

## Rectangular Lattice Boltzmann Equation for Gaseous Microscale Flow

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**Abstract.** The lattice Boltzmann equation (LBE) is considered as a promising approach for simulating flows of liquid and gas. Most of LBE studies have been devoted to regular square LBE and few works have focused on the rectangular LBE in the simulation of gaseous microscale flows. In fact, the rectangular LBE, as an alternative and efficient method, has some advantages over the square LBE in simulating flows with certain computational domains of large aspect ratio (e.g., long micro channels). Therefore, in this paper we expand the application scopes of the rectangular LBE to gaseous microscale flow. The kinetic boundary conditions for the rectangular LBE with a multiple-relaxation-time (MRT) collision operator, i.e., the combined bounce-back/specular-reflection (CBBSR) boundary condition and the discrete Maxwell's diffuse-reflection (DMDR) boundary condition, are studied in detail. We observe some discrete effects in both the CBBSR and DMDR boundary conditions for the rectangular LBE and present a reasonable approach to overcome these discrete effects in the two boundary conditions. It is found that the DMDR boundary condition for the square MRT-LBE can not realize the real fully diffusive boundary condition, while the DMDR boundary condition for the rectangular MRT-LBE with the grid aspect ratio  $a \neq 1$  can do it well. Some numerical tests are implemented to validate the presented theoretical analysis. In addition, the computational efficiency and relative difference between the rectangular LBE and the square LBE are analyzed in detail. The rectangular LBE is found to be an efficient method for simulating the gaseous microscale flows in domains with large aspect ratios.

**AMS subject classifications:** 76M28, 76D05, 76P05

**Key words:** Lattice Boltzmann equation, gaseous microscale flow, rectangular lattice, boundary conditions, multiple-relaxation time.

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## 1 Introduction

The wide applications of micro-electro-mechanical-systems (MEMS) and nano-electro-mechanical-systems (NEMS) have stimulated a great interest in the development of simulation methods for gaseous microscale flow [1, 2]. For non-continuum flows, the characteristic parameter is the Knudsen number  $Kn = \lambda/h$ , where  $\lambda$  represents the mean-free path of the gas and  $h$  is the characteristic length of the flow. According to the value of  $Kn$ , the flow can be classified into four flow regimes, i.e., the continuum flow ( $Kn \leq 0.001$ ), the slip flow ( $0.001 < Kn \leq 0.1$ ), the transition flow ( $0.1 < Kn \leq 10$ ), and free molecular flow ( $Kn > 10$ ). Therefore, when  $Kn$  is greater than around 0.001, the continuum assumption will break down and the traditional simulation approaches based on the Navier-Stokes equations are not valid.

The lattice Boltzmann equation (LBE), which is a special discrete form of the continuous Boltzmann equation [3, 4], is considered as a promising method for simulating gaseous microscale flow [5]. Recently, numerous LBE studies have been devoted to gaseous microscale flow and most of them have focused on the LBE with a regular square lattice [6–25]. However, to our knowledge, there are few LBE works to study gaseous microscale flow based on a rectangular lattice. In fact, the rectangular LBE, as an alternative and efficient method, has some advantages over the square LBE for simulating flows in some cases.

Recently, the two-dimensional nine-velocity (D2Q9) LBE model with a rectangular lattice has been received particular attention and further studied [26–30]. As pointed out in [30], the rectangular LBE schemes can be constructed in three distinct approaches: the first method is to decouple the discretization of the velocity space from spatial and temporal discretizations [31], the second one is to construct a multiple-relaxation-time (MRT) operator [26], and the third one is to introduce some more discrete velocities [30]. Compared to the second approach mentioned above, the first approach loses the simplicity of the LBE and the third approach can not generate real rectangular grids. Therefore, in this work we choose the rectangular D2Q9 MRT-LBE model presented in [26] to study gaseous microscale flow.

The aim of this paper is to analyze two kinds of boundary conditions for the rectangular LBE and to apply the method to gaseous microscale flows in slip regime. The rest of the paper is organized as follows. In Section 2, we present the Chapman-Enskog analysis and derive the relationship between the relaxation parameter and the Knudsen number for the rectangular LBE model. In Section 3, we analyze the combined bounce-back/specular-reflection (CBBSR) boundary condition and the discrete Maxwells diffuse-reflection (DMDR) boundary condition for the rectangular LBE, and show how to choose the reasonable combination parameters (i.e., the bounce-back fraction for the CBBSR scheme and the accommodation coefficient for the DMDR scheme) in the two boundary conditions. In Section 4, the numerical tests are performed to validate the presented theoretical analysis. Finally, we conclude the paper in Section 5.