Modified mass-conservative curved boundary scheme for lattice Boltzmann simulations

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Abstract

In this paper, we firstly investigate the performance of three types of curved boundary schemes in two-phase lattice Boltzmann (LB) simulations through modeling a droplet resting on a circular cylinder. All of the investigated schemes are found to result in mass leakage, i.e., the droplet unphysically “evaporates” under the no-slip and isothermal conditions. Subsequently, numerical analysis is carried out to figure out the origin of mass leakage of the curved boundary schemes by simulating static flow under gravity. It is found that mass leakage occurs in all the cases except when the curved boundary schemes reduce to the halfway bounce-back scheme. According to the numerical results, it is clear that the mass leakage is caused by the imbalance between the amount of mass streamed out by the post-collision outgoing distribution functions and the amount of mass streamed into the system by the incoming (unknown) distribution functions at each boundary node. On the basis of the numerical investigations, we propose two modified mass-conservative boundary schemes for treating no-slip curved boundaries. Numerical simulations are performed for steady flow past a circular cylinder, natural convection in a square enclosure with a circular cylinder, and droplet resting on a circular cylinder to validate the numerical accuracy of the modified curved boundary schemes and their capability of conserving mass in two-phase LB simulations.

Keywords: lattice Boltzmann model; curved boundary scheme; mass leakage.
1. Introduction

In the past three decades, the lattice Boltzmann (LB) method [1-5] has been developed into an efficient and powerful numerical approach for simulating fluid flow and heat transfer. Compared with traditional numerical methods, the LB method has some major advantages. First, in the LB method the fluid flow is described by a discrete kinetic equation based on the particle distribution functions, which is a more fundamental level than normal continuum approaches [6]. Second, the fluid pressure and the strain tensor are available locally in the LB method, while the pressure field in traditional numerical methods is usually obtained by solving the Poisson equation. Moreover, the LB method is easy to parallelize because of its explicit algorithm and local interactions.

Unlike traditional numerical methods, which usually specify the macroscopic variables such as $\rho$ and $\mathbf{u}$ at the boundaries, the LB method applies the boundary condition to the particle distribution functions, giving more degrees of freedom [7] than the set of macroscopic variables. The oldest and simplest boundary condition or scheme in the LB community is the bounce-back scheme, which assumes that, when a particle hits a solid wall, it is reflected back to where it originally came from. Besides its simplicity, the bounce-back scheme is also well-known for its advantage in conserving mass [7]. When the physical boundary nodes lay at the lattice nodes, the bounce-back scheme is called the standard bounce-back scheme. On the contrary, when the solid wall locates at the middle of the fluid boundary node and the node inside the solid, the scheme is referred to as the halfway bounce-back scheme [8].

The bounce-back scheme is usually applicable to straight walls and it leads to staircase shaped boundaries for curved walls. Using a stair-shaped approximation, the fidelity of real geometry is lost and additional errors may be introduced [9]. In order to improve the accuracy of LB simulations involving curved boundaries, various curved boundary schemes have been developed. The first attempt which considers the accurate shape of a curved solid wall was made by Filippova and Hanel [10]. The basic
idea of their scheme is to create ghost nodes inside the solid and then apply a linear interpolation to
determine the unknown distribution functions at the boundary node. However, this scheme suffers from
numerical instability when the boundary node is close to the solid wall and the relaxation time is close to
1. Later, Mei et al. [11] proposed an improved curved boundary scheme based on the work of Filippova
and Hanel, which enhances the numerical stability. These two schemes have been demonstrated to be of
second-order accuracy.

Subsequently, Bouzidi et al. [12] devised a curved boundary scheme that does not require the
interpolation from a ghost node inside the solid. The motivation of their scheme is to interpolate the
distribution functions in the interior fluid region and to include additional information about the wall
location during the bounce-back process. Nevertheless, they employed separate treatments for different
regions. In order to avoid discontinuity in the boundary treatment, Yu et al. [13] developed a unified
scheme of Bouzidi et al.’s algorithm. This type of boundary schemes is also second-order accurate and
usually referred to as the interpolated bounce-back scheme. However, it introduces viscosity-dependence
boundary slip. To solve this issue, Ginzburg and d’Humières [14] proposed a multi-reflection boundary
scheme, which can be viewed as an enhanced interpolated bounce-back scheme. The main feature of
their scheme lies in that it determines the coefficients of the interpolation through the second-order
Chapman-Enskog expansion on the interpolated distribution functions [7].

Another type of curved boundary schemes involves only a single lattice node and is free of
interpolation, which is often called “one-point” or “single-node” boundary scheme. The advantage of
this type of boundary schemes is its local computations. The first one-point curved boundary scheme
was proposed by Junk and Yang [15]. Nevertheless, this scheme needs to compute the inverse of a matrix
at each boundary node. Recently, Zhao and Yong [16] devised an alternative single-node boundary
scheme. They considered a linear combination of the pre-collision and equilibrium distribution functions
at the fluid boundary node and introduced five parameters, which were determined by the Maxwell
iteration. Moreover, Tao et al. [17] recently developed a single-node curved boundary scheme for LB simulations of suspended particles. Besides the aforementioned schemes, there are some other developments of boundary schemes for LB simulations involving curved walls, which have been summarized in a recent book written by Krüger et al. [7].

Although various curved boundary schemes have been developed, they mostly suffer from the violation of mass conservation in LB simulations [7], i.e., there will be mass leakage (loss or gain) at each time step during the simulations. In order to enhance the mass conservation, several improved curved boundary schemes have been proposed. Kao and Yang [18] presented an interpolation-free boundary scheme to improve the mass conservation of the boundary condition. Bao et al. [19] devised an improved version of Mei et al.’s boundary scheme by redefining the density term in the equilibrium distribution function of the ghost node in the solid. In addition, Le Coupanec and Verschaeve [20] developed a mass-conservative boundary scheme for LB simulations with tangentially moving walls. Recently, Sanjeevi et al. [9] found that the interpolation-free boundary scheme proposed by Kao and Yang [18] still leads to mass leakage.

In the present study, we aim at developing alternative mass-conservative curved boundary schemes for LB simulations. Actually, for certain flows, such as two-phase flows, the mass conservation is a very crucial requirement. In the literature the halfway bounce-back scheme is usually employed in two-phase LB simulations involving curved boundaries [21, 22]. However, as previously mentioned, the fidelity of a curved boundary is lost and additional errors will be introduced when using the stair-shaped approximation of the halfway bounce-back scheme. Particularly, for two-phase flows with phase change [23-25], e.g., boiling heat transfer involving curved surfaces [26], the stair-shaped approximation will introduce many “artificial” nucleation sites and cause significant errors. A mass-conservative boundary scheme that is not only able to describe the accurate shape of a curved boundary but also capable of conserving mass is highly demanded for two-phase LB simulations.
The rest of the present paper is organized as follows. In Sec. 2 we briefly introduce the LB method and some of the existing curved boundary schemes. In Sec. 3 we investigate the performance of three types of curved boundary schemes in two-phase LB simulations through modeling a droplet on a circular cylinder. Subsequently, numerical analysis is carried out to figure out the origin of mass leakage of the curved boundary schemes. On the basis of the numerical investigations, two modified mass-conservative curved boundary schemes are proposed in Sec. 4. Numerical validation and discussion are made in Sec. 5, and finally a brief summary is given in Sec. 6.

2. Lattice Boltzmann method and curved boundary schemes

2.1. The lattice Boltzmann method

The LB equation using the Bhatnagar-Gross-Krook (BGK) collision operator can be written as [27]

\[
\begin{align*}
    f^e_\alpha (x + e_\alpha \delta_i, t + \delta t) - f_\alpha (x, t) &= - \frac{1}{\tau} \left[ f_\alpha (x, t) - f^e_\alpha (x, t) \right] + \delta_i F_\alpha (x, t), \tag{1}
\end{align*}
\]

where \( f_\alpha \) is the density distribution function, \( f^e_\alpha \) is the equilibrium density distribution function, \( x \) is the spatial position, \( e_\alpha \) is the discrete velocity in the \( \alpha \)th direction, \( t \) is the time, \( \delta_i \) is the time step, \( \tau \) is the non-dimensional relaxation time, and \( F_\alpha \) is the forcing term. The space is usually discretized in such a way that \( e_\alpha \delta_i \) is the distance between two neighboring nodes. Hence after one time step, \( f_\alpha (x, t) \) will arrive at its neighboring node along the lattice velocity direction \( e_\alpha \).

Therefore the LB equation can be split into two processes: the “collision” process

\[
\begin{align*}
    f^* \alpha (x, t) &= f_\alpha (x, t) - \frac{1}{\tau} \left[ f_\alpha (x, t) - f^e_\alpha (x, t) \right] + \delta_i F_\alpha (x, t), \tag{2}
\end{align*}
\]

and the “streaming” process

\[
\begin{align*}
    f_\alpha (x + e_\alpha \delta_i, t + \delta t) &= f^* \alpha (x, t), \tag{3}
\end{align*}
\]

where \( f^* \alpha (x, t) \) is the post-collision state of the density distribution function.

From Eqs. (2) and (3) it can be seen that the collision process is completely local and the streaming
process is completely linear. Using the two-dimensional nine-velocity (D2Q9) lattice model \[1-3, 27\],
the equilibrium density distribution function is given by

\[ f_{eq}^{α} = ω_{α}ρ \left[ 1 + \frac{e_{α} \cdot u}{c_{s}^2} + \frac{(e_{α} \cdot u)^2}{2c_{s}^4} - \frac{(u \cdot u)}{2c_{s}^2} \right], \tag{4} \]

where \( c_{s} = \frac{1}{\sqrt{3}} \) is the lattice sound speed and the weights \( ω_{α} \) are defined as \( ω_{0} = 4/9 \), \( ω_{4} = 1/9 \), and \( ω_{8} = 1/36 \). The kinematic viscosity is related to the non-dimensional relaxation time through

\( ν = c_{s}^2 (τ - 0.5) δ_{s} \), and the macroscopic density and velocity are calculated by, respectively

\[ ρ = \sum_{α} f_{α}, \quad ρu = \sum_{α} f_{α} e_{α} + \frac{δ_{s}}{2} F, \tag{5} \]

where \( F \) is the total force of the system and is incorporated into the LB equation through the forcing term \( F_{α}(x, t) \) \[3\].

2.2. Curved boundary schemes

Figure 1 illustrates a curved wall together with the neighboring lattice nodes. The link between the fluid boundary node \( x_{b} \) and the solid node \( x_{s} \) is cut by the wall at the point \( x_{w} \). The fraction of the intersected link in the fluid region is defined as \[7, 8\]

\[ q = \frac{|x_{b} - x_{w}|}{|x_{s} - x_{w}|}, \tag{6} \]

where \( 0 < q ≤ 1 \) and \( |x_{b} - x_{w}| \) depends on \( e_{α} \).

![FIG. 1. Sketch of a curved wall and the lattice nodes near the wall.](image)
The first LB boundary scheme for curved solid walls is proposed by Filippova and Hanel [10]. In order to determine the unknown distribution function \( f_\pi(x_s, t + \delta_t) \) at the fluid boundary node (the subscript \( \alpha \) denotes the opposite direction of \( \alpha \)), Filippova and Hanel [10] defined a post-collision density distribution function at the solid node \( x_s \),

\[
f_\pi(x_s, t) = (1 - \chi) f_\pi^a(x_s, t) + \chi f_\pi^{eq}(x_s, t). \tag{7}
\]

Then the unknown distribution function at the boundary node is obtained by \( f_\pi(x_s, t + \delta_t) = f_\pi^a(x_s, t) \) after the streaming process. The feature of this type of boundary schemes lies in that it introduces a fictitious equilibrium distribution function at the solid node, and Eq. (7) can be interpreted as a linear combination of the bounce-back distribution function and the fictitious equilibrium distribution function, which is defined as

\[
f_\pi^{eq}(x_s, t) = \omega_s \rho(x_s, t) \left[ 1 + \frac{\mathbf{e}_s \cdot \mathbf{u}_s}{c_s^2} + \frac{(\mathbf{e}_s \cdot \mathbf{u}_s)^2}{2c_s^4} - \frac{\mathbf{u}_a \cdot \mathbf{u}_a}{2c_s^2} \right], \tag{8}
\]

where \( \mathbf{u}_b = \mathbf{u}(x_s, t) \) and \( \mathbf{u}_s \) is a fictitious velocity. The parameter \( \chi \) in Eq. (7) depends on the choice of the fictitious velocity \( \mathbf{u}_s \). In Ref. [10], Filippova and Hanel utilized the following choices:

\[
q < 1/2: \quad \mathbf{u}_s = \mathbf{u}_b, \quad \chi = \frac{2q - 1}{\tau - 1}, \tag{9}
\]

\[
q \geq 1/2: \quad \mathbf{u}_s = \frac{q - 1}{q} \mathbf{u}_b + \frac{1}{q} \mathbf{u}_w, \quad \chi = \frac{2q - 1}{\tau}, \tag{10}
\]

where \( \mathbf{u}_w \) is the velocity at the point \( x_w \). In the present work, we only consider non-moving no-slip boundaries. Hence \( \mathbf{u}_w = 0 \). Obviously, when \( q = 1/2 \) (\( \chi = 0 \)), the scheme of Filippova and Hanel reduces to the halfway bounce-back scheme, i.e., \( f_\pi(x_s, t + \delta_t) = f_\pi^a(x_s, t) \).

It can be found that the parameter \( \chi \) will become very large when \( \tau \) is close to 1 as \( q < 1/2 \), and then the scheme of Filippova and Hanel will suffer from severe numerical instability [8]. To solve this problem, Mei et al. [11] proposed an improved scheme, which still uses Eq. (10) for \( q \geq 1/2 \) but employs the following choice for \( q < 1/2 \):
\[ \mathbf{u}_s = \mathbf{u}_f, \quad \mathbf{x} = \frac{2q - 1}{\tau - 2}, \]  

where \( \mathbf{u}_f = \mathbf{u}(\mathbf{x}_f, t) \) and \( \mathbf{x}_f = \mathbf{x}_b - \mathbf{e}_\alpha \delta \) is the location of the fluid node beyond the boundary node (cf. Fig. 1). Mei et al. [11] showed that the above modification significantly improves the numerical stability of the boundary scheme.

The interpolated bounce-back scheme proposed by Bouzidi et al. [12] employs an interpolation of the distribution functions in the interior fluid region. Using a linear interpolation, the boundary scheme of Bouzidi et al. is given by

\[
 f_\sigma (\mathbf{x}_b, t + \delta \tau) = \begin{cases} 
 2q f_\sigma (\mathbf{x}_b, t) + (1 - 2q) f_\sigma (\mathbf{x}_f, t), & q < \frac{1}{2} \\
 \frac{1}{2q} f_\sigma (\mathbf{x}_b, t) + \frac{2q - 1}{2q} f_\sigma (\mathbf{x}_f, t), & q \geq \frac{1}{2} 
\end{cases} \tag{12}
\]

As \( q = 1/2 \), Eq. (12) reduces to the halfway bounce-back scheme. Alternatively, when a quadratic interpolation is used, the scheme takes the following form [12]:

\[
 f_\sigma (\mathbf{x}_b, t + \delta \tau) = \begin{cases} 
 q(1 + 2q) f_\sigma (\mathbf{x}_b, t) + (1 - 4q^2) f_\sigma (\mathbf{x}_f, t) - q(1 - 2q) f_\sigma (\mathbf{x}_f, t), & q < \frac{1}{2} \\
 \frac{1}{q(2q + 1)} f_\sigma (\mathbf{x}_b, t) + \frac{2q - 1}{q} f_\sigma (\mathbf{x}_b, t) - \frac{2q - 1}{2q + 1} f_\sigma (\mathbf{x}_f, t), & q \geq \frac{1}{2} 
\end{cases} \tag{13}
\]

where \( \mathbf{x}_f = \mathbf{x}_b - 2\mathbf{e}_\alpha \delta \). Some other versions of the interpolated bounce-back boundary scheme can be found in Ref. [7].

Another type of boundary schemes is the one-point or single-node boundary scheme. In comparison with the original single-node boundary scheme proposed in Ref. [15], Zhao and Yong [16] recently devised a simpler single-node boundary scheme. They suggested a non-convex combination of \( f_\sigma (\mathbf{x}_b, t) \) and \( f_\alpha (\mathbf{x}_b, t) \) at the fluid boundary node, which is defined as

\[
 f_\pi (\mathbf{x}_b, t + \delta \tau) = \frac{2q}{1 + 2q} f_\sigma (\mathbf{x}_b, t) + \frac{1}{1 + 2q} f_\alpha (\mathbf{x}_b, t). \tag{14}
\]

In this scheme, the parameters/coefficients are determined based on the analysis using the Maxwell iteration. Obviously, Eq. (14) only involves local computations. Moreover, it can be found that Eq. (14) does not reduce to the halfway bounce-back scheme when \( q = 1/2 \).
3. Numerical investigations

In this section, numerical investigations are performed for the scheme of Mei et al. [11], the scheme of Bouzidi et al. [12], and the scheme proposed by Zhao and Yong [16], which can be regarded respectively as the representative schemes of the aforementioned three types of boundary schemes. In the remaining of this paper, these three boundary schemes are referred to as the MLS scheme, the Bouzidi scheme, and the Zhao-Yong scheme, respectively. Moreover, we use “L-Bouzidi” and “Q-Bouzidi” to represent the Bouzidi scheme employing the linear and quadratic interpolations, respectively.

3.1. Simulations of droplet resting on a circular cylinder

The test of a droplet on a circular cylinder is utilized to investigate the performance of the MLS scheme, the Bouzidi scheme, and the Zhao-Yong scheme in two-phase LB simulations. Under the no-slip and isothermal conditions, no evaporation will occur when a droplet is placed on a circular cylinder. However, if there exists mass leakage in the LB simulations such as mass loss at the curved wall boundary, the droplet will gradually become smaller, like an evaporating droplet. In our simulations, the isothermal pseudopotential multiphase LB method [3, 28-31] is adopted, in which the fluid-fluid interaction force is defined as follows:

\[
F = -G\psi(x) \sum_{\alpha} w_{\alpha}\psi(x + \vec{e}_\alpha \delta)\vec{e}_\alpha, \tag{15}
\]

where \(\psi\) is the pseudopotential, \(G\) is the interaction strength, and \(w_{\alpha}\) are the weights. For the nearest-neighbor interactions on the D2Q9 lattice, the weights are given by \(w_{\alpha} = 1/3\) for \(|\vec{e}_\alpha| = 1\) and \(w_{\alpha} = 1/12\) for \(|\vec{e}_\alpha| = 2\).

The pseudopotential is chosen as \(\psi(\rho) = \psi_0 \exp(-\rho_0/\rho)\), where \(\psi_0\) and \(\rho_0\) are both set to 1.0, which leads to the liquid density \(\rho_L = 2.783\) and the vapor density \(\rho_V = 0.3675\) when the interaction strength is taken as \(G = 10/3\) [32]. For this type of pseudopotentials, the forcing scheme proposed by Guo et al. [33] is employed to incorporate the fluid-fluid interaction force into the LB equation. The
contact angle is implemented via a constant virtual wall density [6, 34, 35]. A recent study of the contact angle schemes with curved boundaries can be found in Ref. [36]. In simulations, the computational domain is divided into $N_x \times N_y = 300 \times 350$ lattices. A circular cylinder of radius $R = 70$ is located at $(150, 130)$ and a droplet is initially placed on the circular cylinder, as shown in Fig. 2. The periodic boundary condition is utilized in the $x$ and $y$ directions and the kinematic viscosity is taken as $\nu = 0.15$ for both the liquid and vapor phases.

![Diagram of droplet on circular cylinder](image)

**FIG. 2** Initial setting of a droplet resting on a circular cylinder.

Some snapshots of the density contours obtained by the MLS scheme, the L-Bouzidi scheme, the Q-Bouzidi scheme, and the Zhao-Yong scheme are displayed in Figs. 3(a), 3(b), 3(c), and 3(d), respectively. From the figures it can be seen that, for all the investigated schemes, the simulated droplet gradually becomes smaller as time goes by, behaving like an evaporating droplet. However, the present simulations are performed using the isothermal pseudopotential LB model and the periodic boundary condition is applied in both the $x$ and $y$ directions, which means that there exists mass leakage at the surface of the circular cylinder due to the curved boundary schemes employed in the simulations. Among these boundary schemes, the Zhao-Yong scheme has the advantage of local computations since it is a single-node scheme, while the other schemes usually require the information of two or more nodes. However, from Fig. 3(d) we can clearly see that the Zhao-Yong scheme also suffers from the violation

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1 The present work had been finished before we conducted the study in Ref. [36].
of mass conservation although it does not involve any interpolation or extrapolation. Particularly, the

FIG. 3. Snapshots of density contours obtained by different boundary schemes. (a) MLS scheme, (b) L-Bouzidi scheme, (c) Q-Bouzidi scheme, and (d) Zhao-Yong scheme.
rate of mass loss caused by the Zhao-Yong scheme is much larger than those caused by the other boundary schemes, as shown in Fig. 4, which plots the variations of the normalized mass of the system during the simulations. The normalized mass is defined as \( \bar{m} = m/m_0 \), where \( m \) is the transient mass of the system and \( m_0 \) is the initial mass of the system at \( t = 0 \). From Fig. 4 we can also observe that the MLS scheme performs best among the investigated schemes, i.e., the mass of the system decreases relatively slowly in the test of using the MLS scheme. Besides, the figure shows that the performance of the Bouzidi scheme is better than that of the Zhao-Yong scheme, but worse than the MLS scheme.

**FIG. 4.** Simulations of droplet on a circular cylinder using different boundary schemes. Variations of the normalized mass of the system against time.

### 3.2. Numerical analysis of mass leakage through simulating static flow under gravity

In the preceding subsection, the fraction \( q \) defined by Eq. (6) varies between 0 and 1 along the surface of the circular cylinder. Hence, from the above numerical results it is difficult to identify the performance of the boundary schemes with a specific value of \( q \). To this end, we consider the test of static flow under gravity, which is illustrated in Fig. 5. The grid system is taken as \( N_x \times N_y = 100 \times 50 \) and the non-dimensional relaxation time \( \tau \) is set to 1. The aforementioned three types of boundary schemes are employed at the upper and lower solid walls and the periodic boundary condition is applied.
in the $x$ direction. The gravity force is given by $\mathbf{F}_g = (0, -\rho g)$, in which the gravitational acceleration is chosen as $g = 0.001$.

![Diagram](image)

**FIG. 5.** Configuration of static flow under gravity with an arbitrary $q$.

In our simulations, the fraction $q$ is taken as $q = n/10$ with $n = 1, 2, \ldots, 9$. The variations of the normalized mass of the system are plotted in Figs. 6(a), 6(b), 6(c), and 6(d) for the MLS scheme, the L-Bouzidi scheme, the Q-Bouzidi scheme, and the Zhao-Yong scheme, respectively. As can be seen in these figures, all the investigated boundary schemes basically exhibit different performance when different values of $q$ are applied. Specifically, for the MLS scheme, the L-Bouzidi scheme, and the Q-Bouzidi scheme, the mass of the system is conserved in the case of $q = 0.5$, but is decreased in other cases. In fact, from Sec. II it can be found that the MLS scheme and the Bouzidi scheme (regardless of using the linear or quadratic interpolation) reduce to the halfway bounce-back scheme as $q = 0.5$, which also numerically confirms that the halfway bounce-back scheme is capable of conserving mass.

To quantify the numerical results, an averaged mass change rate is evaluated at $t = 6 \times 10^4 \delta t$, which is defined as $\varepsilon = \left| m - m_0 \right| / m_0 \times 100\%$. Here $m$ is the mass of the system at $t = 6 \times 10^4 \delta t$. The results are displayed in Fig. 7. From the figure we can clearly see that the mass change rate caused by the Zhao-Yong scheme is much larger than those produced by other schemes in all the cases. Such a finding is consistent with the phenomenon observed in Fig. 4, which shows that the mass of the system decreases fastest in the test of using the Zhao-Yong scheme. Moreover, Fig. 7 shows that there are no
FIG. 6. Simulations of static flow under gravity using different boundary schemes. Variations of the normalized mass of the system against time.

FIG. 7. Simulations of static flow under gravity using different boundary schemes. Variations of the averaged mass change rate against the fraction $q$ defined by Eq. (6).
significant differences between the results of the MLS and Bouzidi schemes when \( q < 0.5 \), but the MLS scheme performs better as \( q > 0.5 \). In other words, the overall mass loss caused by the MLS scheme will be smaller than that produced by the Bouzidi scheme when the fraction \( q \) in the modeling varies from 0 to 1, which also explains why in Fig. 4 the MLS scheme exhibits better performance than the Bouzidi scheme.

The mass loss can also be evaluated at the mesoscopic level, i.e., in terms of the distribution functions. For the lower wall depicted in Fig. 5, the mass loss at a boundary node can be defined as

\[
\Delta m^L = f_4^*(x_b^L, t) + f_5^*(x_b^L, t) + f_6^*(x_b^L, t) - \left[ f_2(x_b^L, t + \delta_i) + f_3(x_b^L, t + \delta_i) + f_7(x_b^L, t + \delta_i) \right],
\]

where \( f_4^* \), \( f_5^* \), and \( f_6^* \) are the post-collision outgoing distribution functions at the boundary node, which will prorogate from the boundary node to the ghost nodes below the lower wall during the streaming step. The sum of \( f_4^* \), \( f_5^* \), and \( f_6^* \) denotes the amount of mass that is streamed out of the system through the boundary node. On the contrary, the sum of the incoming (unknown) distribution functions, i.e., \( f_2 \), \( f_3 \), and \( f_7 \) at \( t + \delta_i \) time level, which are obtained by the boundary schemes, represents the amount of mass that is streamed into the system via the boundary node. Similarly, for a boundary node near the upper wall in Fig. 5, the following mass loss \( \Delta m^U \) can be established:

\[
\Delta m^U = f_2^*(x_b^U, t) + f_3^*(x_b^U, t) + f_4^*(x_b^U, t) - \left[ f_5(x_b^U, t + \delta_i) + f_6(x_b^U, t + \delta_i) + f_7(x_b^U, t + \delta_i) \right].
\]

Owing to the periodicity, we choose a pair of boundary nodes at \( x = N_x/2 \) to monitor \( \Delta m^L \) and \( \Delta m^U \). The mass loss of such a pair of boundary nodes is given by \( \Delta m = \Delta m^L + \Delta m^U \).

The numerically obtained \( \Delta m \) is plotted in Fig. 8 against time for the cases of \( q = 0.3 \), \( 0.5 \), \( 0.6 \), and \( 0.8 \). Actually, from Eqs. (16) and (17) it can be easily found that \( \Delta m^L = \Delta m^U = 0 \) when the halfway bounce-back scheme is applied. Hence it can be seen that in Fig. 8 \( \Delta m \) is zero at \( q = 0.5 \) for the MLS scheme, the L-Bouzidi scheme, and the Q-Bouzidi scheme as these schemes reduce to the halfway bounce-back scheme when \( q = 0.5 \). In other cases, \( \Delta m \) is non-zero. The results displayed in Fig. 8 are
FIG. 8. Simulations of static flow under gravity using different boundary schemes. Variations of the mass loss of a pair of boundary nodes at $x = N_x/2$. The mass loss is defined as $\Delta m = \Delta m^L + \Delta m^U$, in which $\Delta m^L$ and $\Delta m^U$ are given by Eqs. (16) and (17), respectively.

consistent with those reported in Fig. 7. For example, at $q = 0.6$ and 0.8, the mass loss caused by the Bouzidi scheme is smaller than that caused by the Zhao-Yong scheme, but is larger than that produced by the MLS scheme. By making use of the periodicity in the $x$ direction, the averaged mass change rate of the system can be evaluated according to the data in Fig. 8. Taking the case of using the Zhao-Yong scheme at $q = 0.5$ as an example, the mass loss at each time step is around $1.3 \times 10^{-4}$, as shown in Fig. 8(b). Then the mass loss after $6 \times 10^4$ time steps is approximately given by $1.3 \times 10^{-4} \times 6 \times 10^4 = 7.8$ l.u., where l.u. represents lattice units. Hence the averaged mass change rate of the system at $t = 6 \times 10^4 \delta_t$
can be calculated by \( \epsilon \approx 7.8/\langle 49 \rho_0 \rangle \approx 16\% \), in which \( 49 \rho_0 \) (\( \rho_0 = 1 \)) is the initial mass on the forty-nine lattice nodes in the \( y \) direction (a pair of boundary nodes and forty-seven interior nodes). It can be found that such a result is consistent with that in Fig. 7.

To sum up, the numerical results clearly show that the mass leakage is caused by the *imbalance* between the amount of mass streamed out by the post-collision outgoing distribution functions and the amount of mass streamed into the system by the incoming (unknown) distribution functions at each boundary node. According to the above numerical investigations, we can establish the following mass loss for each boundary node:

\[
\Delta m(x_b, t + \delta t) = \sum_{\text{outgoing}} f_{\text{o}}(x_b, t) - \sum_{\text{incoming}} f_{\text{i}}(x_b, t + \delta t).
\]  \( \text{(18)} \)

Specifically, Fig. 9 illustrates the distribution functions that will propagate across a curved wall through a boundary node during the streaming step. In the figure the blue arrows denote the outgoing distribution functions, which propagate from the boundary node to the ghost nodes in the solid, while the red arrows represent the incoming distribution functions that propagate from the ghost nodes to the boundary node.

**FIG. 9.** Sketch of the distribution functions that propagate across a curved wall through a boundary node.

The blue arrows denote the outgoing distribution functions, which propagate towards the ghost nodes in the solid, while the red arrows represent the incoming distribution functions that propagate from the ghost nodes to the boundary node.
4. Modified mass-conservative curved boundary schemes

In this section, two modified boundary schemes with mass conservation are proposed for treating curved boundaries. On the basis of the consideration that the MLS boundary scheme yields the smallest mass loss among the investigated boundary schemes, the modified boundary schemes are devised based on the MLS scheme. According to the MLS scheme, the unknown distribution functions at each boundary node are determined by

\[
    f_{\alpha} (x, t + \delta t) = \left(1 - \chi\right) f_{\alpha}^e (x, t) + \chi f_{\alpha}^{eq} (x, t),
\]

(19)

where \( f_{\alpha}^{eq} (x, t) \) is defined by Eq. (8) and the parameter \( \chi \) is given by Eqs. (11) and (10) for \( q < 0.5 \) and \( q \geq 0.5 \), respectively. A simple treatment to conserve the mass of a system is to add the mass loss to each boundary node. However, if the mass loss is averagely added to the known distribution functions, the momentum at the boundary node may be changed. To avoid such an influence, the mass loss established in Eq. (18) can be added to the rest distribution function, i.e.,

\[
    f_{\alpha}^0 (x, t + \delta t) = f_{\alpha}^e (x, t) + \sum_{\text{outgoing}} f_{\alpha}^* (x, t) - \sum_{\text{incoming}} f_{\alpha} (x, t + \delta t),
\]

(20)

where \( f_{\alpha}^* (x, t + \delta t) \) are calculated by Eq. (19). In the remaining of the present paper, this modified curved boundary scheme based on the MLS scheme is referred to as the modified scheme A.

On the other hand, the mass of a system can also be conserved by directly guaranteeing the balance between the amount of mass carried by the outgoing and incoming distribution functions at each boundary node. When \( \Delta m (x, t + \delta t) \) in Eq. (18) is set to zero, we can obtain

\[
    \sum_{\text{incoming}} f_{\alpha} (x, t + \delta t) = \sum_{\text{outgoing}} f_{\alpha}^* (x, t).
\]

(21)

To satisfy the above requirement, an additional parameter is needed. Inspired by the study of Bao et al. [19], we can redefine the density in the fictitious equilibrium distribution function of the ghost nodes

\[
    f_{\alpha}^{eq} (x, t) = \omega_\alpha \rho (x, t) \left[ 1 + \frac{e_{\alpha} \cdot u_i}{c_i^2} + \frac{(e_{\alpha} \cdot u_i)^2}{2c_i^4} - \frac{(u_i \cdot u_i)}{2c_i^2} \right],
\]

(22)

where the density is changed to a fictitious density \( \rho (x, t) \). Substituting Eq. (19) into Eq. (21), the
requirement given by Eq. (21) can be transformed to

\[ \sum_{\text{outgoing}} \chi f_{\alpha}^{\ast}(x_s,t) = \sum_{\text{outgoing}} \chi f_{\alpha,\ast}^{\ast}(x_s,t). \]  \hspace{1cm} (23)

Combining Eq. (23) with Eq. (22), the fictitious density in Eq. (22) can be obtained as follows:

\[ \rho(x_s,t) = \frac{\sum_{\text{outgoing}} \chi f_{\alpha}^{\ast}(x_s,t)}{\sum_{\text{outgoing}} \chi b_{\alpha} \left[ 1 + \frac{e_{\alpha} \cdot u_{\alpha}}{c_{\alpha}^2} + \frac{(e_{\alpha} \cdot u_{\alpha})^2}{2c_{\alpha}^4} - \frac{(u_{\alpha} \cdot u_{\alpha})}{2c_{\alpha}^2} \right]} . \]  \hspace{1cm} (24)

Since the parameter \( \chi \) depends on \( e_{\alpha} \) through the fraction \( q \), it cannot be moved out from the summation sign in Eqs. (23) and (24).

It can be readily verified that the requirement given by Eq. (21) is satisfied when employing Eqs. (19), (22), and (24), which constitute another modified curved boundary scheme based on the MLS scheme, and is referred to as the modified scheme B. In Ref. [19], Bao et al. have devised an improved curved boundary based on the MLS scheme. The major difference between the present modified scheme B and the scheme of Bao et al. lies in that the constraint in the present study is given by Eq. (21), while in the study of Bao et al. the constraint is formulated as \( \sum_{\text{incoming}} f_{\pi} = \sum_{\text{outgoing}} f_{\alpha} \).

5. Numerical validation

In this section, numerical simulations are performed to validate the two modified curved boundary schemes. Three tests are considered, i.e., steady flow past a circular cylinder, natural convection in a square enclosure with a circular cylinder, and droplet resting on a circular cylinder with different contact angles. The former two tests are employed to examine the numerical accuracy of the modified schemes for simulating fluid flow and heat transfer, whereas the last test is utilized to validate their capability of conserving mass in two-phase LB simulations.

5.1. Steady flow past a circular cylinder

The steady flow past a circular cylinder is a classical problem in the computational fluid dynamics...
(CFD) and has been studied extensively with a number of numerical and experimental results in the literature. The computational domain is chosen as $N_x \times N_y = 40D \times 25D$, where $D = 40$ is the diameter of the circular cylinder located at $(15D, 12.5D)$. The free-stream velocity is taken as $U_0 = 0.1$ and the Reynolds number is defined as $Re = U_0 D / \nu$. The inlet boundary is given by a uniform velocity profile, which is implemented by the Zou-He boundary scheme [37], while the fully developed boundary condition is employed at the outlet boundary. The periodic boundary condition is applied to the upper and lower boundaries and the modified curved boundary schemes are used on the circular cylinder.

![Streamlines of steady flow past a circular cylinder](image)

**FIG. 10.** Streamlines of steady flow past a circular cylinder obtained by the modified curved boundary scheme A at Re = 20 and 40.

Figure 10 shows the streamlines obtained by the modified scheme A for the cases of Re = 20 and 40. From the figure we can see that a pair of symmetric vortices develops behind the cylinder and the vortices become larger with the increase of the Reynolds number. To quantify the numerical results, the non-dimensional length of the recirculation region, the separation angle, and the drag coefficient obtained by the modified schemes A and B are compared with published results in Table 1. The non-dimensional length of the recirculation region is defined as $2L/D$, where $L$ is measured from the rearmost point of the cylinder. The drag coefficient is defined as $C_d = F_x / \left( 0.5 \rho U_0^2 D \right)$, where $F_x$ is the $x$-component of the force $F$ exerted on the cylinder, which is calculated using the
momentum-exchange method \cite{38, 39}. From the table we can see that the numerical results of the modified schemes A and B are both in good agreement with those reported in the previous studies.

**TABLE 1.** Comparisons of the wake length, the separation angle, and the drag coefficient.

| References                      | $Re = 20$ |           | $Re = 40$ |           |
|---------------------------------|-----------|-----------|-----------|-----------|
|                                 | $2L/D$    | $\theta_s$| $C_d$     | $2L/D$    | $\theta_s$| $C_d$     |
| Scheme A                        | 1.90      | 41.35     | 2.130     | 4.61      | 53.93     | 1.590     |
| Scheme B                        | 1.91      | 41.56     | 2.133     | 4.64      | 53.93     | 1.593     |
| Dennis and Chang \cite{40}      | 1.88      | 43.7      | 2.045     | 4.69      | 53.8      | 1.522     |
| Takeshi et al. \cite{41}        | 1.90      | 40.78     | 2.104     | 4.64      | 50.38     | 1.568     |
| Niu et al. \cite{42}            | 1.89      | 42.95     | 2.144     | 4.52      | 53.86     | 1.589     |

To illustrate the differences between the present modified schemes and the halfway bounce-back scheme, Fig. 11 presents a comparison of local velocity vectors around the bottom of the circular cylinder at $Re = 40$ between the results of the modified schemes and those of the halfway bounce-back scheme. As shown in the figure, the halfway bounce-back scheme leads to unphysical results below the circular cylinder since the velocity obtained by the stair-shaped approximation penetrates the real cylindrical surface. On the contrary, such an unphysical phenomenon is not observed in the results of the modified schemes A and B.

![Fig. 11. Comparison of local velocity vectors around the bottom of the circular cylinder at $Re = 40$ between the modified curved boundary schemes and the halfway bounce-back scheme.](image-url)
5.2. Natural convection in a square enclosure with a circular cylinder

This test consists of a square enclosure with sides of length $L$ and a stationary circular cylinder with the radius $R = 0.2L$, which is located at the centre of the square enclosure. The walls of the square enclosure are kept at a constant low temperature $T_l$ while the circular cylinder is kept at a constant high temperature $T_h$. The fluid properties are assumed to be constant except that the density in the buoyancy term is treated according to the Boussinesq approximation. The temperature field is governed by

$$\partial_t T + \mathbf{u} \cdot \nabla T = \alpha \nabla^2 T,$$

where $\alpha$ is the thermal diffusivity. The natural convection is usually characterized by the Rayleigh number and the Prandtl number, which are defined as follows:

$$Ra = \frac{g \beta L^4 (T_h - T_l)}{\nu \alpha}, \quad \Pr = \frac{\nu}{\alpha},$$

where $\nu$ is the kinematic viscosity, $\beta$ is the thermal expansion coefficient, and $g$ is the gravitational acceleration.

In our simulations, the Prandtl number is fixed at $\Pr = 0.71$ whereas the Rayleigh number varies in the range of $10^4 - 10^6$. The grid system is taken as $N_s \times N_p = 200 \times 200$. The temperature equation is solved by a finite-difference scheme [23] with the immersed boundary method [43] being applied to fix the temperature at the surface of the inner circular cylinder. The modified curved boundary schemes are employed to handle the no-slip boundary condition of the inner circular cylinder.

Figure 12 displays the isotherms and streamlines obtained by the modified curved boundary scheme A for the cases with different Rayleigh numbers. Similar results are given by the modified scheme B and therefore not shown here. At $Ra = 10^4$, the heat transfer in the enclosure is mainly dominated by thermal conduction. From the streamlines shown in Fig. 12(a), we can observe two overall rotating symmetric eddies with two inner vortices respectively. As the Rayleigh number increases to $10^5$, the effect of convection on heat transfer in the enclosure also increases. Consequently, the thermal boundary
FIG. 12. Simulations of natural convection in a square enclosure with a circular cylinder. The streamlines (left) and isotherms (right) obtained by the modified curved scheme A for the cases with different Rayleigh numbers.
layer near the surface of the inner circular cylinder becomes thinner, as can be seen in Fig. 12(b). Meanwhile, a plume appears on the top of the circular cylinder and the isotherms move upward. The thermal gradient at the bottom of the enclosure is very small in comparison with that at the middle and top regions. Correspondingly, the flow field undergoes a bifurcation where two inner vortices merge and the dominant flow is in the upper half of the enclosure.

**TABLE 2.** Comparison of the surface-averaged Nusselt number with published results.

| Ra   | Scheme A | Scheme B | Ref. [44] | Ref. [45] | Ref. [46] |
|------|----------|----------|-----------|-----------|-----------|
| $10^4$ | 3.246    | 3.246    | 3.412     | 3.24      | 3.331     |
| $10^5$ | 5.016    | 5.001    | 5.176     | 4.86      | 5.08      |
| $10^6$ | 9.253    | 9.190    | 9.171     | 8.9       | 9.374     |

When the Rayleigh number is further increased to $10^6$, the heat transfer in the enclosure is mainly dominated by thermal convection. From the isotherms in Fig. 12(c) we can clearly observe the thermal boundary layer in the upper part of the enclosure and the middle and lower parts of the circular cylinder. The thermal boundary layer separates from the cylinder surface near the top of the circular cylinder and consequently a strong plume appears there. Moreover, a pair of tiny symmetric vortices appears at the bottom of the enclosure due to the separation of the boundary layer by the strong convective flow, as can be seen from the streamlines in Fig. 12(c). All of these observations agree well with those reported in Refs. [44-47]. To quantify the numerical results, the surface-averaged Nusselt number (see Ref. [48] about its calculation) at the inner circular cylinder is compared with the results in the previous studies in Table 2, where the results of Ref. [46] were obtained by a control-volume-based numerical method in body-fitted coordinates. The table shows that the results given by the modified scheme A and scheme B are both in good agreement with those reported in the previous studies. Minor differences (within 0.7%) are observed between the results of the two modified schemes at $Ra = 10^5$ and $10^6$, which are acceptable since these two schemes are devised from different points of view.
5.3. Droplet resting on a circular cylinder

Now we turn our attention to the capability of the modified curved boundary schemes in conserving mass in two-phase LB simulations. The test of a droplet placed on a circular cylinder is employed and the initial setting can be found in Fig. 2. Three cases with different contact angles are considered, i.e., \( \theta = 30^\circ, 90^\circ, \) and \( 120^\circ \). The grid system and the simulation parameters are the same as those used in Sec. 3.1. Some snapshots of the density contours obtained by the modified scheme A for the three cases are displayed in Fig. 13. Similar results are obtained by the modified scheme B and not shown here. By comparing the numerical results in Fig. 13 and those in Fig. 3, we can see that the droplet can achieve a stable state when the modified scheme A is employed, rather than behaving like an evaporating droplet as the original MLS scheme is used, which indicates that the modification formulated by Eq. (20) has prevented the mass leakage at the surface of the circular cylinder.
FIG. 13. Simulations of droplet on a circular cylinder using the modified curved boundary scheme A. Snapshots of density contours under the static contact angles $\theta = 30^\circ$, $90^\circ$, and $120^\circ$, respectively. From left to right: $t = 1000\delta$, $5000\delta$, $20000\delta$.

Figure 14 displays the variations of the normalized mass of the system during the simulations using the modified schemes A and B, respectively. For both modified schemes, the maximum variation of the normalized mass of the system is very small (about 0.01%) and it appears in the early stage of the simulations, which is expected because the liquid-vapor interface is initially a sharp interface and it will develop into a diffuse interface with a finite thickness in the early stage of the simulations. Such a change will cause a small fluctuation of the mass of the system since the density varies smoothly within the diffuse liquid-vapor interface. After the early stage, the variations of the normalized mass of the system are much smaller, as can be seen in Fig. 14. In addition, we can also observe some slight differences between the results of the three cases, which are actually attributed to the fact that the perimeter/length of the liquid-vapor interface is slightly different in these cases.

This test demonstrates that both the modified scheme A and scheme B are capable of conserving mass in two-phase LB simulations, although they are devised based on the MLS scheme from different points of view. We have also examined the constraint $\sum_{\text{incoming}} f_\alpha = \sum_{\text{outgoing}} f_\alpha$ employed by Bao et al. [19], and found that mass leakage still exists in the related simulations, which indicates that $\sum_{\text{outgoing}} f_\alpha$ in Eqs. (20) and (21) cannot be replaced by $\sum_{\text{outgoing}} f_\alpha$. Actually, the two-phase LB simulations are
very sensitive to the mass leakage caused by the boundary scheme and considerable numerical errors will be accumulated even the mass loss at each time step is very small.

![Variations of the normalized mass of the system under the static contact angles θ = 30°, 90°, and 120°, respectively.](image)

**FIG. 14.** Variations of the normalized mass of the system under the static contact angles θ = 30°, 90°, and 120°, respectively.

### 6. Summary

In this paper, we have investigated the performance of three well-known types of curved boundary schemes in two-phase LB simulations. Through the modeling of a droplet resting on a circular cylinder, it is found that, for all the investigated schemes, the simulated droplet unphysically “evaporates” under the no-slip and isothermal conditions, revealing the existence of mass leakage at the cylindrical surface due to the curved boundary schemes. Besides, the numerical results showed that the MLS boundary scheme yields the smallest mass loss among the investigated curved boundary schemes. Moreover, numerical analysis has been performed to figure out the origin of mass leakage of the boundary schemes by simulating static flow under gravity, which shows that the mass leakage occurs in all the cases except when the curved boundary schemes reduce to the halfway bounce-back scheme.

By analyzing the mass loss from the macroscopic level and the mesoscopic level in light of distribution functions, a formulation has been established for the mass loss at each boundary node, which
is shown to arise from the imbalance between the amount of mass streamed out by the post-collision outgoing distribution functions and the amount of mass streamed into the system by the incoming distribution functions. On the basis of the numerical investigations, we have devised two modified mass-conservative boundary schemes for curved boundaries based on the MLS boundary scheme. Numerical simulations have been carried out to validate the proposed modified schemes. It is shown that the two modified schemes exhibit better performance than the halfway bounce-back scheme in the flow modeling of steady flow past a circular cylinder. Meanwhile, the simulations of a droplet on a circular cylinder demonstrate that the two modified schemes are capable of conserving mass in two-phase LB simulations.

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