# Lattice Boltzmann study on Kelvin-Helmholtz instability: the roles of velocity and density gradients

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# Abstract

A two-dimensional lattice Boltzmann model with 19 discrete velocities for compressible Euler equations is proposed (D2V19-LBM). The fifth-order Weighted Essentially Non-Oscillatory (5th-WENO) finite difference scheme is employed to calculate the convection term of the lattice Boltzmann equation. The validity of the model is verified by comparing simulation results of the Sod shock tube with its corresponding analytical solutions. The velocity and density gradient effects on the Kelvin-Helmholtz instability (KHI) are investigated using the proposed model. Sharp density contours are obtained in our simulations. It is found that, the linear growth rate  $\gamma$  for the KHI decreases with increasing the width of velocity transition layer  $D_v$  but increases with increasing the width of density transition layer  $D_{\rho}$ . After the initial transient period and before the vortex has been well formed, the linear growth rates,  $\gamma_v$  and  $\gamma_{\rho}$ , vary with  $D_v$  and  $D_{\rho}$  approximately in the following way,  $\ln \gamma_v = a - bD_v$  and  $\gamma_{\rho} = c + e \ln D_{\rho}(D_{\rho} < D_{\rho}^E)$ , where a, b, c and e are fitting parameters and  $D_{\rho}^E$  is the effective interaction width of density transition layer. When  $D_{\rho} > D_{\rho}^E$ the linear growth rate  $\gamma_{\rho}$  does not vary significantly any more. One can use the hybrid effects of velocity and density transition layers to stabilize the KHI. Our numerical simulation results are in general agreement with the analytical results [L. F. Wang, *et al.*, Phys. Plasma **17**, 042103 (2010)].

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**Keywords:** lattice Boltzmann method; Kelvin-Helmholtz instability; velocity gradient effect; density gradient effect

# I. INTRODUCTION

As a mesoscopic approach and a bridge between the molecular dynamics method at the microscopic level and the conventional numerical method at the macroscopic level, the lattice Boltzmann(LB) method[1] has been successfully applied to various fields during the past two decades, ranging from the multiphase system[2–4], magnetohydrodynamics[5–7], reaction-diffusion system[8–10], compressible fluid dynamics[11–18], simulations of linear and nonlinear partial differential equations[19], etc. Its popularity is mainly owed to its kinetic nature[20], which makes the physics associated with the molecular level interaction can be incorporated easily in the model. As a result, this approach contains more physical connotation than Navier-Stokes or Euler equations based on the continuum hypothesis. Its popularity is also owed to its linear convention term, easy implementation of boundary conditions, simple programming and high efficiency in parallel computing, etc.

The Kelvin-Helmholtz instability(KHI) occurs when two fluids flow with proximity to each other exhibiting a tangential velocity difference[21]. Under the condition of the KHI, small perturbations along the interface between two fluids undergo linear[22–26] and nonlinear growth stages [27–31], and may evolve into turbulent mixing through nonlinear interactions. The KHI has attracted much attentions because of its significance in both fundamental research and engineering applications[32]. On the one hand, in fundamental research, KHI is of great importance in the fields of turbulent mixing[33], supernovae dynamics [34–36], and the interaction of the solar wind with the earth's magnetosphere[37], etc. On the other hand, in engineering applications, the KHI plays a key role in small-scale mixing of Rayleigh-Taylor(RT)[38, 39] and Richtmyer-Meshkov(RM) instabilities in inertial confinement fusion(ICF)[40, 41]. In the final regime of RT and RM instabilities, KHI is initiated due to the shear velocity difference at the spike tips [42], and, therefore, the appearance of the KHI aggravates the development of final nonlinearity of RT instability or RM instability, and quickens the process of fluid flock mixing round the interface.

In the present work, we propose a two-dimensional LB mode to simulate the KHI. The model consists of 19 discrete velocities in six directions and allows to recover the compressible Euler equations in the continuum limit. Actually, this phenomenon has been studied extensively by many researchers using experimental measurements, theoretical analysis and more recently by numerical simulations(NS) during the past decades[21, 25, 26, 31–33]. Those

results indicate that the evolution of KHI depends on the density ratio, viscosities, surface tension, compressibility and others. Although the basic behavior of the KHI has been studied extensively, to the best of our knowledge, the use of the LB method to investigate the evolution of this phenomenon is still very limited. In this paper, with the LB method we focus on the velocity and the density gradient effects on KHI. The rest of the paper is organized as follows. In Section II, using the Chapman-Enskog analysis, we show that the current model can recover the Euler equations in the continuum limit. The numerical scheme and the validation of the model will be performed in Section III. In Section IV, we show numerical simulation results on the KHI for various widths of velocity and density transition layers. Both the two kinds of gradients effects are investigated carefully. Finally, in Section V conclusions and discussions are drawn.

# **II. FORMULATION OF THE LB MODEL**

The model described here is inspired by the previous work of Watari and Tsutahara[14, 43], which is based on a multispeed approach and where the truncated local equilibrium distribution uses global coefficients.

#### A. Designing of the discrete velocity model

To formulate a finite difference LB model, the first step is to chose an appropriate discretevelocity-model(DVM). For a DVM described by

$$\mathbf{v}_0 = 0, \mathbf{v}_{ki} = v_k \left[\cos(\frac{i2\pi}{N}), \sin(\frac{i2\pi}{N})\right],\tag{1}$$

where subscript k indicates the kth group of the particle velocities whose speed is  $v_k$  and i = 1, 2, ..., N indicates the direction of particle's speed.

The nth rank tensor is defined as

$$T^{(n)}_{\alpha_1\alpha_2\dots\alpha_n} = \sum_{i=1}^n v_{i\alpha_1} v_{i\alpha_2}\dots v_{i\alpha_n},\tag{2}$$

where  $\alpha_1, \alpha_2, ..., \alpha_n$  indicate either the x or y component. The tensor is isotropic if it is invariant under the coordinate rotation and the reflection. As for being isotropic, the odd rank tensors should be zero and the even rank tensors should be the sum of all possible products of Kronecker delta. In this study, the DVM with N = 6 is used to construct a finite difference LB model. For this DVM it is easy find that the odd rank tensors are zero, and the even rank tensors generally have the following forms

$$\sum_{i=1}^{6} v_{ki\alpha} v_{ki\beta} = 3v_k^2 \delta_{\alpha\beta},\tag{3}$$

$$\sum_{i=1}^{6} v_{ki\alpha} v_{ki\beta} v_{ki\gamma} v_{ki\chi} = \frac{3}{4} v_k^4 \Delta_{\alpha\beta\gamma\chi},\tag{4}$$

where

$$\Delta_{\alpha\beta\gamma\chi} = \delta_{\alpha\beta}\delta_{\gamma\chi} + \delta_{\alpha\gamma}\delta_{\beta\chi} + \delta_{\alpha\chi}\delta_{\beta\gamma}.$$
(5)

Therefore, this DVM is isotropic up to, at least, its fifth rank tensor.

## B. Recovering of the Euler equations

The evolution of the distribution function  $f_{ki}$  for the particle velocity  $\mathbf{v}_{ki}$  is governed by the following Boltzmann equation with a BGK collision operator[44]

$$\frac{\partial f_{ki}}{\partial t} + \mathbf{v}_{ki} \cdot \frac{\partial}{\partial \mathbf{r}} f_{ki} = -\frac{1}{\tau} (f_{ki} - f_{ki}^{(0)}), \tag{6}$$

where  $f_{ki}^{(0)}$ , **r** and  $\tau$  denote the local equilibrium distribution function, the spatial coordinate and the relaxation time due to collision, respectively. The macroscopic density  $\rho$ , momentum  $\rho$ **u** and temperature *T* are calculated as the moments of the local equilibrium distribution function:

$$\sum_{ki} f_{ki}^{(0)} \begin{pmatrix} 1 \\ \mathbf{v}_{ki} \\ \frac{1}{2} (\mathbf{v}_{ki} - \mathbf{u})^2 \end{pmatrix} = \begin{pmatrix} \rho \\ \rho \mathbf{u} \\ \rho T = P \end{pmatrix}.$$
 (7)

Besides the moments in Eq.(7), Chapman-Enskog analysis indicates the following additional ones are needed to satisfy in order to recover the hydrodynamic equations at Euler level:

$$\sum_{ki} v_{ki\alpha} v_{ki\beta} f_{ki}^{(0)} = P \delta_{\alpha\beta} + \rho u_{\alpha} u_{\beta}, \tag{8}$$

$$\sum_{ki} \frac{1}{2} v_{ki}^2 v_{ki\alpha} f_{ki}^{(0)} = u_\alpha (2P + \frac{1}{2}\rho u^2).$$
(9)

To perform the Chapman-Enskog expansion on the two sides of Eq.(6), we introduce expansions

$$f_{ki} = f_{ki}^{(0)} + \epsilon f_{ki}^{(1)} + \epsilon^2 f_{ki}^{(2)} + \cdots,$$
(10)

$$\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_0} + \epsilon^2 \frac{\partial}{\partial t_1} + \cdots,$$
(11)

$$\frac{\partial}{\partial r_{\alpha}} = \epsilon \frac{\partial}{\partial r_{1\alpha}},\tag{12}$$

where  $\epsilon \ll 1$  is the Knudsen number. The introducing of  $\epsilon$  is equivalent to stipulating that

the gas is dominated by large collision frequency. The  $f_{ki}^{(0)}$  is the zeroth order,  $f_{ki}^{(1)}$ ,  $\frac{\partial}{\partial t_0}$  and  $\frac{\partial}{\partial r_{1\alpha}}$  are the first order,  $f_{ki}^{(2)}$  and  $\frac{\partial}{\partial t_1}$  are the second order terms of the Knudsen number  $\epsilon$ . Substituting Eqs.(10)-(12) into Eq.(6) and comparing the coefficients of the same order of  $\epsilon$  gives

$$\epsilon^1 : \frac{\partial f_{ki}^{(0)}}{\partial t_0} + \frac{\partial}{\partial r_{1\alpha}} (f_{ki}^{(0)} v_{ki\alpha}) = -\frac{1}{\tau} f_{ki}^{(1)}, \qquad (13)$$

$$\epsilon^2 : \frac{\partial f_{ki}^{(0)}}{\partial t_1} + \frac{\partial f_{ki}^{(1)}}{\partial t_0} + \frac{\partial}{\partial r_{1\alpha}} (f_{ki}^{(1)} v_{ki\alpha}) = -\frac{1}{\tau} f_{ki}^{(2)}, \qquad (14)$$

$$\epsilon^{j} : \frac{\partial f_{ki}^{(0)}}{\partial t_{j-1}} + \frac{\partial f_{ki}^{(1)}}{\partial t_{j-2}} + \dots \frac{\partial f_{ki}^{(j-1)}}{\partial t_{0}} + \frac{\partial}{\partial r_{1\alpha}} (f_{ki}^{(j-1)} v_{ki\alpha})$$
$$= -\frac{1}{\tau} f_{ki}^{(j)}.$$
(15)

Summing Eq.(13) over k, i gives

$$\frac{\partial \rho}{\partial t_0} + \frac{\partial}{\partial r_{1\alpha}} (\rho u_\alpha) = 0.$$
(16)

Summing Eq.(15) over k, i gives

$$\frac{\partial \rho}{\partial t_{j-1}} = 0, (j \ge 2). \tag{17}$$

Using Eq.(11) and Eq.(12) gives

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial r_{\alpha}} (\rho u_{\alpha}) = 0.$$
(18)

It is clear that the continuity equation can be derived at any order of  $\epsilon$ . Performing the operator  $\sum_{ki} v_{ki\alpha}$  to the two sides of Eq.(13) gives

$$\frac{\partial}{\partial t_0}(\rho u_\alpha) + \frac{\partial}{\partial r_{1\beta}}[\rho(T\delta_{\alpha\beta} + u_\alpha u_\beta)] = 0.$$
(19)

Performing the operator  $\sum_{ki} v_{ki\alpha}$  to the two sides of Eq.(14) gives

$$\frac{\partial}{\partial t_1}(\rho u_\alpha) = 0. \tag{20}$$

Using Eq.(11) and Eq.(12) gives the moment equation at the Euler level

$$\frac{\partial}{\partial t}(\rho u_{\alpha}) + \frac{\partial}{\partial r_{\beta}}[\rho(T\delta_{\alpha\beta} + u_{\alpha}u_{\beta})] = 0.$$
(21)

Performing operator  $\sum_{ki} v_{ki}^2/2$  to both sides of Eq.(13) gives

$$\frac{\partial}{\partial t_0} \left[ n(T + \frac{u^2}{2}) \right] + \frac{\partial}{\partial r_{1\beta}} \left[ \rho u_\beta \left( 2T + \frac{u^2}{2} \right) \right] = 0.$$
(22)

Performing operator  $\sum_{ki} v_{ki}^2/2$  to both sides of Eq.(14) gives

$$\frac{\partial}{\partial t_1} [n(T + \frac{u^2}{2})] = 0.$$
(23)

Using Eq.(11) and Eq.(12) gives the energy equation at the Euler level

$$\frac{\partial}{\partial t}\left[n(T+\frac{u^2}{2})\right] + \frac{\partial}{\partial r_\beta}\left[\rho u_\beta(2T+\frac{u^2}{2})\right] = 0.$$
(24)

# C. Formulation of the discrete equilibrium distribution function

We now formulated the discrete equilibrium distribution function based on the DVM with N = 6. The requirement Eq.(9) contains up to the third order of the flow velocity u. It is reasonable to expand the local equilibrium distribution  $f_{ki}^{(0)}$  in polynomial of the flow velocity up to the third order:

$$f_{ki}^{(0)} = \frac{\rho}{2\pi T} \exp\left[-\frac{v_k^2}{2T}\right] \exp\left[-\frac{u^2 - 2uv_k}{2T}\right]$$
$$= \rho F_k \left[\left(1 - \frac{u^2}{2T}\right) + \frac{v_{ki\varepsilon}u_\varepsilon}{T}\left(1 - \frac{u^2}{2T}\right) + \frac{v_{ki\varepsilon}v_{ki\eta}u_\varepsilon u_\eta}{2T^2} + \frac{v_{ki\varepsilon}v_{ki\eta}v_{ki\xi}u_\varepsilon u_\eta u_\xi}{6T^3}\right] + \cdots,$$
(25)

where

$$F_k = \frac{1}{2\pi T} \exp\left[-\frac{v_k^2}{2T}\right] \tag{26}$$

is a function of temperature T and particle velocity  $v_k$ . The truncated equilibrium distribution function  $f_{ki}^{(0)}$  contains the third rank tensor of the particle velocity and the requirement Eq.(8) contains the second rank tensor. Thus, the DVM should have an isotropy up to its fifth rank tensor. So the DVM with N = 6 is an appropriate choice.

To numerically calculate the equilibrium distribution function, one needs first calculate the global factor  $F_k$ . It should be noted that  $F_k$  can not be calculate directly from its definition Eq.(26). It should take values in such a way that satisfies Eqs.(7)-(9).

To satisfy the first equation in Eq.(7), we require

$$\sum_{ki} F_k = 1, \tag{27}$$

$$\sum_{ki} F_k v_{ki\varepsilon} v_{ki\eta} u_{\varepsilon} u_{\eta} = T u^2.$$
<sup>(28)</sup>

To satisfy the second equation in Eq.(7), we require

$$\sum_{ki} F_k v_{ki\alpha} v_{ki\varepsilon} u_{\varepsilon} = T u_{\alpha}, \tag{29}$$

$$\sum_{ki} F_k v_{ki\alpha} v_{ki\varepsilon} v_{ki\eta} v_{ki\xi} u_\varepsilon u_\eta u_\xi = 3T^2 u^2 u_\alpha.$$
(30)

To satisfy the third equation in Eq.(7), we require

$$\sum_{ki} F_k \frac{v_k^2}{2} = T,\tag{31}$$

$$\sum_{ki} F_k \frac{v_k^2}{2} v_{ki\varepsilon} v_{ki\eta} u_\varepsilon u_\eta = 2T^2 u^2.$$
(32)

To satisfy Eq.(8), we require

$$\sum_{ki} F_k v_{ki\alpha} v_{ki\beta} = T \delta_{\alpha\beta},\tag{33}$$

$$\sum_{ki} F_k v_{ki\alpha} v_{ki\beta} v_{ki\varepsilon} v_{ki\eta} u_{\varepsilon} u_{\eta} = T^2 (u^2 \delta_{\alpha\beta} + 2u_{\alpha} u_{\beta}).$$
(34)

To satisfy Eq.(9), we require

$$\sum_{ki} F_k \frac{v_k^2}{2} v_{ki\alpha} v_{ki\varepsilon} u_{\varepsilon} = 2T^2 u_{\alpha}, \tag{35}$$

$$\sum_{ki} F_k \frac{v_k^2}{2} v_{ki\alpha} v_{ki\varepsilon} v_{ki\eta} v_{ki\xi} u_\varepsilon u_\eta u_\xi = 9T^3 u^2 u_\alpha.$$
(36)

If further consider the isotropic properties of the DVM, the above ten requirements reduces to four ones. Requirement Eq.(27) gives

$$\sum_{ki} F_k = 1. \tag{37}$$

Requirements Eqs.(28),(29),(31),(33) give

$$\sum_{k} F_k v_k^2 = \frac{T}{3}.$$
(38)

Requirements Eqs.(30),(32),(34),(35) give

$$\sum_{k} F_k v_k^4 = \frac{4}{3} T^2.$$
(39)

Requirement Eq.(36) gives

$$\sum_{k} F_k v_k^6 = 8T^3.$$
 (40)

To satisfy the above four requirements, four particle velocities  $v_k$  are necessary. We choose a zero speed  $v_0 = 0$ , and other three nonzero ones. Eqs.(37)-(40) are easily solved to the following solution

$$F_k = \frac{24T^3 - 4(v_{k+1}^2 + v_{k+2}^2)T^2 + v_{k+1}^2v_{k+2}^2T}{3v_k^2(v_k^2 - v_{k+1}^2)(v_k^2 - v_{k+2}^2)},$$
(41)

$$F_0 = 1 - 6(F_1 + F_2 + F_3), \tag{42}$$

with

$$\begin{cases} k+l, & \text{if } k+l \le 3; \\ k+l-3, \text{if } k+l > 3. \end{cases} l = 1, 2.$$
(43)

As far as a simulation being stably conducted, the specific values of  $v_1$ ,  $v_2$  and  $v_3$  do not affect the accuracy of the results. The flexibility can be used to obtain the temperature range as wide as possible. In our simulations we set  $v_1 = 1$ ,  $v_2 = 2$  and  $v_3 = 3$ .

# III. SPATIOTEMPORAL DISCRETIZATIONS AND VERIFICATION OF THE

## MODEL

#### A. Time and space discretizations

In this section, we will confirm validity of the model by conducting numerical simulations. Here the time derivative is calculated using the forward Euler finite difference scheme. Spatial derivatives in convection term  $\mathbf{v}_{ki} \cdot \frac{\partial}{\partial \mathbf{r}} f_{ki}$  are calculated using fifth order Weighted Essentially Non-Oscillatory(5th-WENO) finite difference scheme[45]. The WENO scheme is an improvement of the ENO scheme, which changes the method of choosing smooth template with logical judgment into weighted average of all templates, thereby improving the adaptability of calculation format for flow field. Specifically, the discrete evolution equation of distribution function  $f_{ki}^{n+1}$  is

$$f_{ki,I}^{n+1} = f_{ki,I}^{n} - \frac{\partial (v_{ki\alpha} f_{ki,I}^{n})}{\partial x_{\alpha}} \Delta t - \frac{1}{\tau} (f_{ki,I}^{n} - f_{ki,I}^{n,(0)}) \Delta t$$
  
$$= f_{ki,I}^{n} - \frac{1}{\Delta x_{\alpha}} (h_{i,I+1/2} - h_{i,I-1/2}) \Delta t$$
  
$$- \frac{1}{\tau} (f_{ki,I}^{n} - f_{ki,I}^{n,(0)}) \Delta t, \qquad (44)$$

where the superscripts n, n + 1 indicate the consecutive two iteration steps,  $\Delta t$  is the time step,  $h_{i,I+1/2}$  is the numerical flux and can be defined as

$$h_{i,I+1/2} = \omega_1 h_{i,I+1/2}^1 + \omega_2 h_{i,I+1/2}^2 + \omega_3 h_{i,I+1/2}^3.$$
(45)

Under the condition  $v_{ki\alpha} \ge 0$ , interpolation functions  $h^q_{i,I+1/2}(q=1,2,3)$  are given by

$$h_{i,I+1/2}^{1} = \frac{1}{3}F_{i,I-2} - \frac{7}{6}F_{i,I-1} + \frac{11}{6}F_{i,I}, \qquad (46)$$

$$h_{i,I+1/2}^2 = -\frac{1}{6}F_{i,I-1} + \frac{5}{6}F_{i,I} + \frac{1}{3}F_{i,I+1}, \qquad (47)$$

$$h_{i,I+1/2}^3 = \frac{1}{3}F_{i,I} + \frac{5}{6}F_{i,I+1} - \frac{1}{6}F_{i,I+2}, \tag{48}$$

where  $F_{i,I} = v_{ki\alpha} f_{ki,I}$ .

The weighting factors  $\omega_q$  reflect the smooth degree of the template. They can be defined as follows

$$\omega_q = \frac{\tilde{\omega}_q}{\tilde{\omega}_1 + \tilde{\omega}_2 + \tilde{\omega}_3}, \\ \tilde{\omega}_q = \frac{\delta_q}{\left(10^{-6} + \sigma_q\right)^2},$$
(49)

where  $\delta_1 = 1/10$ ,  $\delta_2 = 3/5$  and  $\delta_3 = 3/10$ . The small value  $10^{-6}$  is added to the denominator to avoid dividing by zero. The coefficients  $\sigma_q$  in Eq.(49) are the smoothness indicators, and can be obtained by

$$\sigma_1 = \frac{13}{12} (F_{i,I-2} - 2F_{i,I-1} + F_{i,I})^2 + \frac{1}{4} (F_{i,I-2} - 4F_{i,I-1} + 3F_{i,I})^2,$$
(50)

$$\sigma_2 = \frac{13}{12} (F_{i,I-1} - 2F_{i,I} + F_{i,I+1})^2 + \frac{1}{4} (F_{i,I-1} - F_{i,I+1})^2,$$
(51)

$$\sigma_3 = \frac{13}{12} (F_{i,I} - 2F_{i,I+1} + F_{i,I+2})^2 + \frac{1}{4} (3F_{i,I} - 4F_{i,I+1} + F_{i,I+2})^2.$$
(52)

Similarly, under the condition  $v_{ki\alpha} < 0$ , a mirror image procedure of the procedure from Eqs.(45) to (52) can be carried out.



FIG. 1: (Color online) Comparisons between LB results and exact ones for the one-dimensional Sod problem, where t = 0.2.

# B. Numerical test: one-dimensional Sod shock tube[46]

The validity of the formulated LB model is verified through a one-dimensional Riemann problem, the Sod shock tube. This is a classical test in the research of compressible flows, which contains the shock wave, the rarefaction wave and the contact discontinuity.

For the problem considered, the initial condition is described by

$$\begin{cases} (\rho, u_1, u_2, T)|_L = (1.0, 0.0, 0.0, 1.0), & x \le 0; \\ (\rho, u_1, u_2, T)|_R = (0.125, 0.0, 0.0, 0.8), & x > 0. \end{cases}$$
(53)

Subscript "L" and "R" indicate macroscopic variables at the left and right sides of the discontinuity. Figure 1 shows the computed density, pressure, velocity, and temperature profiles at t = 0.2, where the circles are for simulation results and solid lines are for analytical solutions. The size of grid is  $\Delta x = \Delta y = 10^{-3}$ , time step and relaxation time are  $\Delta t = \tau = 10^{-5}$ . The two sets of results have a satisfying agreement. The unphysical numerical oscillation at discontinuity[16, 17] is effectively eliminated by the WENO scheme. Moreover, the shock waves are spread over only three grid cells, which shows that the LB model with the WENO scheme has a high ability to capture shocks for this test.

# IV. EFFECTS OF VELOCITY AND DENSITY GRADIENTS ON KHI

In this section, the LB model is used to simulate the KHI and investigate how the velocity and density transition layers influence the evolution of this kind of instability.

#### A. Linear growth rate and velocity gradient effect

The initial configurations in our simulation are described by

$$\rho(x) = \frac{\rho_L + \rho_R}{2} - \frac{\rho_L - \rho_R}{2} \tanh(\frac{x}{D_{\rho}}),$$
(54)

$$v(x) = \frac{v_L + v_R}{2} - \frac{v_L - v_R}{2} \tanh(\frac{x}{D_v}),$$
(55)

$$P_L = P_R = P, (56)$$

where  $D_{\rho}$  and  $D_{v}$  are the widths of density and velocity transition layers. The velocity(density) is discontinuous at x = 0 when  $D_{v} = 0(D_{\rho} = 0)$ .  $\rho_{L} = 5.0(\rho_{R} = 2.0)$  is the density away from the interface of the left(right) fluid.  $v_{L} = 0.5(v_{R} = -0.5)$  is the velocity away from the interface in y-direction of the left(right) fluid and  $P_{L}(P_{R}) = 2.5$  is the pressure in the left(right) side. The whole calculation domain is a rectangle with length 0.6 and height 0.2, which is divided into  $600 \times 200$  uniform meshes. A simple velocity perturbation in the x-direction is introduced to trigger the KH rollup and it is in the following form

$$u = u_0 \sin(ky) \exp(-kx),\tag{57}$$

where  $u_0 = 0.02$  is the amplitude of the perturbation. Here, k is the wave number of the initial perturbation, and is set to  $\pi/100$ . Periodic boundary conditions are used in the y-direction. Boundary conditions in the horizontal directions are as below. At the left side, we set  $(\rho, u, v, P)_{ix=1} = (\rho, u, v, P)_{ix=2}$ , and at the right side  $(\rho, u, v, P)_{ix=nx} =$  $(\rho, u, v, P)_{ix=nx-1}$ , where  $ix = 1, 2, \dots, nx$  is the index of the lattice node in the x-direction. Such a boundary condition is valid when the horizontal scale of computational domain is large enough so that the disturbance could not arrive at the left and right boundaries during the checking period.

Figure 2 shows the temporal evolution of the density field for  $D_v = 4$  and  $D_\rho = 8$  at four different times. It is clear that at t = 0.3 the interface is wiggling due to the initial perturbation and the velocity shear. After the initial linear growth stage, there is a nicely rolled vortex developing around the initial interface. A larger vortex is observed in the snapshot at t = 0.7, and a mixing layer is expected to be formed around the initial interface. The interface is continuous and smooth, which indicates the LB model has a good capturing ability of interface deformation.



FIG. 2: (Color online) Density evolutions of KHI simulated using the LB model, where  $D_v = 4$ and  $D_{\rho} = 8$ , t = 0.1 in (a), t = 0.3 in (b), t = 0.5 in (c), and t = 0.7 in (d).



FIG. 3: (Color online) Averaged density profiles along the x-axis at t = 0.1 (solid line), t = 0.3 (dash dot line), t = 0.5 (dash dot dot line), and t = 0.7 (short dash line) for  $D_{\rho} = 8$  and  $D_{v} = 4$ .

To quantitatively describe the characteristics of the vortex or the mixing layer, in Fig.3 we plot the averaged density profile  $\overline{\rho}(x)$  against the *x*-axis at t = 0.1, 0.3, 0.5 and 0.7. The averaged density in the mixing layer is defined as

$$\overline{\rho}(x) = \frac{1}{L} \int_0^L \rho(x, y) dy.$$
(58)

The averaged density profiles vary from being smooth to being irregular. The thickness of the mixing layer and the amplitude of the density oscillation increase with time. The zigzags in the profiles indicate the transfer of fluids from the dense to the rarefactive regions and the irregularity in the mixing layer.

To consider the velocity gradient effect, the simulations with various  $D_v$  have been performed and the density maps for  $D_v = 4, 8, 12$ , and 16 with five contour lines at t = 0.6are plotted in Fig.4. We see that the width of the velocity transition layer can significantly affect the evolution of KHI. For fixed density gradient and velocity difference, the larger the



FIG. 4: (Color online) Vortices in the mixing layer as a function of  $D_v$  at t = 0.6, where  $D_v = 4$  in (a),  $D_v = 8$  in (b),  $D_v = 12$  in (c), and  $D_v = 16$  in (d). The density transition layer  $D_{\rho}$  is fixed to be 8.



FIG. 5: (Color online) Time evolution of the perturbed peak kinetic energy  $E_x$  along the x-axis in In-linear scale for various widths of velocity transition layer. The dash-dotted lines represent the linear fits to the initial linear growth regimes.

value of  $D_v$ , i.e., the wider the initial transition zone, the weaker the KHI, and the later the vortex appears. In Fig.4(a) and Fig.4(b), the appearance of large vortices demonstrates that the evolution is embarking on the nonlinear stage. While in Fig.4(c) and Fig.4(d), the



FIG. 6: (Color online) Linear growth rate as a function of the width  $D_v$  of velocity transition layer.

width of the mixing layers is rapidly decreased by the increase of  $D_v$  and the evolution is in the weakly nonlinear stage. Figures 4(a)-(d) show that a wider velocity transition zone has a better stabilization effect on KHI.

At the beginning of the KHI, the perturbation grows exponentially and a linear growth rate can be determined. Taking the logarithm of the perturbed peak kinetic energy  $E_x = 0.5\rho u^2$  of each time step, this exponential growth can be obtainted[47, 48] (see Fig.5). The linear growth rate is obtained from the slope of a linear function fitted to the initial growth stage. The peak kinetic energy  $E_x$  can represent the interacting strength of two different fluids. It is clear from Fig.5 that the logarithm of the perturbed kinetic energy first grows linearly in time and then arrives at a nonlinear saturation procedure at late times.

For a fixed  $D_v$  and  $D_\rho$ ,  $E_x$  increases with time t during the linear growth stage. However, at the same time, the larger the value of  $D_v$ , the smaller the perturbed peak kinetic energy  $E_x$ . This means when the transition layer becomes wider, the evolution of the density field becomes slower. Moreover, we find that the dependence of  $\gamma_v$  on  $D_v$  can be fitted by a logarithmic function with the form

$$\ln \gamma_v = a - bD_v,\tag{59}$$

with a = 3.39 and b = 0.07 as displayed in Fig.6. The numerical simulation result is in general agreement with the analytical results (see Eq.(18) and Fig.3 in recent work of Wang, et al [26]). In the classical case, the linear growth rate is  $\gamma_c = k\sqrt{\rho_1\rho_2}(u_1-u_2)/(\rho_1+\rho_2) \propto \Delta u$ , where  $\Delta u$  is the shear velocity difference. A wider transition layer decreases the local or the effective shear velocity difference  $\Delta u$ , which results in a smaller linear growth rate, a smaller



FIG. 7: (Color online) Time evolution of the logarithm of the peak kinetic energy  $E_x$  along the x-axis for various widths of density transition layers.



FIG. 8: (Color online) Linear growth rate as a function of the width  $D_{\rho}$  of density transition layer. saturation energy, and a longer linear growth time  $t_{lin}$ .

# B. Linear growth rate and density gradient effect

In this section, the density gradient effect is investigated in a similar way. The initial conditions are described as:  $(\rho_L, v_L, P_L) = (5.0, 0.5, 1.5)$  and  $(\rho_R, v_R, P_R) = (1.25, -0.5, 1.5)$ . Parameters are set to be dx = dy = 0.002,  $\tau = 10^{-5}$ . Figure 7 shows time evolution of the logarithm of the peak kinetic energy  $E_x$  along the x-axis with various widths of density transition layers. It is seen in Fig.7, for fixed width  $D_v$  of velocity transition layer and fixed density difference, the linear growth rate first increases with the width  $D_{\rho}$  of density transition layer. But when  $D_{\rho} > 6$ , the linear growth rate does not vary significantly any

more (see Fig.8 for details), which indicates the effective interaction width of  $D_{\rho}$  is less than that of  $D_{v}$ . Moreover, we find when  $D_{\rho} < 6$ , the dependence of  $\gamma_{\rho}$  on  $D_{\rho}$  can be fitted by the following equation

$$\gamma_{\rho} = c + e \ln D_{\rho},\tag{60}$$

with c = 10.55 and e = 1.23 as shown in the legend of Fig.8. The numerical simulation results are also in general agreement with the analytical results (see Fig.2 in previous work by Wang, et al [25], Eq.(18) and Fig.2 in recent work of Wang, et al [26]). In the classical case, the square of the linear growth rate is  $\gamma_c^2 = k^2 \rho_1 \rho_2 (u_1 - u_2)^2 / (\rho_1 + \rho_2)^2 \propto (1 - A^2) \Delta u^2$ , where  $A = (\rho_1 - \rho_2) / (\rho_1 + \rho_2)$  is the Atwood number. A wider density transition zone reduces the Atwood number around the interface. Then in the process of exchanging momentum in the direction normal to the interface, the perturbation can obtain more energy from the shear kinetic energy than in cases with sharper interfaces. Therefore, a wider density transition layer increases the linear growth rate of the KHI.

## C. Hybrid effects of velocity and density gradients

In practical systems, at the interface of two fluids with a tangential velocity difference, both the velocity and the density gradients exist. The wider velocity transition layer decreases the linear growth rate of the KHI, but the wider density transition layer strengthens it. Consequently, there is a competition between these two gradient effects. In this section, we investigate how these two effects compete with each other. For convenience, we introduce a coefficient  $R = D_{\rho}/D_v$  to analyze the combined effect. The linear growth rate at various velocity and density gradients for R = 0.5, 1, 2, and 5 are illustrated in Fig.9.

As shown in Fig.9, on the whole, the hybrid effect of velocity and density transition layers reduces the linear growth rate. Only at small  $D_{\rho}$  and when R > 1, the hybrid effect of velocity and density transition layers makes larger the linear growth rate. This indicates that the effective interaction width of the velocity transition layer  $D_v^E$  is wider than that of density transition layer  $D_{\rho}^E$ .

For a fixed value of R (> 1), when  $D_{\rho}$  is small, the transfer efficiency of kinetic energy between neighboring layers increases with decreasing the density gradient, so the linear growth rate increases with  $D_{\rho}$  and reaches a peak. When  $D_{\rho}$  greater than the peak value, the stabilizing effect of velocity transition layer becomes more significant and stronger than



FIG. 9: (Color online) The linear growth rate versus the width of density transition layer for R = 0.5, 1, 2, and 5. The initial density, shear velocity and pressure of the two fluids are  $(\rho_L, v_L, P_L) = (5.0, 0.5, 1.5)$  and  $(\rho_R, v_R, P_R) = (1.25, -0.5, 1.5)$ .

the destabilizing effect of the density transition layer, which leads to the decreasing of linear growth rate with  $D_{\rho}$ , as shown in Fig.9 of R = 1, 2, and 5 cases. However, when R < 1, the linear growth rate decreases monotonically with  $D_{\rho}$ , no matter it is small or large.

#### V. CONCLUSIONS AND DISCUSSIONS

In this paper, a two-dimensional LB model with 19 discrete velocities in six directions is proposed. The model allows to recover the compressible Euler equations in the continuum limit. With the introduction of WENO finite difference scheme, the unphysical oscillations at discontinuities are effectively suppressed. The validity of the model is verified by its application to the Sod shock tube and excellent agreement between the simulation results and the analytical solutions.

Using the proposed LB model, the velocity and density gradient effects on the KHI have been studied. The averaged density profiles, the peak kinetic energy are used to quantitatively describe the evolution of KHI. It is found that evolution of the KHI is damped with increasing the width of velocity transition layer but is strengthened with increasing the width of density transition layer. After the initial transient period and before the vortex has been well formed, the linear growth rates,  $\gamma_v$  and  $\gamma_\rho$ , vary with  $D_v$  and  $D_\rho$  approximately in the following way,  $\ln \gamma_v = a - bD_v$  and  $\gamma_\rho = c + e \ln D_\rho (D_\rho < D_\rho^E)$ , where a, b, c and e are fitting parameters and  $D_{\rho}^{E}$  is the effective interaction width of density transition layer. When  $D_{\rho} > D_{\rho}^{E}$  the growth rate  $\gamma_{\rho}$  goes to nearly a constant and the destabilizing effect of density gradient on KHI is fixed. These can be understood as follows. As noted above, in the classical case, the square of the linear growth rate is  $\gamma_{c}^{2} = k^{2}\rho_{1}\rho_{2}(u_{1}-u_{2})^{2}/(\rho_{1}+\rho_{2})^{2} \propto (1-A^{2})\Delta u^{2}$ . The wider velocity transition layer reduces the the local velocity difference  $\Delta u$  and the wider density transition zone reduces local Atwood number A. Therefore, the linear growth rate can be decreased by  $D_{v}$  but made larger by  $D_{\rho}$ . In practical system, both the two transition layers exist and there is a competition between these two gradient effects. One can use the hybrid effects of density and velocity transition layers to stabilize the KHI. By incorporating an appropriate equation of state, or equivalently, a free energy functional, or an external force, the present model may be used to simulate the liquid-vapor transition and the surface tension effects on KHI.

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[4] V. Sofonea, K. Mecke, Eur. Phys. J. B 8, 99 (1999); V. Sofonea, A. Lamura, G. Gonnella, A. Cristea, Phys. Rev. E 70, 046702 (2004); G. Gonnella, A. Lamura, V. Sofonea, Phys. Rev. E

S. Succi, The Lattice Boltzmann Equation for Fluid Dynamics and Beyond, (Oxford University Press, New York, 2001).

<sup>[2]</sup> Aiguo Xu, G. Gonnella, A. Lamura, Phys. Rev. E 67, 056105 (2003); Phys. Rev. E 74, 011505 (2006); Physica A 331, 10 (2004); Physica A 344, 750 (2004); Physica A 362, 42 (2006).

<sup>[3]</sup> Aiguo Xu, G. Gonnella, A. Lamura, G. Amati, F. Massaioli, Europhys. Lett. 71, 651 (2005);
Aiguo Xu, Commun. Theor. Phys. 39, 729 (2003); C. Wang, Aiguo Xu, Guangcai Zhang, Y. Li, Sci. China Ser. G-Phys. Mech. Astron. 52, 1337 (2009).

76, 036703 (2007); A. Cristea, G. Gonnella, A. Lamura, V. Sofonea, Commun. Comput. Phys.7, 350 (2010).

- [5] S. Y. Chen et al., Phys. Rev. Lett. 67, 3776 (1991).
- [6] S. Succi, M. Vergassola and R. Benzi, Phys. Rev. A 43, 4521 (1991).
- [7] G. Vahala et al., Comm. Comp. Phys. 4, 624 (2008).
- [8] J. Yepez, Int. J. Mod. Phys. C 12, 1285 (2001).
- [9] G. P. Berman et al., Phys. Rev. A 66, 012310 (2002).
- [10] K. Furtado and J. Yeomans, Phys. Rev. E 73, 066124 (2006).
- [11] C. H. Sun, Phys. Rev. E 58, 7283 (1998).
- [12] G. W. Yan, Y. S. Chen, and S. X. Hu, Phys. Rev. E 59, 454 (1999).
- [13] T. Kataoka, M. Tsutahara, Phys. Rev. E 69, 035701(R) (2004); Phys. Rev. E 69, 056702 (2004).
- [14] M. Watari, M. Tsutahara, Phys. Rev. E 67, 036306 (2003); Phys. Rev. E 70, 016703 (2004).
- [15] Aiguo Xu, Europhys. Lett. 69, 214 (2005); Phys. Rev. E 71, 066706 (2005); Prog. Theor.
   Phys. (Suppl.) 162, 197 (2006).
- [16] Yanbiao Gan, Aiguo Xu, Guangcai Zhang, Xijun Yu, and Y. J. Li, Physica A 387, 1721 (2008).
- [17] Feng Chen, Aiguo Xu, Guangcai Zhang, Yingjun Li and Sauro Succi, Europhys. Lett. 90, 54003 (2010).
- [18] Q. Li, Y. L. He, Y. Wang, and W. Q. Tao, Phys. Rev. E 76, 056705 (2007); Q. Li, Y.L. He,
  Y. Wang, G.H. Tang, Phys. Lett. A 373, 2101 (2009); Y. Wang, Y. L. He, T. S. Zhao, G.
  H.Tang and W. Q. Tao, Int. J. Mod. Phys. C 18, 1961 (2007).
- [19] J. Y. Zhang and G. W. Yan, Phys. Rev. E 81, 066705 (2010); Chaos 20, 023129 (2010).
- [20] Q. F. Wu, W. F. Chen, DSMC method for heat chemical nonequilibrium flow of high temperature rarefied gas, (in Chinese), (National Defence Science and Technology University Press, Beijing, 1999).
- [21] S. Chandrasekhar, Hydrodynamic and Hydromagnetic Stability, (Oxford University, London, 1961).
- [22] Walker J. S., Talmage G., Brown S. H. and Sondergaard N. A., Phys. Fluids A 5, 1466 (1993).
- [23] Bau H. H., Phys. Fluids **25**, 1719 (1982).
- [24] Miles J. W., Phys. Fluids **23**, 1719 (1980).

- [25] L. F. Wang, C. Xue, W. H. Ye, and Y. J. Li, Phys. Plasma 16, 112104 (2009).
- [26] L. F. Wang, W. H. Ye, and Y. J. Li, Phys. Plasma 17, 042103 (2010).
- [27] Miura A., Phys. Rev. Lett. 83, 1586 (1999).
- [28] Blaauwgeers R., Eltsov V. B., Eska G., Finne A. P., Haley R. P., Krusius M., Ruohio J. J., Skrbek L. and Volovik G. E., Phys. Rev. Lett. 89, 155301 (2002).
- [29] Bodo G., Mignone A. and Rosner R., Phys. Rev. E 70, 36304 (2004).
- [30] Horton W., Perez J. C., Carter T. and Bengtson R., Phys. Plasmas 12, 22303 (2005).
- [31] L. F. Wang, W. H. Ye, Z. F. Fan, Y. J. Li, X. T. He and M. Y. Yu, Europhys. Lett. 86, 15002 (2009).
- [32] R. Paul Drake, High-Energy-Density Physics: Fundamentals, Inertial Fusion and Experimental Astrophysics, (Springer, New York, 2006).
- [33] M. Lesieur, *Turbulence in Fluids*, (Kluwer Academic Publishers, Dordrecht, 1997).
- [34] V.N. Gamexo, A.M. Khokhlo, E.S. Oran, et al., Science **299**, 77 (2003).
- [35] A. Burrows, Nature (London) **430**, 727 (2000).
- [36] K. Nomoto, K. Iwamoto, and N. Kishimoto, Science **276**, 1378 (1997).
- [37] H. Hasegawa1, M. Fujimoto, T.D. Phan, et al., Nature (London) 430, 755 (2004).
- [38] L. F. Wang, W. H. Ye, and Y. J. Li, Phys. Plasma 17, 052305 (2010).
- [39] L. F. Wang, W. H. Ye, Z. F. Fan and Y. J. Li, Europhys. Lett. **90**, 15001 (2010).
- [40] Remington B. A., Drake R. P., Takabe H. et al., Phys. Plasmas 7, 1641 (2000).
- [41] Remington B. A., Drake R. P. and Ryutov D. D., Rev. Mod. Phys. 78 755 (2006).
- [42] G. Chimonas, Phys. Fluids **29**, 2061 (1986).
- [43] M. Watari, Phys. Rev. E **79**, 066706 (2009).
- [44] P. Bhatnagar, E. P. Gross, and M. K. Krook, Phys. Rev. 94, 511 (1954).
- [45] G. S. Jiang, C. W. Shu, J. Comput. Phys. **126**, 202 (1996).
- [46] G. A. Sod, J. Comput. Phys. 27, 1 (1978).
- [47] U. V. Amerstorfer, N. V. Erkaev, U. Taubenschuss, and H. K. Biernat, Phys. Plasma 17, 072901 (2010).
- [48] Ashwin J. and R. Ganesh, Phys. Rev. Lett. **104**, 215003 (2010).