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One-point second-order curved boundary condition for lattice Boltzmann simulation of suspended particles

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ABSTRACT

The lattice Boltzmann method (LBM) has been widely considered as a distinctive and reliable approach for simulating the complex particulate flows. As an intrinsic kinetic scheme, it is quite convenient for LBM to apply the bounce-back (BB) type methods to handle the moving boundaries with complicated geometry, which is a tricky task for general interface-resolved methods. However, the two major schemes in LBM, i.e., the simple BB rule and the curved boundary condition (CBC) are presently encountered by the problems of low precision and loss of local computation, respectively. To overcome those two deficiencies in the boundary treatment simultaneously, a one-point second-order CBC is proposed in this paper. Information of only a single node is required in the present scheme, and the second-order accuracy is validated in the channel flow and cylindrical Couette flow. Applications to the particulate flows are further implemented to verify the present scheme. Numerical results are in good agreement with those in the literature.

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1. Introduction

Particulate flow is widely encountered in the natural and engineering processes, such as the haze weather, watercourse silt, pharmacy industry and coal combustion [1,2]. Over the past two decades, the lattice Boltzmann method (LBM) has been developed and advanced into a popular numerical approach for the interface-resolved simulation of that kind of complex flow [3,4]. One important reason is for the inherent characteristics of LBM generally based on the fixed Cartesian grids, which removes the complicated procedure for mesh-generation and remeshing involved in other methods, such as the Arbitrary-Lagrange-Euler (ALE) [5]. Furthermore, compared with the remaining particle-resolved schemes, for example the immersed boundary (IB) [6], fictitious domain (FD) [7] and force coupling (FC) [8] methods, LBM considers the thickness of the fluid-solid interface to be sufficiently thin, other than smeared in several grids. That feature enables LBM to be more accurate for the description of the flow details near the interface with limited grid resolution, which essentially is attributed to the bounce back (BB) rule [4] used in the treatment of solid boundary. Since the BB scheme mimics the fictitious fluid particle [9]. The simple and efficient BB method, with the addition of the general merits of LBM, for instance, unnecessary to solve the time-consuming Poisson equation for pressure but determined directly by the equation of state, easy implementation and natural parallelism, have together formed the competitive advantages of LBM, and been increasingly used to solve the interface-resolved particulate flows [4,10].

The BB scheme (simple BB) was first proposed by Ladd [11] in the famous Shell model, where the body surface is assumed to locate at the middle of a lattice link. Hence, the fluid particles can exactly return to their starting point after rebounding.

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The value of the unknown distribution function (UDF), which is the main concern in the boundary treatment of LBM [12] can then be obtained. Such simplification makes the original smooth particle surface to be discretized into a series of zigzag lines, rendering a collapse of geometry integrity [13]. As a result, the simple BB has a deficiency of low precision (just first-order) in the boundary treatment, which is insufficient in the simulation of complex particulate flows. Furthermore, many authors found in some cases it would obtain seriously wrong results [14,15]. Those shortages for the simple BB had not been improved in the subsequent ALD [16] and Qi [17] models of LBM. However, it should be clearly noted that, the local computation property of the original LBM has been completely preserved in the simple BB scheme, because there is no extra fluid node involved in the boundary treatment.

To improve the accuracy of the simple BB scheme, some refined methods, called curved boundary conditions (CBCs) are then developed for considering the real shape of the solid boundary [13,18–20]. Those remedies reach a consensus that the value of the UDF should be connected with the relative position for the boundary node to solid surface. This is consistent with existing knowledge that the portion of the bounce back part is determined by such distance. Generally, the CBCs can be categorized into two groups: the construction scheme and the interpolated BB scheme. In the former category, Filippova et al. [21] considered the UDF to be a combination of the BB and virtual equilibrium parts. This pioneering CBC has an inferior performance on the numerical stability, which was improved by Mei et al. [22] subsequently. Ginzburg et al. [20] proposed the multireflection BC using the theoretical analysis. This scheme can achieve higher accuracy with more distribution functions combined. On the other hand, the non-equilibrium extrapolation scheme was extended by Guo et al. [23] for curved boundary treatment, where the UDF was obtained by coupling the equilibrium and non-equilibrium parts. Furthermore, Dorschner et al. [24] constructed the UDF with the Grad function. For the interpolated BB scheme, Bouzidi et al. [25] and Lallemand et al. [26] presented a UDF by interpolation, according to the position of fluid particle after rebounding. Yu et al. [27] elucidated a unified scheme to solve the problem that the interpolation had to be implemented separately at a threshold value of 1/2 in the previous methods. Those described CBCs [21-27] all dramatically improve the accuracy to be second-order in the treatment of solid boundaries. However, most of them obtain the UDF at the boundary node with the aid of the information of neighboring fluid nodes. It is inevitable to undermine the local computation property and further the parallel performance of LBM [28,29].

As outlined above, most methods in the boundary treatment cannot integrate the two properties of the accuracy and local computation of LBM simultaneously. Therefore, the development of a one-point and second-order accurate CBC seems to be an open question in the particulate flow simulations. Note that some significant achievements have been made in developing such boundary schemes for lattice Boltzmann modeling of convection–diffusion equation in recent years [30–34]. Particularly, Zhao et al. [35] proposed a one-point CBC for viscous flows in LBM. The key point of that boundary scheme is to obtain the constant parameters involved in the formula, which must be determined by the Maxwell iteration [36,37]. As up to five parameters included, the overall second-order accuracy can be achieved for their scheme, but that may complicate the treatment of curved boundaries at the same time. More importantly, the implementation of that boundary scheme [35] may be model-dependent (presently only for the lattice Bhatnagar–Gross–Krook (LBGK) model [38]). In general, this study is motivated to develop a simple one-point second-order CBC for the interface-resolved simulation of particulate flows in LBM. The remaining part of the paper is organized as follows. A methodology introduction is provided in Section 2. The numerical scheme is validated in Section 3. Finally, conclusions are summarized in Section 4.

2. Numerical methodology

2.1. Lattice Boltzmann method

Originally derived from the lattice gas automate (LGA), the lattice Boltzmann method has been advanced in recent years to be an alternative incompressible flow solver [39]. As an intrinsic kinetic scheme, the LBM evolves a set of velocity distribution functions $f_i(\mathbf{x}, t)$ with position \mathbf{x} , time t and discrete velocity \mathbf{e}_i , rather than the macroscopic quantities as

$$f_i(\mathbf{x} + \mathbf{e}_i \delta_t, t + \delta_t) - f_i(\mathbf{x}, t) = \Omega_i(f), \quad i = 0, 1, \dots, b - 1.$$

$$\tag{1}$$

In the above lattice Boltzmann equation, $\Omega_i(f)$, δ_t and *b* respectively denote the discrete collision operator, the temporal step and the total number of discrete velocities. Eq. (1) is solved generally by the following two steps as

Collision:
$$f_i^+(\mathbf{x}, t) = f_i(\mathbf{x}, t) + \Omega_i(f)$$
,
Streaming: $f_i(\mathbf{x} + \mathbf{e}_i \delta_t, t + \delta_t) = f_i^+(\mathbf{x}, t)$.
(2)

For the collision term, the multi-relaxation-time (MRT) model will be adopted instead of the LBGK to avoid the unphysical numerical artifact and improve the stability, which is written as [40]

$$\Omega_i(f) = -\sum_{j=1}^{b-1} \left(\boldsymbol{M}^{-1} \boldsymbol{S} \boldsymbol{M} \right)_{ij} \left(f_j - f_j^{eq} \right), \tag{3}$$

with **M** a $b \times b$ transform matrix and **S** a relaxation matrix. f_j^{eq} is the equilibrium distribution function typically determined by the density ρ , velocity **u** and temperature *T* of the fluid,

$$f_{j}^{eq} = \omega_{j}\rho \left[1 + \frac{\boldsymbol{e}_{j}.\boldsymbol{u}}{c_{s}^{2}} + \frac{(\boldsymbol{e}_{j}.\boldsymbol{u})^{2}}{2c_{s}^{4}} - \frac{\boldsymbol{u}^{2}}{2c_{s}^{2}} \right],\tag{4}$$

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