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An overview of boundary implementation in lattice Boltzmann method for computational heat and mass transfer☆

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ABSTRACT

The ability to deal with the complex geometries precisely and accurately has always been the most integral part of any computational fluid dynamics approach. The lattice Boltzmann method has already achieved considerable success in the simulation of unsteady flow with arbitrary boundary shapes. To include boundaries in the lattice Boltzmann simulations, several methods have been presented in the past to satisfy the standard boundary implementation of macroscopic flows. In spite of the considerably vast body of literatures that discuss in this field, the study still is in progress. The current study is an overview of the adopted boundary conditions in lattice Boltzmann method.

1. Introduction

The lattice Boltzmann method (LBM) is an innovative technique of computational fluid dynamics based on the Boltzmann transport equation, which is supported by the advanced kinetic theory [1–7]. In the last few decades, LBM has changed into a successful alternative method for simulating complex physical, chemical, and fluid mechanics problems [8,9]. The LBM utilizes the ensemble-averaged distribution functions to explain the system by this assumption that the collective behavior of the fictitious particles which, comprised of the system, is consistent with the principles of the macroscopic physics. An interesting aspect of the LBM is its ability to process the complicated boundary geometries easily with acceptable accuracy [10]; hence, investigating the suitable boundary conditions' treatment for LB simulations has become a highly researched area in many engineering and scientific applications [11–16]. The computational efficiency of LBM in comparison with the traditional CFD methods establishes it as a potent applicant. The quantitative behavior of LBM was investigated in comparison with FVM in many research studies [17–20]. The results show that, concerning complex geometries, the lattice Boltzmann method showed more efficiency than the well accepted finite volume approach. The CPU times with increasing complexity of the obstacle structure was increased for both method and for highly complex structures became almost independent from it for LBM. Furthermore, based on review by Chen and Doolen [21] the approximated computational cost for moving solid particle simulation, in suspension simulation, in LBM had been convenient and efficient. The work for simulation of N particles in LBM moving boundary method scales linearly with N while in finite element method this scale is N^2 [22]. A method with the capability of accurate inter-phase calculation and simple boundary condition implementation can be a very good option for replacing the current methods of complex flow simulation. Adding to these advantages, parallel scalability has made it exceptional to many other numerical approaches. In this paper, we are willing to review the different boundary condition developing trend in the frame of LBM. In the next section lattice Boltzmann method will be briefly touched and on followings the most popular studies of LBM boundary conditions will be summarized and discussed based on the CFD standard categories.

2. Review of lattice Boltzmann method

The LBM has its ancestry from the lattice gas automata (LGA), a kinetic model that was constructed in discrete space and time. The discretized velocity distribution function can be obtained by solving the Boltzmann equation with different collision models. The LGA is frustrated by some unwanted issues. First, the density dependent factor in nonlinear advection term and a velocity dependent pressure that does not lead to the Galilean invariance system of lattice gases. Second, it is overwhelmed by noise. To overcome these undesirable problems LBM replaced the Boolean variable in LGA by a single particle distribution function [23]. This process eliminated the statistical noise in LGA and single particle distribution function f_i was defined as an ensemble average of particle occupation variable ($f_i = n_i$). The practical approach, interpreted in the LBM, consists of solving the Boltzmann equation for the evolution of a single distribution function $f\,(x, v, t)$ of particles as they move and collide on a lattice. The solution of the equation includes

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two main steps; the stream step or advection term propagates information through the lattice cells, while the collision step normalizes the distribution functions to the equilibrium distribution function. The collision operator represents the rate of change of the distribution function due to the colliding process and depends only on the local equilibrium state. The discrete Boltzmann equation with the BGK [24] collision model for the particle velocity distribution function, $f_i\,(x,t)$ ignoring the external force term can be expressed as:

$$f_i(x+e_i\Delta t, t+\Delta t) = f_i(x,t) + \frac{1}{\tau}\left(f_i(x,t) - f_i^{eq}(x,t)\right), (i = 0, 1, 2, 3, \ldots, N) \tag{1}$$

where τ is the relaxation time, Δt is the time step, $e_i(=\Delta x/\Delta t)$ is the particle velocity in the i-direction. f_i is the particle velocity distribution along the ith direction, which represents the fraction of the particles with velocities in the range of e_i and $e_i + d\,e_i$. The number of discrete velocity directions standing for the lattice is chosen based on certain symmetry requirements to recover the isotropy of the viscous stress tensor of the fluid flow [25]. The zero index symbolizes the rest particle with the zero velocity. The relaxation time is related to the kinematic viscosity of the fluid via the relation:

$$\tau = 3\nu + \frac{1}{2}. \tag{2}$$

The equilibrium distribution function which appears in the collision operator is an expansion of the Maxwellian distribution function in an equilibrium state for the low Mach number.

$$f^{eq}(x,t) = \frac{\rho}{(2\pi RT)^{\frac{d}{2}}}\, exp\left(-\frac{(e-u)\cdot(e-u)}{2RT}\right) \tag{3}$$

where R, T, ρ and u are gas constant, temperature, macroscopic density and macroscopic velocity respectively. d stands for space dimension. The general structure of the equilibrium function can be written up to $O(u^2)$ [26]:

$$f_i^{eq}(\rho,u) = \rho\left[a + b\,(e_i.u) + c\,(e_i.u)^2 - d\,(u.u)\right] \tag{4}$$

where a, b, c, and d are the lattice constants. $\rho(=\Sigma f_i)$ is the fluid density, $u\,(\rho u = \Sigma f_i e_i)$ is the fluid velocity. The coefficients of the above equation can be obtained analytically [27] and results in:

$$f_i^{eq}(\rho,u) = \rho w_i\left[1 + \frac{1}{c_s^2}\,(e_i.u) + \frac{1}{2c_s^4}\,(e_i.u)^2 - \frac{1}{2c_s^2}\,(u.u)\right] \tag{5}$$

where c_s is the speed of sound and w is the weighting factor in the lattice fluid density. This equation is used for lattice nodes within the fluid domain and the boundary nodes need extra treatments due to insufficient number of known distribution functions. In the simulations of LBM, the distribution functions f_i on the fluid nodes are known after each time step of streaming, but some distribution functions on the boundary nodes are unknown. Only if distribution functions on the boundary nodes are determined, the next computation step can proceed. So, the distribution functions on the boundary nodes need to be determined based on the known macroscopic boundary conditions. When boundary appears physical characteristics, including periodicity, symmetry, and fully developed flow conditions, unknown distribution functions can be simply determined by the motion pattern of particles.

3. Boundary condition in LBM

One of the most important and critical issues in the LBM is imposing the proper boundary condition for flow simulation. Applying the boundary condition in NS method is somehow straightforward, while in LBM, because of the mesoscopic nature, it is not so clear and it needs translation from macroscopic to mesoscopic scale. Hence, remarkable efforts have been devoted to develop effective and precise boundary schemes for different situations. Depending on the flow structure and problem geometries, various types of boundary condition, including free slip, no-slip, periodic, sliding walls, moving walls, in-flux, and out-flux boundaries might be applied to the evolution of the distribution functions. In the frame of LBM, different approaches have been presented for simulating BCs [28–32].

3.1. Periodic boundary condition

Through the aforementioned BCs the easiest one is the periodic boundary at the sides of the computational domain. In this case, the system is assumed to be isolated in a closed domain so the number of particles remains constant due to conservation law. The periodic conditions are applied as a natural part of the streaming operation, so that outgoing particles at one end of the lattice become incoming particles at the other end. These make sure that mass is neither gained nor lost through the periodic boundaries. The concerns about positivity of the population are somewhat the key of numerical stability and the major drawback of the proposed methods is laid in that the distribution function is lost during the BC applying [33]. However, there is an agreement on the methods of treatment for this type of BC, but a more specified study in this field can be found in the literatures.

In a reported study of Zhang and Kwok [34] the general periodic BC of the lattice Boltzmann method has been altered to include the pressure variance for fully developed periodic flows (Fig. 1). They stated Q2 that the proposed treatment does not generate nonphysical inlet or outlet disturbance and it is applicable for systems with periodic electric and temperature fields. Later on, Kim et al. [35] proposed a new boundary closure for fully developed pressure driven flow, which is of higher accuracy than of Zhang et al. [34] and it is applicable for both compressible and incompressible flows. Subsequently, Gräser and Grimm [36] have combined the Kim and Pitsch method with a controller loop that adapted a perpendicular pressure gradient to restrain any net momentum, perpendicular to the outer walls and developed an algorithm for an adaptive BC for fully developed pressure driven flow simulation.

3.2. Pressure and velocity boundary condition

Successful fluid flow numerical simulations desire the proper velocity and pressure boundary conditions implementation. The general velocity and pressure boundaries are still under further development for the lattice-Boltzmann method. In LBM, most previous researches concerned with pressure and the velocity boundary condition concentrate somehow on the wall Dirichlet boundary condition based on the

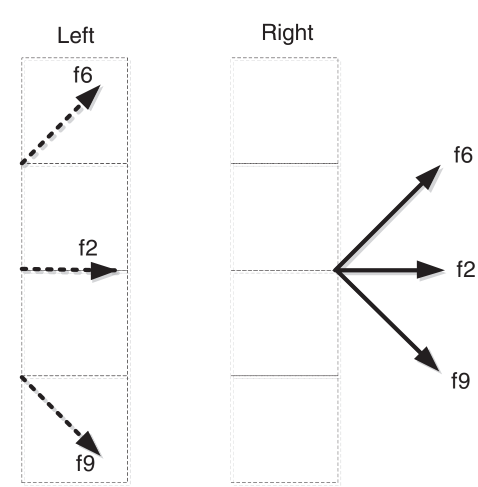

Fig. 1. The periodic boundary for left and right sides of a domain (D2Q9).

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