A wall function approach in lattice Boltzmann method: algorithm and validation using turbulent channel flow

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Abstract

In the lattice Boltzmann method (LBM), the widely utilized wall boundary is the bounce-back (BB) boundary, corresponding to the no-slip boundary. The BB boundary prevents the LBM from capturing the accurate shear drag on the wall when addressing high Reynolds number flows using coarse-grid systems. This study proposed the ‘wall-function bounce (WFB)’ boundary, a general framework to incorporate wall functions into the LBM’s boundary condition, independent of specific information of discrete velocity schemes and collision functions. The WFB boundary calculates the appropriate shear drag on the wall using a wall function model, and thereafter just modifies partial diagonal distribution functions to reflect the shear drag. The Spalding’s law was utilized as the wall function in WFB. Simulations of turbulent channel flow at \( \text{Re}_\tau = 640 \) and 2003 using the LBM-based large-eddy simulation were conducted to validate the effectiveness of the proposed boundary condition. The results indicate that the BB boundary underestimated the time-averaged velocity in the buffer layer at \( \text{Re}_\tau = 640 \), and the averaged velocity in the entire domain at \( \text{Re}_\tau = 2003 \), when using coarse-grid systems. However, WFB obtained the proper shear drag on the wall and thus, compensated for the underestimation and agreed better with the experimental or direct numerical simulation data, especially at the 1st-layer grid. In addition, WFB improved the Reynolds normal stress in the near-wall region to some extent. The distributions of shear drag...

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stress on the wall by WFB were analogous to those by the wall model function in the finite volume method.

Keywords: lattice Boltzmann method, wall function, wall-function bounce, large-eddy simulation, turbulent channel flow

Nomenclature

| Symbol | Definition |
|--------|------------|
| BB     | bounce-back boundary, |
| $D$    | half-height of the channel (m), |
| $e_s$  | speed of sound in LBM, |
| $f_a$  | distribution function of the virtual particle, |
| $p$    | local pressure (Pa), |
| $Re_f$ | friction Reynolds number, $= u_\tau D/\nu$, |
| $t$    | time step (s), |
| $u_\tau$ | friction velocity (m s$^{-1}$), $= \tau_{w}/\rho$, |
| $\nu$  | a virtual velocity vector utilized for the free-slip boundary (m s$^{-1}$), |
| $y^+$  | dimensionless distance from the wall, $= y u_\tau/\nu$, |
| $\Delta t$ | discrete time interval (s), |
| $\kappa$ | Karman constant, |
| $\rho$ | local fluid density (kg m$^{-3}$), |
| $\tau_w$ | shear stress on the wall (kg m$^{-1}$ s$^{-2}$), |
| $x, y, z$ | streamwise, normal, and spanwise components of the spatial coordinate, respectively (m), |
| $v_x, v_y, v_z$ | components of $v$ in the $x, y, z$ directions, respectively (m s$^{-1}$), |
| $C_s$ | Smagorinsky constant, |
| $e_a$ | discrete velocity vector of the virtual particle in the $a$-direction, |
| $F_a$ | external force term in the $a$-direction, |
| $N$ | number of total grids, |
| $r$ | position vector of the virtual particle, |
| $T$ | parameter for time normalization (s), $T = D/u_\tau$, |
| $u^+$ | dimensionless velocity, $= u/u_\tau$, |
| WFB | wall-function bounce boundary, |
| $\Delta f$ | difference of the distribution function on wall boundary after and before WFB collision, |
| $\epsilon_{u^+}$ | L2 error norm of $u^+$, |
| $\nu$ | molecular kinematic viscosity (m$^2$ s$^{-1}$), |
| $\tau$ | stress (kg m$^{-1}$ s$^{-2}$), |
| $\Omega_a(r, t)$ | collision function, |
| $u_x, u_y, u_z$ | components of $u$ in the $x, y, z$ directions, respectively (m s$^{-1}$), |
| $\sqrt{u_x'^2}, \sqrt{u_y'^2}, \sqrt{u_z'^2}$ | components of standard deviations of the fluctuating velocity in the $x, y, z$ directions, respectively (m s$^{-1}$). |

Subscripts and superscripts

| Symbol | Definition |
|--------|------------|
| $f_a^*$ | distribution function $f_a$ updated by the collision step, |
| $\Phi_{(i,j,k)}$ | a property $\Phi$ or $\Phi_a$ at the grid $(i,j,k)$, |
| $|\Phi|$ | magnitude of the vector property $\Phi$, |
| $\bar{\Phi}$ | spatial-average of property $\Phi$, |
| $f_a^*$ | distribution function $f_a$ that is modified by the WFB, |
| $\Phi_{(i,j,k)}^t$ | a property $\Phi$ at time step $t$, |
| $\langle \Phi \rangle$ | time-average of property $\Phi$. |
1. Introduction

In recent years, the lattice Boltzmann method (LBM) has been applied to high Reynolds number (high-Re) turbulent flows (Dong and Sagaut 2008, Fernandino et al 2009), such as the built environment (Béghein et al 2005, Sajjadi et al 2017, Han et al 2018, 2019), analogous to the conventional finite volume method (FVM). Based on the lattice Boltzmann equation (1), as well known, the LBM simulates the fluid motion by using distribution functions to represent the properties of the collection of particles. The simulation results are dependent on the collective collide-and-stream behavior of the particles in the system, rather than solving physical quantities on the macro scale (Inamuro 1999). In addition, the macroscopic fluid quantities are calculated through the integration of the distribution functions (equation (2)). Furthermore, the LBM can also be utilized for the large-eddy simulation (LBM-LES) to solve high-Re flows and several applications have been reported (Dong and Sagaut 2008, Wu and Guan 2009, Zhuo and Zhong 2013, Kuwata and Suga 2015, Suga et al 2017, Han et al 2018, 2019, Zhou et al 2019)

\[ f_a (r + \Delta t e_a, t + \Delta t) - f_a (r, t) = \Omega_a (r, t) + F_a. \]  
\[ \rho = \sum_a f_a (r, t), \quad \mathbf{u} = \frac{1}{\rho} \sum_a \mathbf{e}_a f_a (r, t), \quad p = \rho e_s^2. \]

In the viscous sublayer, which is a thin layer near the wall, the inertia force is in almost the same order as the viscous force, or only slightly larger than the viscous force, manifesting as \( \text{Re} \sim 1 \). In this sublayer, the fluid suffers from viscosity such that the motion does not follow the free flow pattern. In other words, the fluid pattern in this sublayer should not be modeled with a high-Re model (Versteeg and Malalasekera 2007). An ideal handling method is to densify the grids near the wall such that the fluid pattern in the sublayer can be calculated directly while not being modeled. Unfortunately, in many instances, the 1st-layer grid is not placed in the viscous sublayer when solving high-Re problems to reduce the computational cost, thus resulting in that unsatisfactory results in the near-wall region with the no-slip wall boundary. In the FVM, a widely utilized approach to overcome the deficiency is a wall function that models the appropriate velocity profile near the wall region. Some commonly used wall function models include the logarithmic law (Grötzbach 1987), the two-layer model (Werner and Wengle 1993), and the Spalding’s law (Spalding 1961, Launder and Spalding 1974). Among them, the Spalding’s law is increasingly widely utilized in high-Re turbulence problems; because its curve is continuous and is the asymptote of the curves of both the viscous sublayer and the logarithmic layer (figure 1), hence, it describes the law of the wall using one equation. Hitherto, the Spalding’s law has been applied to the FVM (Stathopoulos and Baskaran 1996, Toparlar et al 2015, Kikumoto et al 2018).

In the LBM, the most widely adopted wall boundary is the bounce-back (BB) boundary condition (Carnubert et al 1991, Ziegler 1993), because of its advantages of the simple algorithm and easy implementation. In this boundary, after hitting the wall, the fluid particles completely bounce back to the path in which they come from rather than move forward. Therefore, no flux across the wall, and no relative transverse motion exist between the fluid and wall. Researchers have applied the BB boundary to both isothermal and non-isothermal fluid problems (Béghein et al 2005, Liu and Guo 2013, Zhuo and Zhong 2013, Kuwata and Suga 2015, Han et al 2019), especially in relatively low-Re flow problems (Breuer et al 2000, Geller et al 2006, Fakhari and Lee 2015). However, the BB corresponds to the no-slip boundary, which may lead to a misprediction of the flow pattern in the viscous sublayer when solving high-Re flow problems. On the other hand, the widely adopted discrete velocity scheme in the LBM hitherto is
the DdQq scheme (Qian et al 1992) that typically utilizes uniform cubic lattices for the entire simulation domain. This may cause the misprediction of the shear drag on the wall by the BB boundary more significant when using coarse-grid systems in solving high-Re flow. Currently, several new technologies are being developed to improve grid features such as the local grid refinement for the DdQq scheme (Lagrava et al 2012, Gendre et al 2017), and the finite volume LBM with unstructured meshes (Li and Luo 2016); however, these methods will not be discussed in this study.

In such situations, although the mass and momentum can be conserved, the BB boundary cannot describe the shear drag on the wall accurately in turbulent flows, especially if the near-wall grids are coarse. Therefore, although the LBM-LES can be utilized in turbulent flows, it exhibits the same problem of mispredicting the shear drag on the wall as the FVM-LES. In some studies to solve relatively high-Re problems with LBM-LES, there are reports that the near-wall velocity errors may partly be due to defects of the BB. Fernandino et al (2009) indicated that the error of the results was apparent near the wall unless finer grid systems were employed in their simulation of the free surface flow in a wide rectangular duct using LBM-LES. Han reported that in the simulation of indoor flow (Han et al 2019) and the flow around a building (Han et al 2018) using LBM-LES, the simulated velocity near the walls agreed inaccurately with the experimental data; they supposed that it was partly owing to the lack of the wall function. It should be noted that the turbulent flow simulation using LBM-LES is challenging. It is because that several other factors will affect the result accuracy in addition to the boundary condition, such as the collision functions (Geier et al 2015, Gehrke et al 2017), sub-grid scale (SGS) models, grid resolutions (Kawai and Larsson 2012), and the number of discrete speeds of the lattice. However, in this study, we have mainly focused on the effect of the boundary conditions. Therefore, an enhanced wall treatment is necessary for LBM in addressing turbulent flows, similar to the wall function models in FVM.

Hitherto, reports regarding the progress of the wall function in LBM suited to high-Re turbulent flows are not sufficient. This is partly because the LBM is primarily applied to small-scale or medium range Reynolds number flow problems; thus, implementing the wall function is not urgent because the simulation accuracy is sufficient in solving these problems. Norouzi and Esfahani (2014) implemented both the power-law and exponential wall functions into two relaxation time LBM (TRT-LBM) to consider the effect of the Knudsen layer in the transition

Figure 1. Non-dimensional velocity profile obtained by Spalding’s law in a boundary layer.
flow regime. Their results of Poiseuille gas flow through a micro/nanochannel indicated that the TRT-LBM using the wall function could satisfactorily predict the flow behavior up to the upper end of the transition flow regime. Ahangar et al (2020) also utilize the power-law analytical function to improve the near-wall slippage velocity of rarefied gas flow in a microchannel with multi throats using TRT-LBM. Regarding high-Re turbulent flows, Wilhelm et al (2018) proposed an explicit wall model based on a power-law velocity profile and implemented it for the LBM-based Reynolds-averaged Navier–Stokes simulations of the incompressible flow around airfoils at high-Re numbers. Haussmann et al (2019) compared three wall function models (Musker profile, Werner an Wengle model, and power-law model) in LBM-LES for solving the turbulent channel flow at Re_τ = 1000, 2000, and 5200. Malaspinas and Sagaut (2014) established a wall model for LBM-LES for high-Re wall-bounded flows, by relying on the analytical profile of the velocity profile within the 1st off-wall cell or the solution of turbulent boundary layer equations. Their model obtained accurate averaged velocity, Reynolds stress, and friction coefficient compared to the direct numerical simulation (DNS) or semi-analytical profiles in the turbulent channel flow at Re_τ = 950, 2000, and 16 000. Pasquali et al (2020) proposed a wall function model for the cumulant LBM that sets a partial slip velocity on the wall by computing a skin frictional coefficient. Their model yielded results that were in good agreement with the DNS data in the case of the velocity profile, Reynolds shear, and normal stresses for the turbulent channel flow at Re_τ = 950, 2000, and 16 000.

In most previous studies, the implementation of the wall function depended on the specific information of the discrete velocity schemes, e.g. weight function, lattice velocity, lattice sound velocity, and equilibrium distribution (Malaspinas and Sagaut 2014, Haussmann et al 2019, Pasquali et al 2020). Some implementations depended on the type of collision functions (Norouzi and Esfahani 2014, Ahangar et al 2020). Therefore, the generality of the implementation of the wall function is somehow limited. In this study, we proposed a wall boundary, named the ‘wall-function bounce (WFB)’ boundary, which can incorporate wall function models. WFB is a general boundary framework that is independent of the specific information of discrete velocity schemes or collision functions. With WFB, LBM-LES can be applied for turbulent flows without densifying near-wall grids to reduce the computational cost in LES. The Spalding’s law was employed for the incorporation, because of its prevalence in the FVM when solving turbulent flows. LBM-LES simulations of the turbulent channel flow at Re_τ = 640 and 2003 were employed to validate the effectiveness of the WFB boundary. The turbulent channel flow is a high-Re flow problem and is sensitive to the drag on the wall, which makes it appropriate for validating the effectiveness of the WFB boundary.

2. Algorithm of WFB boundary for LBM

2.1. How can a wall function model be realized in LBM?

For brevity, we hereinafter abbreviate the BB boundary and proposed WFB boundary as BB and WFB, respectively. We first compare the difference between the no-slip (BB) boundary and the free-slip boundary in the LBM to obtain the principal idea of the realization of a wall function model. These explanations are based on the two-dimensional D2Q9 scheme (Qian et al 1992) (see appendix: figure A1(a)) for clarity. Subsequently, we derive the WFB in detail based on the three-dimensional D3Q19 scheme (see appendix: figure A1(b)).

In the LBM, the most straightforward approach for the walls is the BB boundary, which corresponds to the no-slip wall boundary. In this boundary, the particles hit a wall while not penetrating it, implying that no particles move across the boundary. Subsequently, the particles bounce back rather than bounce forward, implying that no relative transverse movement occurs
between the fluid and boundary (i.e. the fluid velocity on the wall is zero). BB boundary only affects the solid wall boundary particles while does nothing to the fluid region particles. Take the D2Q9 discrete velocity as an example (see appendix: figure A2), this process can be described as (Krüger et al 2017):\[ f_{2}^{\ast}|_{(i,0)} = f_{4}|_{(i,0)}, \quad f_{6}^{\ast}|_{(i,0)} = f_{8}|_{(i,0)}, \quad f_{5}^{\ast}|_{(i,0)} = f_{7}|_{(i,0)} \] (3)

where, $f_{a}^{\ast}$ means $f_{a}$ updated by the collision step. With increasing Re, the uniform grid system near the walls becomes too coarse to capture the accurate shear drag at the wall and will consequently affect the accuracy of the subsequent calculations. Hence, it is necessary to introduce a new boundary that contains a wall function to overcome this shortcoming of the BB boundary.

Meanwhile, in the free-slip boundary, the distribution functions on the boundary become mirror-symmetrical about the boundary after the collision step (see appendix: figure A3), as equation (4). Therefore, the normal velocity at the boundary grids toward the boundary is zero. However, the tangential velocity at the boundary remains.

\[ f_{2}^{\ast}|_{(i,0)} = f_{4}|_{(i,0)}, \quad f_{6}^{\ast}|_{(i,0)} = f_{8}|_{(i,0)}, \quad f_{5}^{\ast}|_{(i,0)} = f_{7}|_{(i,0)}, \] (4)

By comparing equations (3) and (4), it is clear that in the stream process, a particle moves to the boundary grid; subsequently, in the collision step, the particle bounces back to the incident direction in the no-slip boundary (figure 2(a)) or bounces forward in the free-slip boundary (figure 2(b)). On the other hand, if a wall function is implemented, its effect is equivalent to applying a reverse drag force on the velocity direction to the wall compared to the free-slip boundary, causing the particles near the wall to decelerate, as demonstrated in figure 2(c).

We observed that the difference in the distribution functions between the BB and free-slip boundaries is just that the values of $f_{5}^{\ast}$ and $f_{6}^{\ast}$ (i.e. distribution functions in the diagonal directions and pointing to the interior of the flow field) are swapped. Therefore, it is straightforward that we can reassign the values of $f_{5}^{\ast}$ and $f_{6}^{\ast}$, to achieve the effect of the wall function (drag).

### 2.2. Derivation of WFB boundary

We now return to the three-dimensional problems and derive the algorithm of WFB for D3Q19 scheme. The core task is to determine the adjustment of the distribution functions on the boundary, which are in the diagonal directions and pointing to the interior of the flow field (analog with $f_{5}^{\ast}$ and $f_{6}^{\ast}$ in D2Q9 scheme). We assume that the plane normal to the $y$-direction is the wall boundary and the positive direction of $y$ points to the flow field. In addition, positive $x$ is the streamwise direction. To clarify, from here to the end of this section, we define that $f_{a}$ is

![Figure 2. The difference among no-slip, free-slip, and WFB boundaries.](image_url)
the distribution function \( f_a \) revised by the wall function, and \( f_a^* \) represents \( f_a \) updated by the collision step. \( \rho \) and \( u \) are the density and velocity obtained by the WFB boundary, respectively.

Equation (5) is often observed in the fully developed shear flow near the walls, implying that the shear drag is proportional to the velocity temporal variation. In the near-wall region, the flow pattern can be regarded as a simple two-dimensional shear flow parallel to the wall, and the streamwise is positive \( x \)-direction. Equation (5) indicates that the variation of the momentum \( \rho u \) of this shear flow is resulted by the shear stress \( \tau \).

\[
\frac{\partial \rho u}{\partial t} = -\frac{\partial \tau}{\partial y} + \ldots
\]  

where, \( \ldots \) is other terms such as pressure term, which we do not focus on in this study.

As shown in figure 3, by discretizing equation (5), we have a general form as follows.

\[
\frac{\rho u(t_{i+1,1,k}) - \rho u(t_{i,1,k})}{\Delta t} = -\frac{\tau(t_{i,1+\frac{1}{2},k}) - \tau(t_{i,1-\frac{1}{2},k})}{\Delta y} + \ldots
\]  

Equation (6) can be decomposed into equations (7) and (8).

\[
\frac{\rho u(t_{i+1,1,k}) - \rho u(t_{i-\Delta t,1,k})}{\Delta t} = \frac{\tau(t_{i,1+\frac{1}{2},k}) - 0}{\Delta y} + \ldots
\]

\[
\frac{\rho u(t_{i,1,k}) - \rho u(t_{i-\Delta t,1,k})}{\Delta t} = \frac{0 - \tau(t_{i-1,\frac{1}{2},k})}{\Delta y} = \frac{\tau_w(t_{i,0,k})}{\Delta y}
\]

where we introduce a virtual momentum \( \rho v \), which is the momentum in the condition of the free-slip boundary (i.e. no shear drag on the boundary). This is a hypothetical intermediate status for the momentum variation between time step \( t - \Delta t \) and \( t \).

In equation (7), the stream process changes \( \rho u(t_{i,1,k}) \) to the virtual intermediate status \( \rho u(t_{i-\Delta t,1,k}) \) in the condition of the free-slip boundary we hypothesize. The momentum variation is resulted by \( \tau(t_{i,1+\frac{1}{2},k}) \) while \( \tau(t_{i,1-\frac{1}{2},k}) = 0 \) because there is no shear drag on the free-slip
boundary. This process implemented via the stream step in the LBM and does not require any special treatment.

Next, in equation (8), the shear drag $\tau_w\big|_{(i,0,k)}$ on the wall is introduced into the collision step, thus $\rho v\big|_{(i,1,k)}$ turns to $\rho u\big|_{(i,1,k)}$. This process is implemented via the collision step and realized by WFB. And $\rho u\big|_{(i,1,k)}$ is the modified momentum we obtain, which we consider more ‘correct’ because it is calculated by the wall function model.

Next, we can decompose equation (8) along x- and z-directions (y-direction is the normal direction and the corresponding velocity component is zero). Thus, $\tau_w$ can be decomposed to $x$-component $\tau_{w,x}$ and $z$-component $\tau_{w,z}$. Likewise, $\rho u$ and $\rho v$ are decomposed to $\rho u_x$, $\rho u_z$, and $\rho v_x$, $\rho v_z$, respectively. Therefore, we have:

$$\rho u_{x}\big|_{(i,1,k)} - \rho v_{x}\big|_{(i,1,k)} = \frac{\Delta t}{\Delta y} \tau_{w,x}\big|_{(i,0,k)}$$

$$\rho u_{z}\big|_{(i,1,k)} - \rho v_{z}\big|_{(i,1,k)} = \frac{\Delta t}{\Delta y} \tau_{w,z}\big|_{(i,0,k)}.$$  

The above equation indicates that in the $x$-component, there is a momentum loss ($\frac{\Delta t}{\Delta y} \tau_{w,x}$) caused by the shear drag $\tau_{w,x}$ compared to the free-slip boundary, resulting in that the momentum near the wall reduces from $\rho v_x$ of the hypothetical free-slip boundary to $\rho u_x$ of the actual WFB boundary. The same situation also happens in the $z$-component.

The next problem is to convert the momentum to the distribution functions. By considering the particle velocity of D3Q19 (see appendix: table A1), we can expand equation (2) on the free-slip boundary as:

$$f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7 + f_8 + f_9 + f_{10} + f_{11} + f_{12} + f_{13} + f_{14} + f_{15} + f_{16} + f_{17} + f_{18} = \rho$$

$$f_1 - f_2 + f_3 - f_4 + f_5 - f_6 + f_7 + f_8 - f_9 - f_{10} = \rho v_x$$

$$f_3 - f_4 + f_5 - f_6 + f_7 - f_8 + f_9 - f_{10} = \rho v_y$$

$$f_5 - f_6 + f_7 - f_8 + f_9 - f_{10} = \rho v_z.$$  

Meanwhile, in the condition of WFB boundary, the density $\rho$ is as same as in BB while the velocity varies to $u_x$, $u_z$, and $u_t$. Here, $v_r = v_y = 0$ is tenable. Based on our previous assumptions, only the distribution functions in the diagonal direction and pointing to the interior of the flow field are reassigned while those in the direction of the axis remain unchanged. Therefore, $f_1$, $f_{11}$, $f_{14}$, and $f_{17}$ become $\tilde{f}_1$, $\tilde{f}_{11}$, $\tilde{f}_{14}$, and $\tilde{f}_{17}$ in WFB boundary, respectively. This means, in the WFB, we have:

$$f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + \tilde{f}_7 + f_8 + f_9 + f_{10} + \tilde{f}_{11} + f_{12} + f_{13} + f_{14} + f_{15} + f_{16} + \tilde{f}_{17} + f_{18} = \rho$$

$$f_1 - f_2 + \tilde{f}_7 - f_8 + f_9 - f_{10} = \tilde{f}_{13} - \tilde{f}_{14} + f_{15} - f_{16} = \rho u_x$$

$$f_3 - f_4 + \tilde{f}_7 - f_8 + \tilde{f}_{11} - f_{12} - f_{13} + f_{14} + \tilde{f}_{17} - f_{18} = \rho v_y$$

$$f_5 - f_6 + f_7 - f_8 + \tilde{f}_{11} - f_{12} - f_{13} + f_{14} + f_{17} - f_{18} = \rho u_z.$$  

And $\rho u_{x}$, $\rho u_{z}$, $\rho v_{x}$, $\rho v_{z}$, $\rho v_{y}$ are the modified momentum we obtain, which we consider more ‘correct’ because it is calculated by the wall function model.

The next problem is to convert the momentum to the distribution functions. By considering the particle velocity of D3Q19 (see appendix: table A1), we can expand equation (2) on the free-slip boundary as:

$$f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + \tilde{f}_7 + f_8 + f_9 + f_{10} + \tilde{f}_{11} + f_{12} + f_{13} + f_{14} + f_{15} + f_{16} + \tilde{f}_{17} + f_{18} = \rho$$

$$f_1 - f_2 + \tilde{f}_7 - f_8 + f_9 - f_{10} = \tilde{f}_{13} - \tilde{f}_{14} + f_{15} - f_{16} = \rho u_x$$

$$f_3 - f_4 + \tilde{f}_7 - f_8 + \tilde{f}_{11} - f_{12} - f_{13} + f_{14} + \tilde{f}_{17} - f_{18} = \rho v_y$$

$$f_5 - f_6 + f_7 - f_8 + \tilde{f}_{11} - f_{12} - f_{13} + f_{14} + f_{17} - f_{18} = \rho u_z.$$  

And $\rho u_{x}$, $\rho u_{z}$, $\rho v_{x}$, $\rho v_{z}$, $\rho v_{y}$ are the modified momentum we obtain, which we consider more ‘correct’ because it is calculated by the wall function model.
In addition, we assume that \( f_7, f_{14} \) are independent of \( f_{11}, f_{17} \). Therefore, according to equations (9)–(11), we have:

\[
\tilde{f}_7 + \tilde{f}_{14} = f_7 + f_{14}, \quad \tilde{f}_{11} + \tilde{f}_{17} = f_{11} + f_{17} \tag{12a}
\]

\[
\tilde{f}_7 - \tilde{f}_{14} = f_7 + f_{14} = \frac{\Delta t}{g_y} \tau_{w,x}, \quad \tilde{f}_{11} - \tilde{f}_{17} = f_{11} + f_{17} = \frac{\Delta t}{g_y} \tau_{w,z}. \tag{12b}
\]

Then \( \tilde{f}_7, \tilde{f}_{11}, \tilde{f}_{14}, \tilde{f}_{17} \) can be solved as:

\[
\tilde{f}_7 = f_7 + \frac{\Delta t}{2g_y} \tau_{w,x}, \quad \tilde{f}_{14} = f_{14} - \frac{\Delta t}{2g_y} \tau_{w,x} \tag{13a}
\]

\[
\tilde{f}_{11} = f_{11} + \frac{\Delta t}{2g_y} \tau_{w,z}, \quad \tilde{f}_{17} = f_{17} - \frac{\Delta t}{2g_y} \tau_{w,z}. \tag{13b}
\]

We notice that \( f_7, f_{11}, f_{14}, f_{17} \) in equations (13a) and (13b) are the distribution functions after the collision step under the free-slip boundary. Before the collision step, \( f_7, f_{11}, f_{14}, f_{17} \) correspond to \( f_{13}, f_{18}, f_8, f_{12} \), respectively. Therefore, we can conclude the integrated collision step of WFB boundary as:

\[
\tilde{f}_7^* = f_7 + \frac{\Delta t}{2g_y} \tau_{w,x}, \quad \tilde{f}_{14}^* = f_{14} - \frac{\Delta t}{2g_y} \tau_{w,x} \tag{14a}
\]

\[
\tilde{f}_{11}^* = f_{11} + \frac{\Delta t}{2g_y} \tau_{w,z}, \quad \tilde{f}_{17}^* = f_{17} - \frac{\Delta t}{2g_y} \tau_{w,z} \tag{14b}
\]

\[
f_7^* = f_2, \quad f_{14}^* = f_1, \quad f_8^* = f_4, \quad f_{17}^* = f_3, \quad f_6^* = f_5,
\]

\[
f_1^* = f_7^*, \quad f_3^* = f_9^*, \quad f_{11}^* = f_{10}^*, \quad f_{13}^* = f_{15}^*, \quad f_{17}^* = f_{16}^*, \quad f_{18}^* = f_{17}^*. \tag{14c}
\]

Equations (14a)–(14c) is the algorithm of the WFB. The WFB only occurs on the wall boundary grids and mainly reflects in the collision step, while the stream step is unchanged. Equations (14a) and (14b) are the core operations that implement the wall function. They indicate that the near-wall layer grids acquire an additional shear velocity, which has been reduced by the shear drag \( \tau_w \) on the wall. From equations (14a)–(14c) we can see that the sum of distribution functions before and after the WFB collision step is equal (i.e. sum of \( f_{u} \) is equal to that of \( f_{u}^* \)), further indicating the conservation of mass in the WFB boundary, and it will also be confirmed in the following case study. \( \tau_{w,x} \) and \( \tau_{w,z} \) are the x- and z-components of \( \tau_w \) obtained from the wall function, respectively, and are solved as equation (15). The negative sign indicates that the shear drag \( \tau_{w,x} \) and \( \tau_{w,z} \) should be in the reverse direction of the corresponding components \( u_x \) and \( u_z \) of the shear velocity.

\[
\tau_{w,x} = -\frac{u_x}{\sqrt{u_x^2 + u_z^2}} \tau_w, \quad \tau_{w,z} = -\frac{u_z}{\sqrt{u_x^2 + u_z^2}} \tau_w. \tag{15}
\]

**2.3. Calculation of shear drag \( \tau_w \): Spalding’s law**

The remaining task is to obtain the correct shear drag \( \tau_w \) on the wall. In this study, we choose the Spalding’s law (Spalding 1961, Launder and Spalding 1974) as the wall function to be
incorporated into the boundary, as shown in equation (16). Spalding’s law is chosen due to its simplicity and wide applicability stated in section 1.

\[
y^+ = u^+ + e^{-\kappa B} \left[ e^{e^{-u^+}} - 1 - (\kappa \cdot u^+) - \frac{(\kappa \cdot u^+)^2}{2} - \frac{(\kappa \cdot u^+)^3}{6} \right]
\]

where, \( \kappa = 0.41 \) and \( B = 5.5 \), which are constant in the Spalding’s law (Spalding 1961, Launder and Spalding 1974). \( y^+ \) and \( u^+ \) are the distances from the wall and velocity nondimensionalized by the friction velocity \( u_\tau \), as shown in equation (17). \( u \) is the velocity in the frame of reference of the wall (i.e. \( u - u_{wall} \)), ensuring the Galilean invariant.

\[
y^+ = \frac{yu_\tau}{\nu}, \quad u^+ = \frac{|u|}{u_\tau}, \quad u_\tau = \sqrt{\frac{\tau_w}{\rho}}.
\]

Since the Spalding’s law is an implicit equation, we need an initial value and a root-finding algorithm (here, we have utilized the Newton’s method because it is easy to implement and the error is easy to control). In a single step of WFB collision, the initial \( u_\tau \) is first calculated using the distance of the 1st-layer grid and the shear velocity on it. Thereafter, it is substituted into equation (16), and more approximated values of \( u_\tau \) and \( \tau_w \) are obtained after several iterations of the Newton’s method, controlled by the maximum tolerate error and maximum iteration steps set in advance. Lastly, the corrected value of \( \tau_w \) is reflected in the distribution functions using equations (14) and (15). After completing these operations, we shift to the next stream step.

So far, the WFB boundary has been completely implemented, which can be applied to all straight solid boundaries (e.g. walls, ground, and other solid object surfaces). Two important points should be explained here. One is that the implementation of WFB boundary only requires partial diagonal distribution functions and the shear drag; no specific information of discrete velocity schemes or collision functions are needed. In addition, the wall function model is not restricted to Spalding’s law that was utilized in this study. On the contrary, it is a general framework that can incorporate any wall function model into the LBM, given that the candidate model is capable of providing the appropriate shear drag \( \tau_w \). Therefore, WFB is a general framework to implement a wall function into LBM in a certain extent.

The other point is that although WFB is achieved based on the standard BB boundary, we believe that this concept has the potential to be extended to a more complex BB boundary. For example, in the Bouzidi–Firdaouss–Lallemand linear interpolated BB scheme (Bouzidi et al 2001), the last fluid grid near the wall was the interpolation function of this grid and the adjacent fluid grid in the last time step, and it was related to the dimensionless distance, \( q \), of the fluid grid to the wall. Therefore, it is not difficult to add the shear drag, \( \tau_w \), into the interpolation. The essential point to note is that \( \tau_w \), \( \Delta t \), and \( \Delta y \) should be determined using the dimensionless distance, \( q \).

3. Simulation and validation

3.1. Simulated case description

Isothermal turbulent channel flow was employed to evaluate the proposed boundary. The simulation domain depicted in figure 4, is the same as that proposed by Moin and Kim (1982); the lengths along the streamwise direction \( x \), normal direction \( y \), and span direction \( z \) components were \( 2\pi D, 2D, \) and \( \pi D \), respectively. \( Re_\tau = 640 \) and 2003 were utilized for the validation (\( Re_\tau = u_\tau D/\nu \), \( D \): half height of channel; \( u_\tau \): the friction velocity). The channel was driven by a constant body force and ran long enough to ensure \( Re_\tau \). Simulations of LBM-LES were
implemented using the multi-relaxation-time model (d’Humières et al 2002). To simplify the problem, we chose the standard Smagorinsky SGS model ($C_s = 0.1$ (Rogallo and Moin 1984)) and added the van-Driest style damping function (van Driest 1956). The $x$- and $z$-direction boundaries were periodic, and the $y$-direction boundary was the wall where we implemented the BB or the WFB boundary. A very small uniform velocity was set in the whole channel as the initial condition.

The case settings are listed in table 1. To validate the wall function, the 1st-layer grid should be in the logarithmic layer or the buffer layer; i.e. the $y^+$ of the 1st-layer grid should be larger. However, it is difficult to place the 1st-layer grid in the logarithmic layer because it may cause the grid system to become too coarse and the results unacceptable. In this study, we set the grid resolutions according to the principle of placing the 1st-layer grid in the buffer layer ($\sim 10 < y^+ < \sim 100$). Although these grid resolutions may be coarse to obtain sufficient satisfying results throughout the channel, they are suitable for validating the wall function. Because the LBM is a weakly-compressible method for addressing incompressible flows, compressibility errors may occur if an improper time interval is utilized (Klainerman and Majda 1982, Martínez et al 1994, Reider and Sterling 1995). Therefore, according to our pre-tests, the time intervals of each case were set to be considerably small to make sure that the $Ma_{LB} \ll 0.3$ and to avoid apparent compressibility errors (Martínez et al 1994, Reider and Sterling 1995).

$\langle u \rangle$ of the 1st-layer grid near the wall and the middle-layer grid was monitored for all the BB cases to ensure time convergence (figure 5). $\langle u \rangle$ became stable after approximately 20 T ($T = D/u_\tau$), and the data at 92 T were utilized as they reached the time convergence. Thereafter, the time-averaged values of the same layer grids in the simulation domain were spatially averaged and utilized as the final result of every $y$-coordinate. After the sufficient sampling period, the force balance state was achieved and $u_\tau$ generally satisfied the theoretical value. Therefore, the results were normalized using $D$ and theoretical value of $u_\tau$.

3.2. Results and discussions

3.2.1. Confirmation of mass conservation in WFB. The mass conservation in the WFB had to be first confirmed. Here, we examined the differences between the distribution functions $f_a$ before the WFB collision and $f_a^*$ after the WFB collision at all the boundary grids. 5000 time steps were checked in all the WFB cases when the turbulence was fully developed. Appendix B shows the detailed results.
Table 1. Case settings.

| Test case   | $Re_{τ}$ and $Re^a$ | Grid resolutions | Mesh size ($x \times y \times z$) | $y^+$ at the 1st layer grid | Time interval (s) | $Ma_{LB}$ | $y$-direction boundary condition |
|-------------|---------------------|-------------------|-----------------------------------|----------------------------|------------------|-----------|----------------------------------|
| A20_BB      | $Re_{τ} = 640$; $Re \sim 13800$ | $D/20$            | 128 $\times$ 40 $\times$ 64      | 32                        | 1/800            | 0.060     | BB                               |
| A20_WFB     |                      |                   |                                   |                           |                  |           | WFB                              |
| A40_BB      | $Re_{τ} = 2003$; $Re \sim 48000$ | $D/40$            | 256 $\times$ 80 $\times$ 128     | 16                        | 1/1600           | 0.069     | BB                               |
| A40_WFB     |                      |                   |                                   |                           |                  |           | WFB                              |
| B40_BB      |                      |                   |                                   |                           |                  |           | BB                               |
| B40_WFB     |                      |                   |                                   |                           |                  |           | WFB                              |
| B80_BB      |                      |                   |                                   |                           |                  |           | BB                               |
| B80_WFB     |                      |                   |                                   |                           |                  |           | WFB                              |

$^a$ $Re$ is defined by the time-averaged velocity in the middle of the channel.
Figure 5. Normalized values $\langle u \rangle$ of the 1st-layer grid near the wall and the middle-layer grid at two different frictional. All the values became stable after approximately 20 T; data at 92 T were utilized as they reached the time convergence.

Figure 6. Normalized velocity profiles for two different grid resolutions with two different wall boundary conditions.

Approximately 11%–14% samples of the differences were not zero. However, the orders of the differences were in the range of approximately $1 \times 10^{-16} - 1 \times 10^{-14}$ of the mean $f_a$ at the wall boundary, further indicating that the non-zero differences were considerably smaller than $f_a$, and that it was probably caused by the precision errors of the computer while calculating the floating-point numbers. Therefore, the ‘input’ distribution functions (or mass) before the WFB collision were generally equal to the ‘output’ after the collision, which demonstrates the conservation of mass in the WFB.

3.2.2. Results of time-averaged velocity. The time-averaged velocity profiles are depicted in figure 6. The experimental data from Hussain and Reynolds (1975), and Clark (1968) were used as the basis for $Re_\tau = 640$; the DNS data from Hoyas and Jiménez (2006) were used for $Re_\tau = 2003$.

At $Re_\tau = 640$, an underestimation of the time-averaged velocity was clearly observed in A20_BB and A40_BB in the buffer layer ($y^+ < \sim 100$), especially at the 1st-layer grid. With the increase in grid resolution, the deviations were compensated partially. Meanwhile, in
A20_WFB and A40_WFB, the 1st-layer grids were generally on the Spalding’s law line and they agreed with the experimental data better than the BB cases. However, in the logarithmic layer \((y^+ \geq \sim 100)\), A20_WFB overestimated the velocity whereas A20_BB agreed better with the DNS data.

At \(Re_\tau = 2003\), the differences between BB and WFB became significantly larger. Both B40_BB and B80_BB underestimated \(u^+\) in both buffer and logarithmic layers. This evidently shows that the BB boundary mispredicted \(\tau_w\), which consequently affected the accuracy of the time-averaged velocity. While utilizing WFB, the underestimation of \(u^+\) was compensated, and both B40_WFB and B80_WFB agreed better with the DNS data. In particular, both the cases coincided with the Spalding’s law in the buffer layer, although discrepancies were still visible in the logarithmic layer to some extent.

The error analysis was conducted by utilizing the L2 error norm \(\epsilon_{u^+}\) (Ferziger and Perič 2002) defined by equation (19), and the Spalding’s law was utilized as the basis. \(u^+_{\text{LBM}(i)}\) and \(u^+_{\text{Spalding}(i)}\) represented \(u^+\) at \(y^+ = i\) and were obtained using the LBM and Spalding’s law, respectively. A smaller \(\epsilon_{u^+}\) demonstrated a smaller deviation between the simulation and the Spalding’s law, and thus, exhibited a higher accuracy. The errors in the buffer layer, logarithmic layer, and the entire domain (including both buffer and logarithmic layer) were examined and are listed in table 2, respectively.

\[
\epsilon_{u^+} = \sqrt{\frac{\sum_i \left(u^+_{\text{LBM}(i)} - u^+_{\text{Spalding}(i)}\right)^2}{\sum_i u^+_{\text{Spalding}(i)}^2}}. \tag{19}
\]

In all BB cases, the error of the buffer layer was larger than that of the logarithmic layer, and this affected the accuracy of the entire domain. It is partly because that the turbulent model was failed to predict the transition accurately using such a coarse grid system. This is the reason that a wall function model is needed. Furthermore, this error became larger with the increase in \(Re_\tau\); however, it became smaller with the increase in grid resolution. This also demonstrates that BB boundary will reduce the near-wall accuracy in simulating high-\(Re\) flows when using coarse grid systems. While using WFB, the accuracy of the buffer layer was observed to improve, and the errors became stable (no larger than 5%, which was considered acceptable) in all the cases. This indicates that the WFB boundary implemented a proper shear drag on the wall by following the Spalding’s law, and corrected the near-wall velocity.

As stated previously, the velocity overestimation in the logarithmic layer occurred in A20_WFB, thereby resulting in a larger \(\epsilon_{u^+}\) when compared to A20_BB; however, the reason is not apparent yet. As discussed in the introduction, the accuracy of the results in the off-wall region was comprehensively affected by several other factors in addition to the wall boundary, such as SGS models, collision functions, and discrete velocity schemes. In this study, the effect of the wall boundary on the logarithmic layer was probably not as significant as other factors in the not-too-high-\(Re (Re_\tau = 640)\) case. Meanwhile, the averaged velocity of WFB in the logarithmic layer at \(Re_\tau = 2003\) was better than that of BB, demonstrating that the wall boundary influenced the accuracy of the off-wall region greater in the higher-\(Re\) case.

In the logarithmic layer \((y^+ \geq \sim 100)\), the inertia force became predominant, and all the cases followed the logarithmic law expressed in the following equation:

\[
\frac{|\langle u \rangle|}{u_\tau} = \frac{1}{\kappa} \ln y^+ + b \tag{20}
\]

where, \(\kappa = 0.41\) is the Karman constant, whereas the value of \(b\) refers to the prevalent range of 4.8–5.9 with respect to the experiment based on different conditions (Mathew 2010). In this
| Re_τ | Case name | Buffer layer ($y^+ < \sim 100$) | Logarithmic layer ($y^+ \geq \sim 100$) | Entire domain |
|------|-----------|-------------------------------|-----------------------------------|--------------|
| 640  | A20_BB    | 0.183                         | 0.009                             | 0.156        |
|      | A20_WFB   | 0.069                         | 0.055                             | 0.056        |
|      | A40_BB    | 0.103                         | 0.039                             | 0.048        |
|      | A40_WFB   | 0.071                         | 0.067                             | 0.067        |
|      | B40_BB    | 0.911                         | 0.049                             | 0.420        |
|      | B40_WFB   | 0.049                         | 0.080                             | 0.429        |
| 2003 | B80_BB    | 0.647                         | 0.224                             | 0.235        |
|      | B80_WFB   | 0.057                         | 0.235                             | 0.235        |
Table 3. Value of $b$ for each case.

| Case name | $b$ | Case name | $b$ |
|-----------|-----|-----------|-----|
| A20_BB    | 5.6 | B40_BB    | −0.1|
| D20_WFB   | 6.4 | B40_WFB   | 6.6 |
| D40_WFB   | 6.6 | B80_BB    | −4.1|
| A40_BB    | 6.2 | B80_WFB   | 6.5 |
| Exp (Hussain and Reynolds 1975) | 5.4 | DNS (Hoyas and Jiménez 2006) | 5.4 |

The time-averaged velocity in the logarithmic layer for all the cases was overestimated to some extent compared to the experimental or DNS data. The reason for this may be complex and can be attributed to factors such as grid resolutions, collision functions, and so on. However, all the cases were complied with the logarithmic law in general. Notably, negative values occurred in B40_BB and B80_BB, which further stated that the velocity was universally underestimated due to the improper shear drag produced by the BB boundary.

3.2.3. Results of Reynolds stress. Figure 7 shows the Reynolds normal and shear stresses for all the cases, respectively. At $Re_\tau = 640$, the experimental data proposed by Clark (1968) were added to validate $\sqrt{u_1'r_1'^2}$ and $\sqrt{u_z'^2}$ in addition to the data proposed by Hussain and Reynolds (1975) for validating $\sqrt{u_1'r_1'^2}$. It was observed that WFB improved the normal stresses near the wall to varying degrees at both $Re_\tau = 640$ and 2003 when compared to BB cases. In particular, for $\sqrt{u_1'r_1'^2}$ and $\sqrt{u_z'^2}$ at $Re_\tau = 2003$, the variation was larger than that at $Re_\tau = 640$. This suggests that the effect of WFB on the wall stress is more obvious to some extent in the higher-Re flow simulation. However, $\sqrt{u_z'^2}$ was underestimated at $y^+ < \sim 100$ by both the BB and WFB cases at $Re_\tau = 640$, which was also reported by Piomelli et al (1987). They suggested that this was a typical tendency in the close-to-wall region if the grids are not sufficiently fine. Meanwhile, $\sqrt{u_1'r_1'^2}$ at $Re_\tau = 640$ was overestimated near the channel center in all the BB and WFB cases. In addition, there were also deviations in $\sqrt{u_1'r_1'^2}$ and $\sqrt{u_z'^2}$ approximately at $y^+ = 400$ at $Re_\tau = 2003$ in both BB and WFB cases. A possible reason for these deviations was the coarse grid systems; however, the collision functions or discrete velocity scheme may also have affected the results, as stated earlier. For the shear stress, shear–stress profiles obtained by WFB attained the equilibrium shape that balanced the pressure gradient in the regions away from the walls, similar to that obtained by BB. In the near-wall region, Reynolds shear stress and viscous shear stress together balanced the pressure gradient. At the 1st-layer grid, Reynolds shear stress reproduced by BB was closely related to the grid resolution. WFB improved the stress and reduced the effect of the grid resolution, so that the value became closer.

Figure 8 depicts the normalized probability distribution functions (PDFs) of the coordinate of all the 1st-layer grids off-wall in terms of inner variables for all cases ($y_1^+$). This is an important attribute of the wall function model because it implies the distribution of the instantaneous shear stress on the wall (Pantano et al 2008). The results of FVM-LES with a wall function ($Re_\tau = 2003$) reported by Pantano et al (2008) is also added for reference. Here, $y_1^+$ denotes the wall-parallel spatial averages of $y_1^+$. We observed that the PDF of $y_1^+$ in all WFB cases at different $Re_\tau$ scaled well when normalized with its mean and variance, and it also agreed well with Pantano’s result. The results, therefore, indicate that the distribution of
Figure 7. Reynolds normal and shear stresses for two different grid resolutions with two different wall boundary conditions in the conditions of $Re_\tau = 640$ (left), and $Re_\tau = 2003$ (right). Experimental data from Hussain and Reynolds (1975) and Clark (1968), and DNS data from Hoyas and Jiménez (2006) were compared.
shear stress reproduced by WFB was in close proximity to that produced by FVM-LES with a wall function model.

4. Conclusions

In this study, a general framework ‘WFB’ boundary was proposed to incorporate a wall function into the LBM’s boundary conditions, independent of specific information of discrete velocity schemes and collision functions. Spalding’s law was utilized as the wall function. Simulations of a turbulent channel flow at Re$_{\tau}$ = 640 and 2003 were implemented using LBM-LES (standard Smagorinsky SGS model) to validate the proposed boundary. The conclusions drawn based on the findings of this study are summarized as follows:

(a) The core idea of the WFB is to adjust the distribution functions, which are in the diagonal directions and pointing to the interior of the flow field, to reflect the shear drag obtained from a wall function model. Only partial diagonal distribution functions and shear drag was required when implementing WFB.

(b) The BB boundary underestimated the time-averaged velocity at the 1st-layer grids in the buffer layer for both Re$_{\tau}$ = 640, and 2003. WFB improved it and reduced the L2 error norm $\epsilon_{u^{+}}$ at buffer layer up to approximately 38% (Re$_{\tau}$ = 640) and 9% (Re$_{\tau}$ = 2003) of BB. The velocity at the 1st-layer grids agreed well with the Spalding’s law. This indicates that the WFB obtained the appropriate shear drag on the wall.

(c) The BB boundary underestimated the time-averaged velocity in the entire domain at (Re$_{\tau}$ = 2003) when utilizing coarse grids. The WFB compensated for the underestimation and reduced $\epsilon_{u^{+}}$ of the entire domain up to approximately 27% of BB when Re$_{\tau}$ = 2003. The whole mean velocity profile agreed with the experimental data more accurately when using WFB.
(d) The WFB produced similar distributions of the Reynolds normal and shear stresses with the BB, and it improved the Reynolds normal stress in the near-wall region to a certain extent, as compared to the BB.

(e) The WFB provided analogous distributions of shear stress on the wall with those of FVM-LES with a wall function.

Therefore, the WFB was established and could partially improve the near-wall accuracy of the LBM-LES in solving the turbulent channel flows compared to the BB boundary. Next, to apply the WFB to the irregular building geometries in wind engineering, we plan to extend it to more complex BB boundaries, such as the interpolated BB boundary. Meanwhile, to make WFB broader applicability in complex fluid fields, it is necessary to validate WFB using grid schemes with higher degrees of freedom, such as D3Q27. These will be tested and confirmed in our future work.

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Appendix A

D2Q9 and D3Q19 are the widely-utilized schemes to solve two-dimensional and three-dimensional flows in DdQq schemes (Qian et al 1992); figure A1 depicts the grid of these schemes.

Figures A2 and A3 depict the processes of the BB and no-slip boundary in D2Q9 scheme, respectively.

Table A1 lists the discrete velocity vectors of D3Q19 scheme (Qian et al 1992).
Figure A1. Grid system of D2Q9 and D3Q19 schemes. Modified from Krüger et al (2017) © 2020 Springer Nature Switzerland AG. Part of Springer Nature). With permission of Springer.

Figure A2. Sketch of the BB boundary in D2Q9 scheme. Modified from Krüger et al (2017) © 2020 Springer Nature Switzerland AG. Part of Springer Nature). With permission of Springer.

Figure A3. Sketch of the free-slip boundary in D2Q9 scheme. Modified from Krüger et al (2017) © 2020 Springer Nature Switzerland AG. Part of Springer Nature). With permission of Springer.
Table A1. Discrete velocity vectors $\mathbf{e}_a$ of D3Q19.

| $a$   | $\mathbf{e}_a$       | $a$   | $\mathbf{e}_a$       |
|-------|----------------------|-------|----------------------|
| 0     | $(0, 0, 0)$          | 9, 10 | $(\pm 1, 0, \pm 1)$  |
| 1, 2  | $(\pm 1, 0, 0)$     | 11, 12| $(0, \pm 1, \pm 1)$  |
| 3, 4  | $(0, \pm 1, 0)$     | 13, 14| $(\pm 1, \mp 1, 0)$  |
| 5, 6  | $(0, 0, \pm 1)$     | 15, 16| $(\pm 1, 0, \mp 1)$  |
| 7, 8  | $(\pm 1, \pm 1, 0)$ | 17, 18| $(0, \pm 1, \mp 1)$  |

Table B1. Probability of $\Delta f \neq 0$ in all cases and the order of maximum $\Delta f / f_a$.

| Case name | A20_WFB | A40_WFB | B40_WFB | B40_WFB |
|-----------|---------|---------|---------|---------|
| Rate of $\Delta f \neq 0$ | 13.29%  | 13.81%  | 11.35%  | 11.79%  |
| maximum $\Delta f / f_a$ | $\sim O(10^{-15})$ | $\sim O(10^{-16})$ | $\sim O(10^{-15})$ | $\sim O(10^{-14})$ |

Appendix B

$\Delta f$ was defined to examine the mass conservation at the wall boundary, which is the average of the differences between $f_a$ before WFB collision and $f_a^*$ after WFB collision of all boundary grids, as shown in equation (B1). Here, $i$ represents the $i$th grid at the wall boundary, and $N$ represents the total number of grids on the wall. Furthermore, $\Delta f$ in table B1 lists the rate of $\Delta f \neq 0$ in the 5000 steps in all the cases, and the order of the quotient of maximum $\Delta f$ and spatial average $f_a$ at the wall boundary.

$$\Delta f = \frac{1}{N} \sum_{i=1}^{N} \left( \sum_{a=0}^{18} f_a^* |_{i} - \sum_{a=0}^{18} f_a |_{i} \right). \quad \text{(B1)}$$

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References

Ahangar E K, Ayani M B, Esfahani J A and Kim K C 2020 Lattice Boltzmann simulation of diluted gas flow inside irregular shape microchannel by two relaxation times on the basis of wall function approach Vacuum 173 109104

Béghein C, Jiang Y and Chen Q Y 2005 Using large eddy simulation to study particle motions in a room Indoor Air 15 281–90

Bouzidi M, Firdaouss M and Lallemand P 2001 Momentum transfer of a Boltzmann-lattice fluid with boundaries Phys. Fluids 13 3452–9

Breuer M, Bernsdorf J, Zeiser T and Durst F 2000 Accurate computations of the laminar flow past a square cylinder based on two different methods: lattice-Boltzmann and finite-volume Int. J. Heat Fluid Flow 21 186–96

Clark J A 1968 A study of incompressible turbulent boundary layers in channel flow J. Basic Eng. 90 455

Cornubert R, d’Humières D and Levermore D 1991 A Knudsen layer theory for lattice gases Phys. D: Nonlinear Phenom. 47 241–59
d’Humières D, Ginzburg I, Krafczyk M, Lallemand P and Luo L S 2002 Multiple-relaxation-time lattice Boltzmann models in three dimensions Phil. Trans. R. Soc. A 360 437–51
Dong Y H and Sagaut P 2008 A study of time correlations in lattice Boltzmann-based large-eddy simulation of isotropic turbulence Phys. Fluids 20 035105
Fakhari A and Lee T 2015 Numerics of the lattice Boltzmann method on nonuniform grids: standard LBM and finite-difference LBM Comput. Fluids 107 205–13
Fernando M, Beronov K and Ytrehus T 2009 Large eddy simulation of turbulent open duct flow using a lattice Boltzmann approach Math. Comput. Simul. 79 1520–6
Ferziger J H and Perić M 2002 Computational Methods for Fluid Dynamics vol 46 (Berlin, Heidelberg: Springer Berlin Heidelberg)
Gehrke M, Jannsen C F and Rung T 2017 Scrutinizing lattice Boltzmann methods for direct numerical simulations of turbulent channel flows Comput. Fluids 156 247–63
Geier M, Schönherr M, Pasquali A and Krafczyk M 2015 The cumulant lattice Boltzmann equation in three dimensions: theory and validation Comput. Math. Appl. 70 507–47
Geller S, Krafczyk M, Tölke J, Turek S and Hron J 2006 Benchmark computations based on lattice-Boltzmann, finite element and finite volume methods for laminar flows Comput. Fluids 35 888–97
Gendre F, Ricot D, Fritz G and Sagaut P 2017 Grid refinement for aeroacoustics in the lattice Boltzmann method: a directional splitting approach Phys. Rev. E 96 023311
Grötzbach G 1987 Direct numerical and large eddy simulations of turbulent channel flows En cyc. Fluid Mech. 6 1337–91
Han M, Ooka R and Kikumoto H 2018 Comparison between lattice Boltzmann method and finite volume method for LES in the built environment The 7th Int. Symp. on Computational Wind Engineering 2018 vol m (Seoul) pp 2–5
Han M, Ooka R and Kikumoto H 2019 Lattice Boltzmann method-based large-eddy simulation of indoor isothermal airflow Int. J. Heat Mass. Transf. 130 700–9
Haussmann M, Barreto A C, Kouyi G L, Rivière N, Nirschl H and Krause M J 2019 Large-eddy simulation coupled with wall models for turbulent channel flows at high Reynolds numbers with a lattice Boltzmann method—application to Coriolis mass flowmeter Comput. Math. Appl. 78 3285–302
Hoyas S and Jiménez J 2006 Scaling of the velocity fluctuations in turbulent channels up to $Re_c = 2003$ Phys. Fluids 18 10–14
Hussain A K M F and Reynolds W C 1975 Measurements in fully developed turbulent channel flow J. Fluids Eng. 97 568
Inamuro T 1999 The lattice Boltzmann method and its applications for complex flows J. Soc. Powder Technol. Japan 36 286–91
Kawai S and Larsson J 2012 Wall-modeling in large eddy simulation: length scales, grid resolution, and accuracy Phys. Fluids 24 015105
Kikumoto H, Ooka R, Han M and Nakajima K 2018 Consistency of mean wind speed in pedestrian wind environment analyses: mathematical consideration and a case study using large-eddy simulation J. Wind Eng. Ind. Aerodyn. 173 91–9
Klainerman S and Majda A 1982 Compressible and incompressible fluids Commun. Pure Appl. Math. 35 629–51
Krüger T, Kusumaatmaja H, Kuzmin A, Shadt O, Silva G and Viggen E M 2017 The Lattice Boltzmann Method: Principles and Practice (Berlin: Springer)
Kuwata Y and Suga K 2015 Large eddy simulations of pore-scale turbulent flows in porous media by the lattice Boltzmann method Int. J. Heat Fluid Flow 55 143–57
Lagrava D, Malaspinas O, Latt J and Chopard B 2012 Advances in multi-domain lattice Boltzmann grid refinement J. Comput. Phys. 231 4808–22
Lauder B E and Spalding D B 1974 The numerical computation of turbulent flows Comput. Methods Appl. Mech. Eng. 3 269–89
Li W and Luo L S 2016 Finite volume lattice Boltzmann method for nearly incompressible flows on arbitrary unstructured meshes Commun. Comput. Phys. 20 301–24
Liu X and Guo Z 2013 A lattice Boltzmann study of gas flows in a long micro-channel Comput. Math. Appl. 65 186–93
Malaspinas O and Sagaut P 2014 Wall model for large-eddy simulation based on the lattice Boltzmann method J. Comput. Phys. 275 25–40
Martínez D O, Matthaeus W H, Chen S and Montgomery D C 1994 Comparison of spectral method and lattice Boltzmann simulations of two-dimensional hydrodynamics Phys. Fluids 6 1285–98
Mathew J 2010 Large eddy simulation Def. Sci. J. 60 598–605
Moin P and Kim J 1982 Numerical investigation of turbulent channel flow J. Fluid Mech. 118 341–77
Norouzi A and Esfahani J A 2014 Two relaxation time lattice Boltzmann equation for high Knudsen number flows using wall function approach Microfluid. Nanofluid. 18 323–32
Pantano C, Pullin D I, Dimotakis P E and Matheou G 2008 LES approach for high Reynolds number wall-bounded flows with application to turbulent channel flow J. Comput. Phys. 227 9271–91
Pasquali A, Geier M and Krajczyk M 2020 Near-wall treatment for the simulation of turbulent flow by the cumulant lattice Boltzmann method Comput. Math. Appl. 79 195–212
Piomelli U, Ferziger J H and Moin P 1987 Models for large eddy simulations of turbulent channel flows including transpiration Stanford Univ. Rep. TF–32
Qian Y H, d’Humieres D and Lallemand P 1992 Lattice BGK models for Navier–Stokes equation EPL 17 479–84
Reider M B and Sterling J D 1995 Accuracy of discrete-velocity BGK models for the simulation of the incompressible Navier–Stokes equations Comput. Fluids 24 459–67
Rogallo R S and Moin P 1984 Numerical simulation of turbulent flows Annu. Rev. Fluid Mech. 16 99–137
Sajjadi H, Salmanzadeh M, Ahmadi G and Jafari S 2017 Turbulent indoor airflow simulation using hybrid LES/RANS model utilizing lattice Boltzmann method Comput. Fluids 150 66–73
Spalding D B 1961 A single formula for the ‘law of the wall’ J. Appl. Mech. 28 455
Stathopoulos T and Baskaran B A 1996 Computer simulation of wind environmental conditions around buildings Eng. Struct. 18 876–85
Suga K, Chikasue R and Kuwata Y 2017 Modelling turbulent and dispersion heat fluxes in turbulent porous medium flows using the resolved LES data Int. J. Heat Fluid Flow 68 225–36
Toparlar Y, Blocken B, Vos P, van Heijst G J F, Janssen W D, van Hooff T, Montazeri H and Timmermans H J P 2015 CFD simulation and validation of urban microclimate: a case study for Bergpolder Zuid, Rotterdam Build. Environ. 83 79–90
van Driest E R 1956 On turbulent flow near a wall J. Aeronaut. Sci. 23 1007–11
Versteeg H K and Malalasekera W 2007 An Introduction to Computational Fluid Dynamics - The Finite Volume Method (Harlow: Pearson Education Limited)
Werner H and Wengle H 1993 Large-eddy simulation of turbulent flow over and around a cube in a plate channel Turbulent Shear Flows 8 (Berlin, Heidelberg: Springer Berlin Heidelberg) pp 155–68
Wilhelm S, Jacob J and Sagaut P 2018 An explicit power-law-based wall model for lattice Boltzmann method-Reynolds-averaged numerical simulations of the flow around airfoils Phys. Fluids 30 065111
Wu C-J and Guan H 2009 Lattice Boltzmann dynamics and dynamical system sub-grid models Mod. Phys. Lett. B 23 349–52
Zhou X, Dong B, Chen C and Li W 2019 A thermal LBM-LES model in body-fitted coordinates: flow and heat transfer around a circular cylinder in a wide Reynolds number range Int. J. Heat Fluid Flow 77 113–21
Zhuo C and Zhong C 2013 LES-based filter-matrix lattice Boltzmann model for simulating turbulent natural convection in a square cavity Int. J. Heat Fluid Flow 42 10–22
Ziegler D P 1993 Boundary conditions for lattice Boltzmann simulations J. Stat. Phys. 71 1171–7