose that there is nearly no numerical slip velocity error by applying present method to the no-slip boundary of Poiseuille flow.

Another accuracy assessment is quantified by the root-mean-square of the difference (RMS- ε) between the normalized velocity obtained from the numerical computation and that from the analytic solution at the central station.

$$\varepsilon = \sqrt{\frac{1}{N} \sum_{j=1}^{ny} [u_m(y) - u_{LBM}(y)]^2 / u_{\max}^2} \quad (17)$$

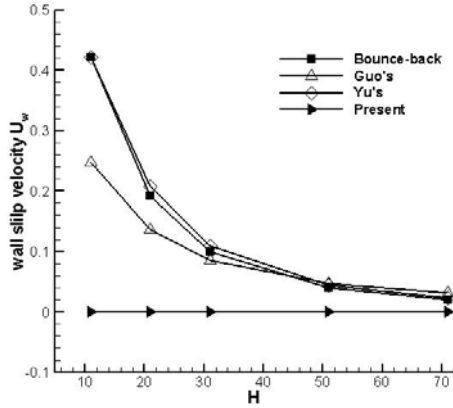


Fig.4 Convergence of wall slip velocity using different boundary methods in Poiseuille flow. ($\Delta = 0.5$, $\tau = 5$, $u_{\max} = 0.01$)

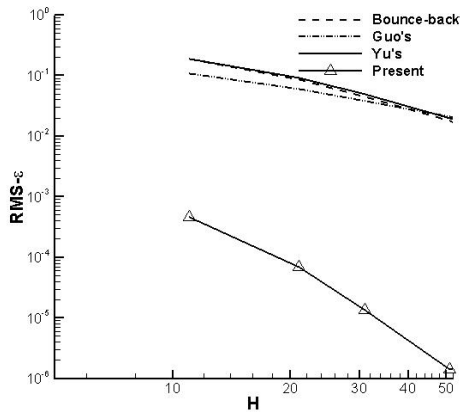


Fig.5 Dependence of RMS- ε on H in Poiseuille flow. ($\Delta = 0.5$, $\tau = 5$, $u_{\max} = 0.01$)

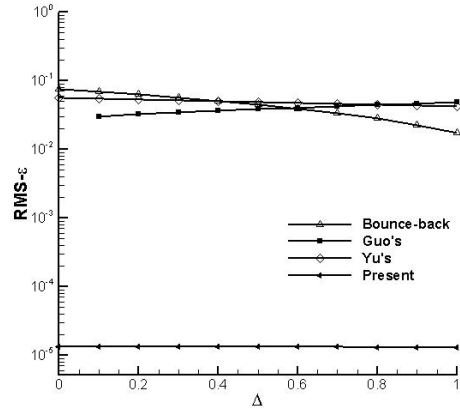


Fig.6 Dependence of RMS- ε on boundary position Δ in Poiseuille flow

Figure 5 shows the RMS- ε by applying different methods. Although these lines are of the similar slope, the magnitude of RMS- ε by present method is pretty small. In Fig. 6, the RMS- ε is given according to different position of physical wall Δ . The result by present method shows not only small error value but also provides a much less dependence on Δ .

4.2 Oscillating Couette flow

For a oscillating Couette flow which is shown in the following figure, the bottom wall is oscillating defined by $u(0, t) = U_0 \sin(\omega t + \phi_0)$, the length of the channel is $L = 4H$. The exact solution is given by

$$u_{\text{exa}} = U_0 e^{-\lambda y} \sin(\omega t - \lambda y) \quad (18)$$

where $\lambda = \sqrt{w/2\nu}$, ν is the kinetic viscosity in lattice unit. In present study, we set $\phi_0 = 0$, $r = 1$, $\beta = 0$, $U_0 = 0.01$. The simulation results in Fig.8 show that the present method can obtain more accurate result in treating this fluid problem.

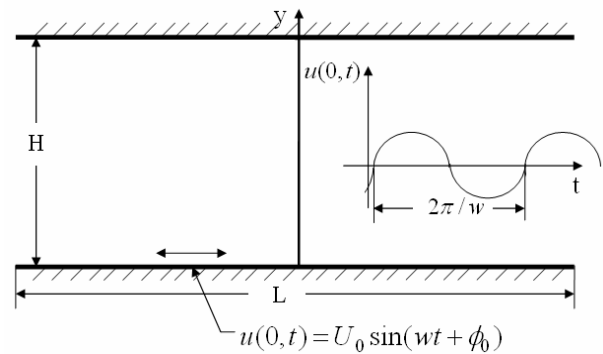


Fig.7 Sketch for oscillating Couette flow

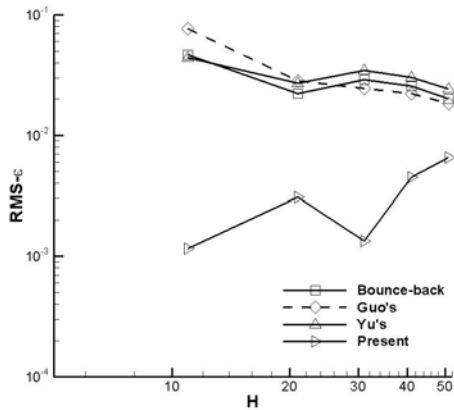


Fig.8 Dependence of RMS- ε on H in oscillating Couette flow.

4.3 Lid-driven Cavity flow

In order to check the flexibility of present method to the singularity problem, we apply it to the boundary implement of lid-driven cavity flow (Fig. 9). The results are obtained by applying Guo's and present methods under following parameter setup, $U_0 = 0.01$, $L = 51$, $\Delta = 0.5$, $\tau = 0.8$, $Re = 5$, and $r = 0.1, \beta = 0$ especially for present method. Figure 10 shows a very good agreement between these two methods' results. But during the implement of present to this fluid problem, the corners of the cavity need special care for the stability problem. Use quadratic extrapolation to get the dynamic wall velocities is considered to be not very suitable at the singular points. We'd better seek more reasonable, e.g. exponential, function in obtaining the wall velocity to fulfill the calculation of fictitious solid node velocity.

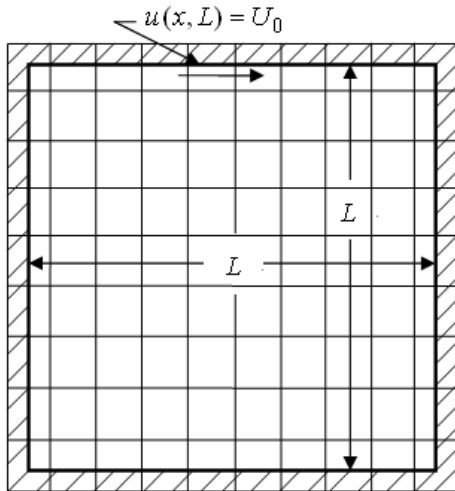


Fig. 9 Lattice system for 2-D lid driven cavity flow

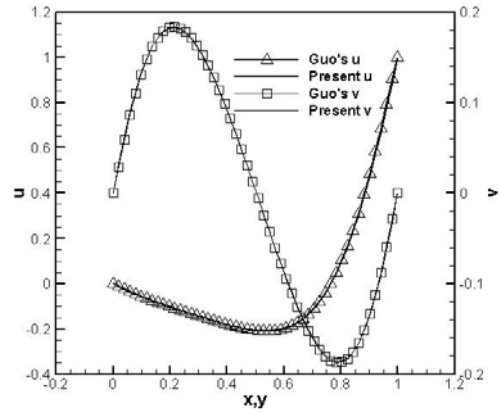


Fig. 10 Comparison of u and v velocities along vertical or horizontal centerline of lid-driven cavity flow by Guo's and present methods.

5. Conclusions and Future Discussions

We demonstrated that the new proposed dynamic boundary treatment has good ability to get higher accuracy. It also turned out that there still exist several problems open to further improvement, the choice of function to evaluate the wall slip velocity, the stability to treat singularity problem and the flexibility to handle complex curved boundary.

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