

# Lattice Boltzmann model for the perfect gas flows with near-vacuum region

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**Abstract:** It is known that the standard lattice Boltzmann method has near-vacuum limit, i. e., when the density is near zero, this method is invalid. In this letter, we propose a simple lattice Boltzmann model for one-dimensional flows. It possesses the ability of simulating near-vacuum area by setting a limitation of the relaxation factor. Thus, the model overcomes the disadvantage of non-physical pressure and the density. The numerical examples show these results are satisfactory.

**Keywords:** lattice Boltzmann method, perfect gas, near-vacuum region, Roe's tests

## Introduction

The Lattice Boltzmann method (LBM) can play a major role in solving fluid flows. In particular, the lattice gas<sup>[1]</sup> and the lattice Boltzmann method have been implemented successfully in the simulation of incompressible flows, magnetohydrodynamics, chemically reacting flows, flow through porous media, turbulent flows *et al.*<sup>[2]</sup> Many results show that the lattice Boltzmann method has three advantages: Firstly, the convection operator of LBM is linear. Secondly, the incompressible Navier-Stokes equations can be obtained in the incompressible limit. Thirdly, LBM uses a minimal set of velocities. Since only a few moving directions are used, if we fix the direction, say  $\alpha$ , the lattice Boltzmann equations is one-dimensional iteration, and the code is greatly simplified. As an important progress, the simple collision model of BGK is applied to the lattice Boltzmann equation, yielding the lattice BGK model<sup>[3-5]</sup>. However, this method is limited to a range of low Mach numbers as an image gas<sup>[6, 7]</sup>. This concerns three aspects of the reason: (1) there exist nonlinear deviations (see Ref. [7]), (2) this model can cause a so-called ideal limitation<sup>[8]</sup>, (3) this model is limited to near-vacuum case. It is known that density and pressure always take positive value. Some numerical methods have no ability to handle the difficulty of near-zero density. From the viewpoint of the gas kinetic theory, the media are not continuous, and the Navier-Stokes equation fails. But the Boltzmann equation resulting from the particle level may be turned into the particle flux equation, i. e., without the collision term. In the view point of computational fluid dynamics, the scheme must have the ability of handling the difficulty of the medium near vacuum. Recently, we have developed a simple lattice Boltzmann model for compressible flow with shock waves and contact interfaces. But this model cannot simulate the flows with near-vacuum area. In this paper, we introduce a limit of relaxation factor, when density  $\rho < 0.01\rho|_{t=0}$ , then the collision vanishes. This assumption agrees with the gas kinetic theory.

In Section 1 of this paper, based on standard lattice Boltzmann method, a new lattice Boltzmann model is proposed. In Section 2, two Roe's tests are calculated to check this model.

## 1 The lattice Boltzmann model

Consider the one-dimensional model. We assume that the particles moving along the link with velocity  $e_\alpha$  are divided into two types,  $|e_\alpha| = c$  and  $|e_\alpha| = 0$ , with two different energy levels  $\varepsilon_A$  and  $\varepsilon_B$ , and the particle at rest possesses energy level  $\varepsilon_D$ . The single particle distribution in the state at site  $x$  and time  $t$  is denoted by  $f_\alpha = f_\alpha(x, t)$  ( $\alpha = 0, 1, \dots, 4$ ). The density  $\rho$ , the momentum  $\rho u$ , and the total energy per site  $\frac{1}{2}\rho u^2 + \rho E$  are defined as

$$\rho = \sum_{\alpha} f_{\alpha}, \quad \rho u = \sum_{\alpha} f_{\alpha} e_{\alpha}, \quad \frac{1}{2}\rho u^2 + \rho E = \sum_{\alpha} f_{\alpha} \varepsilon_{\alpha} \quad (1)$$

In Eqs. (1),  $\rho E$  is the internal energy per site,  $\varepsilon_{\alpha} = \varepsilon_A, \varepsilon_B, \varepsilon_D$ .

The Lattice Boltzmann equation takes the form

$$f_{\alpha}(x + \Delta x, t + \Delta t) - f_{\alpha}(x, t) = -\frac{1}{\tau}[f_{\alpha}(x, t) - f_{\alpha}^{\text{eq}}(x, t)]$$

where  $\tau$  is the relaxation time,  $f_{\alpha}^{\text{eq}}$  is the local equilibrium distribution, which possesses the expressions

$$f_{\alpha}^{\text{eq}} = \begin{cases} D_0 \rho + D_5 \rho u^2, & \alpha = 0 \\ A_0 \rho + A_2 \rho u e_{\alpha} + A_5 \rho u^2 e_{\alpha}^2 + A_5 \rho u^2, & \alpha = 1, 2 \\ B_0 \rho + B_2 \rho u e_{\alpha} + B_5 \rho u^2 e_{\alpha}^2 + B_5 \rho u^2, & \alpha = 3, 4 \end{cases} \quad (2)$$

In Eq. (2), parameters  $D_0, D_5, A_i, B_i$  ( $i = 0, 2, 5$ ) can be determined by the conservation laws of mass, momentum, energy and flux conditions of momentum and energy<sup>[9]</sup>. This local equilibrium distribution function differs from the expressions in Ref. [9], for we are considering an one-dimensional model. The pressure of the perfect gas  $p$  is defined as,  $p = (\gamma - 1)\rho E$ .

By simple algebra, we obtain these coefficients

$$\begin{aligned} D_0 &= 1 - \frac{p}{\rho c^2}, & D_5 &= -\frac{1}{c^2} \\ A_0 &= \frac{\varepsilon_B p (\rho c^2)^{-1} - (E - D_0 \varepsilon_D)}{2(\varepsilon_B - \varepsilon_A)}, & B_0 &= \frac{-\varepsilon_A p (\rho c^2)^{-1} + (E - D_0 \varepsilon_D)}{2(\varepsilon_B - \varepsilon_A)} \\ A_2 &= \frac{\varepsilon_B c^{-2} - c^{-2}(0.5u^2 + \gamma E)}{2(\varepsilon_B - \varepsilon_A)}, & B_2 &= \frac{-\varepsilon_A c^{-2} + c^{-2}(0.5u^2 + \gamma E)}{2(\varepsilon_B - \varepsilon_A)} \\ A_5 &= \frac{\varepsilon_B - 0.5(c^2 + 2\varepsilon_D)}{2(\varepsilon_B - \varepsilon_A)(c^4 + c^2)}, & B_5 &= \frac{-\varepsilon_A + 0.5(c^2 + 2\varepsilon_D)}{2(\varepsilon_B - \varepsilon_A)(c^4 + c^2)} \end{aligned}$$

Using the multi-scale method, i. e., multi-scale time expansion and Chapman-Enskog expansion, we get the Euler equations with the first order accuracy of the truncation errors<sup>[9]</sup>

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} &= O(\varepsilon) \\ \frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} &= O(\varepsilon) \\ \frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho E \right) + \frac{\partial}{\partial x} \left( \frac{1}{2} \rho u^2 + \rho E + p \right) u &= O(\varepsilon) \end{aligned}$$

where  $\varepsilon$  is the Knudsen number, its value being equalized to  $\Delta t$  in this paper. We found that this model has no chosen parameter  $\lambda$ , which differs from Ref. [9]. The reason is that  $\lambda$  disappears when the number of spatial dimensions reduces from two to one.

We use two methods to analyze the stability, (i) Hirt's heuristic stability theory<sup>[10]</sup>, (ii) the consistency criterion. If we set  $\varepsilon_A = \varepsilon_B = e$ , then, this model is the standard lattice Boltzmann model, and equilibrium distribution (2) is the standard lattice Boltzmann equilibrium

distribution in Refs. [3–5]. In our paper, based on method (ii), we obtain the CFL condition of the lattice Boltzmann model. Using the condition  $f_0^{\text{eq}} > 0$ , we have

$$c^2 > u^2 + \frac{D}{\gamma} a^2$$

where  $a$  is the speed of sound,  $a^2 = \gamma p / \rho$ .

Now we focus on the difficulty of near-vacuum area. In the lattice Boltzmann model, the mean free path  $l$  equals to  $c\Delta t$ . We assume that the gas is near-vacuum if collision does not occur in the range of  $l$ . However, if we delay the time, i. e., increase the collision time, collisions will surely occur. Therefore, we define the vacuum as there is no particle collision in the interval of  $t$  to  $t + \Delta t$ . Thus, the limitation of relaxation factor may be expressed as follows

$$\tau = \begin{cases} \tau_0, & \rho > \delta \\ \infty, & \rho < \delta \end{cases} \quad (3)$$

where  $\delta$  is the critical density, and  $\delta = O(\varepsilon)$ . In numerical simulation, we set  $\delta = \varepsilon$ .

## 2 The numerical tests

In this paper, we choose two Roe's tests to simulate. It is difficult to simulate Roe's tests by using the traditional method. The reason is the instability and non-physical pressure in the near-vacuum region.

The Roe's tests with two initial conditions<sup>[11]</sup> are given by

$$\text{Case I} \quad (\rho_L, p_L, u_L) = (1.0, 0.4, -2.0), \quad (\rho_R, p_R, u_R) = (1.0, 0.4, 2.0)$$

$$\text{Case II} \quad (\rho_L, p_L, u_L) = (1.0, 1.8, -1.0), \quad (\rho_R, p_R, u_R) = (1.0, 1.8, 1.0)$$

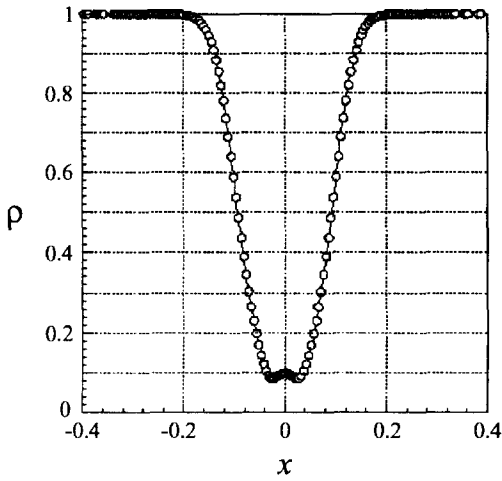
For the sake of comparison, firstly, we give the numerical results by using the model of Ref. [9] (Fig. 1). The numerical results of Case II seem good enough, but we found Case I's numerical pressure value appears negative, and the scheme is unstable when the density tends to zero. Obviously, the model of Ref. [9] can be used to simulate Case II but not Case I.

Fig. 2 shows the numerical results using the relaxation factor Eq. (3). These results show that the model is suitable for Case I but not Case II. In Fig. 2a and Fig. 2b, the density is near 0 and keeps positive. For Case II, see Fig. 2c, there is a large "tip" in the contact interface compared with Fig. 1c. The scheme can restrain the negative value automatically in the near-vacuum area.

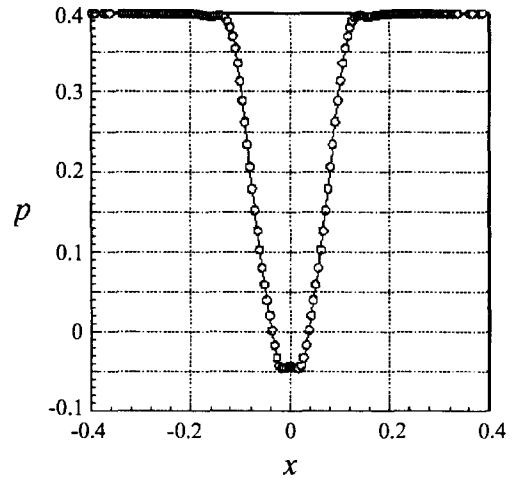
## 3 Conclusions

The Roe's test is a difficult problem in the simulation for the compressible Euler equations, the reason is that scheme relate to the ability of handling near-vacuum area. In this paper, the Case I is an example with the near-vacuum region. If Knudsen number becomes large from the viewpoint of the gas kinetic theory, the Chapman-Enskog expansion and multi-scales method may fail. But, in this paper, we found a simple method to overcome this difficulty, and extend the limits of lattice Boltzmann method.

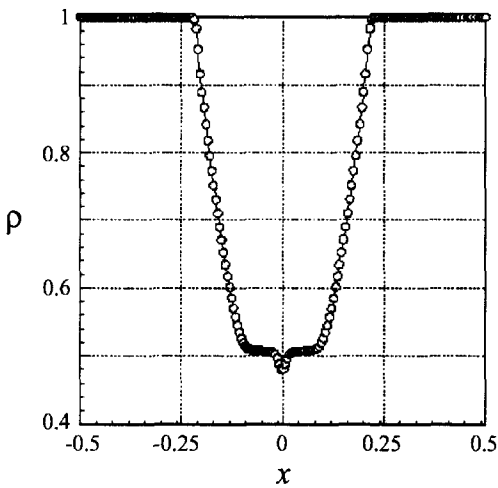
We also unified differential lattice Boltzmann models, constructed the relationship between the compressible lattice Boltzmann model and standard lattice Boltzmann model. When energy-levels  $\varepsilon_A = \varepsilon_B$ , our model reduces to standard lattice Boltzmann model. Thus, the difference between our model and standard lattice Boltzmann model is that the particle in our model have three sizes. Our model also handles compressible flows without near-vacuum region.



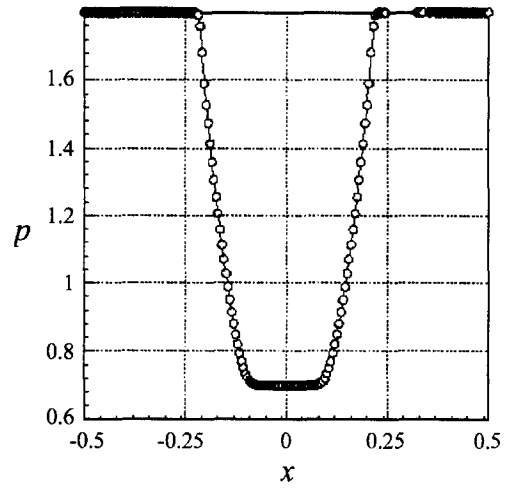
(a) Case I



(b) Case I

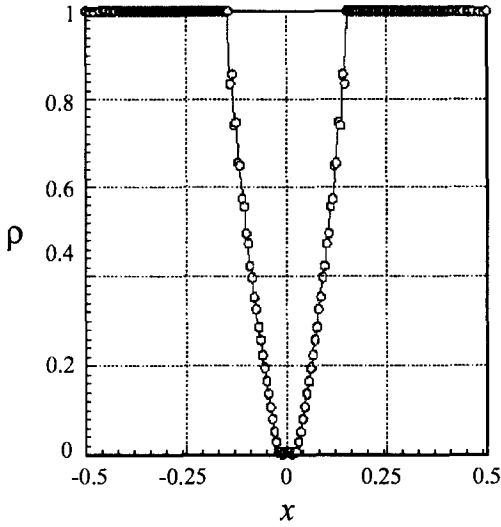


(c) Case II

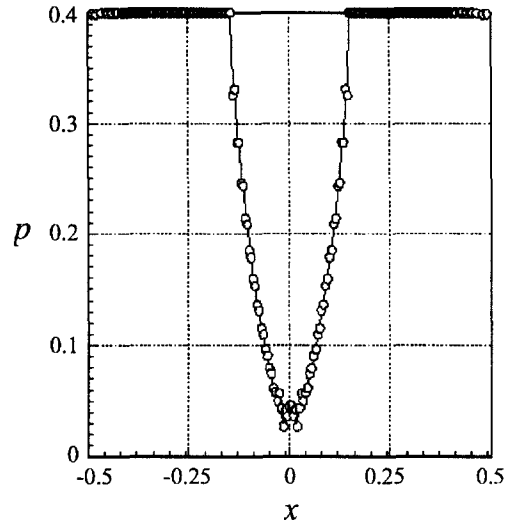


(d) Case II

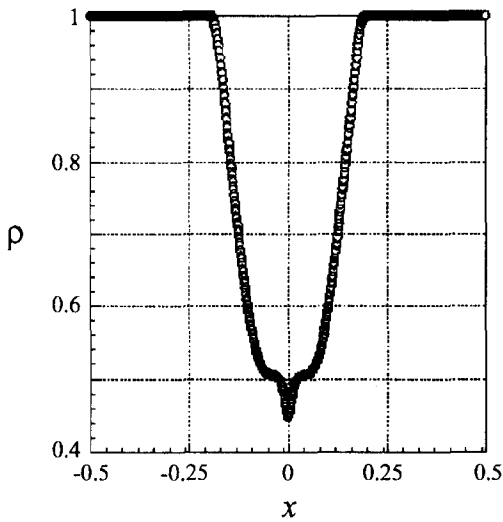
Fig. 1 The numerical results (circles) by using the model in Ref. [9]. (a), (b): Case I, lattice size  $M = 200$ , time  $T = 80\Delta t$ ,  $\gamma = 1.4$ ,  $c = 8.0$ ,  $\lambda = 1.65$ ,  $1/\tau = 1.3$ ,  $\varepsilon_A = 0.65c^2$ ,  $\varepsilon_B = 0.54c^2$ ,  $\varepsilon_D = 0.1c^2$ ; (c), (d): Case II, lattice size  $M = 200$ , time  $T = 50\Delta t$ ,  $\gamma = 1.4$ ,  $c = 3.0$ ,  $\lambda = 1.75$ ,  $1/\tau = 1.35$ ,  $\varepsilon_A = 2.0c^2$ ,  $\varepsilon_B = 0.6c^2$ ,  $\varepsilon_D = 0.1c^2$



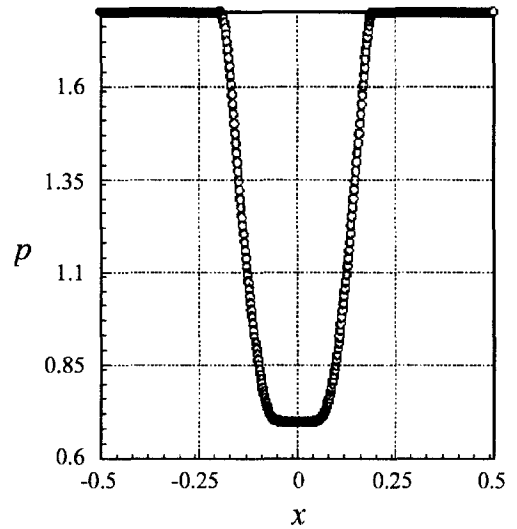
(a) Case I



(b) Case I



(c) Case II



(d) Case II

Fig. 2 The numerical results (circles) by using the model in this paper. (a), (b): Case I, lattice size  $M = 100$ , time  $T = 50\Delta t$ ,  $\gamma = 1.4$ ,  $c = 3.0$ ,  $1/\tau = 1.31$ ,  $\varepsilon_A = 6.5c^2$ ,  $\varepsilon_B = 2.0c^2$ ,  $\varepsilon_D = 0.02c^2$ ; (c), (d): Case II, lattice size  $M = 1000$ , time  $T = 200\Delta t$ ,  $\gamma = 1.4$ ,  $c = 3.0$ ,  $1/\tau = 1.35$ ,  $\varepsilon_A = 2.0c^2$ ,  $\varepsilon_B = 0.6c^2$ ,  $\varepsilon_D = 0.1c^2$

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