



# Non-equilibrium extrapolation method in the lattice Boltzmann simulations of flows with curved boundaries (non-equilibrium extrapolation of LBM)

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## ABSTRACT

The fraction of the intersected link in fluid region is an important parameter in non-equilibrium extrapolation method (NEM) in the lattice Boltzmann study since the NEM adopts different extrapolation schemes when the fraction reaches a critical value. In the present study, effect of the critical value of the fraction on the lattice Boltzmann simulations of flows with curved boundaries is investigated. The flows around a single cylinder and two parallel-placed cylinders under uniform incoming streaming are chosen as typical cases. For these given flows, small critical value of the fraction causes the lattice Boltzmann simulation to suffer severe numerical instability. Moreover, the numerical results also show that large critical value of the fraction can result in more accurate numerical results for flows under large Reynolds numbers, while the numerical accuracy is almost independent of the critical value for flows under small Reynolds numbers.

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## 1. Introduction

The lattice Boltzmann method (LBM), as a novel mesoscopic numerical algorithm, has attracted considerable attention over last decade. In comparison with the conventional numerical approaches in the computational fluid dynamics (CFD) field, this method presents many distinct advantages, such as simple formulations, favorable parallel-computing structure and capability in dealing with complex geometries. More importantly, the lattice Boltzmann model has been demonstrated as a special discrete scheme of the Boltzmann equation. Due to this intrinsic kinetic nature, the LBM has been recognized as one of the promising alternative CFD methods for problems involving mesoscopic/microscopic dynamics. In recent years, the LBM has been widely used in a large variety of scientific researches and engineering applications, such as multiphase and multicomponent fluids [1,2], magnetohydrodynamics [3], reaction-diffusion systems [4], flows through porous media [5], and other complex systems [6–9].

Generally, a complete lattice Boltzmann model consists of four parts: an evolution equation of the distribution function, a polynomial expansion of the equilibrium, an isotropic discrete particle velocity set and a boundary condition of the distribution function. For many flows, however, only the macroscopic fluid velocity and density at the boundaries can be measured and determined. The

corresponding distribution functions at the boundaries are usually unknown and cannot be directly specified by experiments, causing that a solid boundary condition reflecting the real dynamics of particles at the boundaries is hard to give in the LBM. Moreover, even when the distribution functions at the boundaries are fully specified, the LBM still fails to directly use this information for some problems, e.g. flows with a curved boundary, since the LBM carries out the simulations only on the given rectangular lattice. In this case, to close the lattice Boltzmann simulation, we need specify the distribution functions at the nodes nearest the curved boundaries based on the known boundary conditions. In this paper, we grossly call the lattice nodes at the rectangular boundaries and the lattice nodes nearest to the curved boundaries as the boundary nodes. In the literatures, various boundary treatments have been developed to determine the distribution functions on these boundary nodes. One of the most often used boundary treatments is the bounce-back rule [10,11], in which the distribution function of particles streaming to the boundary nodes is set to be equal to those scattering back to the original fluid nodes along the reverse direction. It has been demonstrated that by simply placing the boundary in the middle of the first two rows of lattice nodes, the bounce-back rule can be a second-order approximation of the non-slip boundary conditions of fluid velocity [12,13]. Recently, another boundary treatment based on the known Maxwell's diffusion reflection boundary condition in kinetic theory has been also developed [14]. Unlike the bounce-back rule, this treatment assumes the particles has completely lost their memory of the incoming streaming and reflect diffusively from the wall. The diffusive reflection boundary

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**Nomenclature**

$\mathbf{c}_i$	discrete particle velocity in LBE model (m/s)
$c$	lattice speed (m/s)
$c_s$	speed of sound (m/s)
$D$	cylinder diameter (m)
$E$	average relative error of the velocity
$f_i$	distribution function associated with the $i$ th discrete velocity
$f_i^{\text{eq}}$	equilibrium distribution function in discrete particle velocity space
$f_i^{\text{neq}}$	non-equilibrium distribution function in discrete particle velocity space
Ma	Mach number
$p$	fluid pressure (Pa)
Re	Reynolds number, $U_\infty D/\nu$
$r, \tau$	components of position vector for the coordinate origin at the stagnant point of cylinder
$t$	time (s)
$U^*, V^*$	dimensionless components of fluid velocity, $U_x/U_\infty, U_y/U_\infty$
$U_x, U_y$	components of fluid velocity (m/s)

$U_\infty$	uniform inlet velocity (m/s)
$\mathbf{u}$	fluid velocity (m/s)
$u(\mathbf{x}_w)$	fluid velocity on the node at $\mathbf{x}_w$ (m/s)
$X^*, Y^*$	dimensionless components of Cartesian position vector, $x/D, y/D$
$x, y$	spatial position vector (m)
$\mathbf{x}_w$	lattice node on the solid side next to the boundary (m)
$\mathbf{x}_b$	intersection of the wall with lattice link (m)
$\mathbf{x}_f$	lattice node on the fluid side next to the boundary (m)

**Greek symbols**

$\Delta$	scale factor, $ \mathbf{x}_f - \mathbf{x}_b / \mathbf{x}_f - \mathbf{x}_w $
$\Delta_c$	critical scale factor
$\Delta_{\text{cm}}$	the minimum value for a stable simulation
$\delta t$	time step (s)
$\delta x$	space step (m)
$\nu$	kinematic viscosity of fluid ( $\text{m}^2/\text{s}$ )
$\rho$	fluid density ( $\text{kg}/\text{m}^3$ )
$\rho(\mathbf{x}_w)$	fluid density on the node at $\mathbf{x}_w$ ( $\text{kg}/\text{m}^3$ )
$\tau$	dimensionless relaxation time in LBGK
$\omega_i$	weight coefficient

treatment gives a good prediction of the slip in microscale gas flows. Besides those boundary treatments mimicking the particle dynamics at the boundaries by some *ad hoc* assumptions, Chen et al. [15] developed the other type of boundary treatments using the conventional extrapolation method. He introduced an imaginary layer of lattices inside the boundaries, and then extrapolated the distribution functions inside flow region to those on this extra layer. In each streaming-collision step, the extrapolated distribution functions on the extra layer are used to specify those on the boundary nodes. The idea is of much importance to specify the distribution functions at the boundary nodes by those in the neighborhood using the extrapolation (or interpolation) since by appropriate extrapolation/interpolation, we cannot only control and improve the numerical performance of our boundary treatment, but also gain much more flexibility for flows with complex boundaries. In line with this idea, Filippova and Hänel [16] combined the extrapolation scheme with the bounce-back particle dynamics and developed an extrapolation bounce-back scheme for flows with curved boundaries. Later Mei et al. [17] modified such a scheme and applied it to simulations of channel flow, cavity flow and flow around a column of cylinders.

However, it should be pointed out the extrapolation bounce-back scheme is only suitable for simulations of steady flows. Moreover, owing to its bounce-back feature, this scheme also fails to approximate the macroscopic boundary conditions including the gradients of temperature and velocity [16]. To eliminate these limitations and extend the extrapolation-type boundary treatments to simulations of more general flows, Guo et al. [18] developed a different non-equilibrium extrapolation method (NEM), which does no longer depend on any prior assumption of the underlying particle dynamics. Like that proposed by Chen et al. [15], this extrapolation method first introduces an imaginary layer of lattices inside the wall and then, decomposes corresponding distribution functions at these fictions lattice nodes into the equilibrium and non-equilibrium parts. For the equilibrium part, it is evaluated the same as those at the internal nodes in the flow region but the used fluid density and velocity are extrapolated by those at the boundaries and in the neighboring fluid region. For the non-equilibrium part, it is extrapolated by the non-equilibrium part of

the distribution functions at the nodes in the neighboring fluid region. In simulation, the resulting extrapolated distribution functions inside the walls will be used to determine the corresponding distribution functions at the boundary nodes in the flow region based on the lattice Boltzmann streaming-collision procedure. Such a NEM is simple and robust, and suitable for simulations of flows with curved boundaries. However, it should be also noted that a numerical factor, i.e. the fraction of the intersected link in the fluid region,  $\Delta$ , is introduced in the NEM. When this factor  $\Delta$  reaches a critical values  $\Delta_c$ , the extrapolations of both the equilibrium part and non-equilibrium part will adopt different extrapolation schemes from those with  $\Delta < \Delta_c$ . It can thus be expected that choosing different  $\Delta_c$ s may influence the numerical results, especially for flows with complex boundaries. To understand the effect of  $\Delta_c$  on the numerical performance of lattice Boltzmann simulation, in the present study, we apply the lattice Boltzmann method with the NEM to simulations of flows around a cylinder and two parallel-placed cylinders. By choosing different  $\Delta_c$ s, we test the numerical accuracy and stability of the NEM.

In the rest of this work, we first introduce the LBM in Section 2. In Section 3, the non-equilibrium extrapolation method for flows with curved boundaries is briefly reviewed. Moreover, we detailedly discuss the method determining the extrapolated nodes within the solid wall. In Section 4, the simulations of flows around a cylinder and two parallel-placed cylinders are carried out. Numerical results are analyzed and discussed. Finally, the conclusions are drawn in Section 5.

## 2. The lattice BGK model

In the lattice Boltzmann method, the most popular model is the lattice Bhatnagar–Gross–Krook (BGK) model, which is a specific numerical scheme of the Boltzmann equation with the BGK approximation by discretizing the time and space and projecting the continuous particle velocity space into an isotropic discrete velocity set [19–23]. Without losing generality, in this work, we take the two-dimensional nine-bit (D2Q9) model as an example, whose evolution equation is [20,21]

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