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Lattice Boltzmann model for the compressible Navier-Stokes equations with flexible specific-heat ratio

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We have developed a lattice Boltzmann model for the compressible Navier-Stokes equations with a flexible specific-heat ratio. Several numerical results are presented, and they agree well with the corresponding solutions of the Navier-Stokes equations. In addition, an explicit finite-difference scheme is proposed for the numerical calculation that can make a stable calculation with a large Courant number.

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The kinetic equation approach [1–9] is often used to obtain solutions of the compressible Navier-Stokes (NS) equations. The merits of this approach are the simple basic equation, the linear derivative terms, the high resolution for capturing discontinuities (e.g., shock waves) without any complicated treatment of the numerical scheme, etc. However, to solve the kinetic equation, the molecular velocity space must be considered in addition to the physical space. Therefore, the calculation time naturally becomes larger. By employing the molecular velocities of discrete type, this disadvantage can be avoided to some extent. This is the lattice Boltzmann method (LBM) [1–7].

The LBM for the compressible NS equations was first devised by Alexander *et al.* [1]. Their model includes the nonlinear deviation terms that are proportional to the third-order flow velocity. Later, Chen *et al.* [2] proposed a model without these nonlinear deviation terms. However, an important defect still remains. That is, the specific-heat ratio γ cannot be chosen freely. Especially for the one and two-dimensional models, γ is fixed at unphysical values of 3 and 2, respectively.

In the present paper, we develop a lattice Boltzmann model (without nonlinear deviation terms) of the two-dimensional version that overcomes the defect cited above. For possible future extension to the one and three-dimensional versions, the formulation is presented with ($D=1$, 2, or 3) spatial dimensions, and then the specific two-dimensional model ($D=2$) is given.

For the sake of clarity, we first write down the compressible NS equations:

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u_\alpha}{\partial x_\alpha}=0, \tag{1a}$$

$$\frac{\partial \rho u_\alpha}{\partial t}+\frac{\partial \rho u_\alpha u_\beta}{\partial x_\beta}+\frac{\partial p}{\partial x_\alpha}=-\frac{\partial P'_{\alpha\beta}}{\partial x_\beta}, \tag{1b}$$

$$\frac{\partial \rho(bRT+u_\alpha^2)}{\partial t}+\frac{\partial \rho u_\alpha(bRT+u_\beta^2)+2pu_\alpha}{\partial x_\alpha}=2\frac{\partial}{\partial x_\beta}\left(\lambda\frac{\partial T}{\partial x_\beta}-P'_{\alpha\beta}u_\alpha\right), \tag{1c}$$

where

$$p=\rho RT, \tag{1d}$$

$$P'_{\alpha\beta}=-\mu\left(\frac{\partial u_\alpha}{\partial x_\beta}+\frac{\partial u_\beta}{\partial x_\alpha}-\frac{2}{3}\frac{\partial u_\chi}{\partial x_\chi}\delta_{\alpha\beta}\right)-\mu_B\frac{\partial u_\chi}{\partial x_\chi}\delta_{\alpha\beta} \quad (\alpha,\beta,\chi=1,2,\ldots,D), \tag{1e}$$

and t is the time and x_α is the spatial coordinate. ρ, u_α, T, and p are, respectively, the density, the flow velocity in the x_α direction, the temperature, and the pressure of a gas. R is the specific gas constant and b is a given constant related to the specific-heat ratio γ by

$$\gamma=(b+2)/b. \tag{2}$$

The above NS equations (1a)–(1c) are characterized by γ, $\mu(\rho,T)$ (the viscosity), $\mu_B(\rho,T)$ (the bulk viscosity), and $\lambda(\rho,T)$ (the thermal conductivity). Note that, in the present study, the subscripts α, β, and χ represent the number of spatial coordinates and the summation convention is applied to these subscripts.

Now we present a lattice Boltzmann model that gives the solution of the compressible NS equations (1a)–(1c). Let $c_{i\alpha}$ ($i=1,2,\ldots,I$; I is the total number of discrete molecular velocities) be the molecular velocities in the x_α direction of the ith particle, and η_i be another variable newly introduced to control the specific-heat ratio. $f_i(t,x_\alpha)$ is the velocity distribution function of the ith particle. The macroscopic variables ρ, u_α, and T are defined as

$$\rho=\sum_{i=1}^{I} f_i, \tag{3a}$$

$$\rho u_\alpha=\sum_{i=1}^{I} f_i c_{i\alpha}, \tag{3b}$$

$$\rho(bRT+u_\alpha^2)=\sum_{i=1}^{I} f_i(c_{i\alpha}^2+\eta_i^2). \tag{3c}$$

Note that the summation convention is not applied to the subscript i representing the kind of molecules.

Consider the kinetic equation of the BGK type [10]:

$$\frac{\partial f_i}{\partial t}+c_{i\beta}\frac{\partial f_i}{\partial x_\beta}=\frac{f_i^{\mathrm{eq}}(\rho,u_\alpha,T)-f_i}{\phi(\rho,T)}, \tag{4}$$

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where $\phi(\rho,T)$ (the relaxation time) is a given function of ρ and T [3], and $f_i^{\mathrm{eq}}(\rho,u_\alpha,T)$ (the local equilibrium velocity distribution function) is a given function of the macroscopic variables that satisfies the following relations:

$$\rho=\sum_{i=1}^{I} f_i^{\mathrm{eq}}, \tag{5a}$$

$$\rho u_\alpha=\sum_{i=1}^{I} f_i^{\mathrm{eq}} c_{i\alpha}, \tag{5b}$$

$$p\,\delta_{\alpha\beta}+\rho u_\alpha u_\beta=\sum_{i=1}^{I} f_i^{\mathrm{eq}} c_{i\alpha}c_{i\beta}, \tag{5c}$$

$$\rho(bRT+u_\alpha^2)=\sum_{i=1}^{I} f_i^{\mathrm{eq}}(c_{i\alpha}^2+\eta_i^2), \tag{5d}$$

$$\rho[(b+2)RT+u_\beta^2]u_\alpha=\sum_{i=1}^{I} f_i^{\mathrm{eq}}(c_{i\beta}^2+\eta_i^2)c_{i\alpha}, \tag{5e}$$

$$\rho[RT(u_\alpha\delta_{\beta\chi}+u_\beta\delta_{\chi\alpha}+u_\chi\delta_{\alpha\beta})+u_\alpha u_\beta u_\chi] =\sum_{i=1}^{I} f_i^{\mathrm{eq}} c_{i\alpha}c_{i\beta}c_{i\chi}, \tag{5f}$$

$$\rho\{(b+2)R^2T^2\delta_{\alpha\beta}+[(b+4)u_\alpha u_\beta+u_\chi^2\delta_{\alpha\beta}]RT+u_\chi^2 u_\alpha u_\beta\} =\sum_{i=1}^{I} f_i^{\mathrm{eq}}(c_{i\chi}^2+\eta_i^2)c_{i\alpha}c_{i\beta}. \tag{5g}$$

Then the macroscopic variables ρ, u_α, and T obtained from the solution of the kinetic equation (4) for small values of $\varepsilon\equiv\phi(\rho_0,T_0)\sqrt{RT_0}/L$ (ρ_0, T_0, and L are, respectively, the reference density, temperature, and length) satisfy the compressible NS equations (1a)–(1c) with the relative error of $O(\varepsilon^2)$, whose transport coefficients are given by

$$\mu=\rho RT\phi,\quad \mu_B=2(1/3-1/b)\rho RT\phi,$$
$$\lambda=(b+2)\rho R^2T\phi/2. \tag{6}$$

The method of derivation is a straightforward application of the Chapman-Enskog expansion or the usual asymptotic analysis for $\varepsilon\ll1$. See Refs. [1–5,9,11,12] for details.

We will give a specific form of $c_{i\alpha}$, η_i, and f_i^{eq} of the two-dimensional version ($D=2$ and $I=16$) that satisfies the above constraints (5a)–(5g):

$$(\hat{c}_{i1},\hat{c}_{i2})=\begin{cases}\text{cyc: } (\pm1,0) & \text{for } 1\leqslant i\leqslant4\\ \text{cyc: } (\pm6,0) & \text{for } 5\leqslant i\leqslant8\\ \sqrt{2}(\pm1,\pm1) & \text{for } 9\leqslant i\leqslant12\\ \dfrac{3}{\sqrt{2}}(\pm1,\pm1) & \text{for } 13\leqslant i\leqslant16,\end{cases}$$

$$\hat{\eta}_i=\begin{cases}5/2 & \text{for } 1\leqslant i\leqslant4\\ 0 & \text{for } 5\leqslant i\leqslant16\end{cases} \tag{7}$$

(see Fig. 1), where cyc indicates the cyclic permutation, and

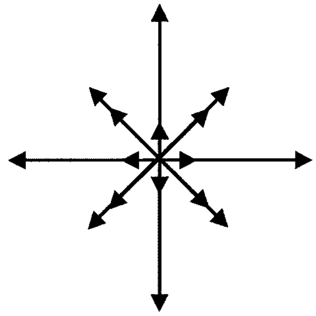

FIG. 1. Distribution of $c_{i\alpha}$ ($\alpha=1,2$; $i=1,2,\dots,16$) for the proposed lattice Boltzmann model.

$$f_i^{\mathrm{eq}}=\rho[a_{0i}+a_{1i}\hat{T}+a_{2i}\hat{T}^2+(a_{3i}+a_{4i}\hat{T})\hat{u}_\alpha^2+a_{5i}\hat{u}_\alpha^2\hat{u}_\beta^2 +(b_{0i}+b_{1i}\hat{T}+b_{2i}\hat{u}_\alpha^2)\hat{u}_\beta\hat{c}_{i\beta}+(d_{0i}+d_{1i}\hat{T}+d_{2i}\hat{u}_\alpha^2) \times\hat{u}_\beta\hat{c}_{i\beta}\hat{u}_\chi\hat{c}_{i\chi}+e_i\hat{u}_\alpha\hat{c}_{i\alpha}\hat{u}_\beta\hat{c}_{i\beta}\hat{u}_\chi\hat{c}_{i\chi}]$$

$$\text{for } i=1,2,\dots,16, \tag{8}$$

where $a_{0i},\dots,e_i$ are given constants whose specific values are arranged in Table I. The variables with a caret are the nondimensional quantities, i.e., $\hat{T}=T/T_0$ and $(\hat{u}_\alpha,\hat{c}_{i\alpha},\hat{\eta}_i)=(u_\alpha,c_{i\alpha},\eta_i)/\sqrt{RT_0}$.

The proposed lattice Boltzmann model, or the kinetic equation (4) with $c_{i\alpha}$, η_i, and f_i^{eq} given above [or by Eqs. (7) and (8)] can take any value of b which is related to the specific-heat ratio γ by Eq. (2). The key is the introduction of η_i that makes it possible to satisfy relations (5c)–(5f) at the same time for any value of b [11]. As for the three-dimensional version ($D=3$), it is, in fact, possible to construct a specific model by using 32 velocities ($I=32$). However, this specific model is not shown here, since the one we derived did not show excellent performance in the numerical computation and it will be possible in the future to construct a better model for computation. For the readers who are interested in the three-dimensional calculation, we introduce Ref. [2] that proposed the three-dimensional model with fixed specific-heat ratio $\gamma=5/3$.

In order to solve the kinetic equation (4) of the above lattice Boltzmann model numerically, here we propose a scheme that utilizes the Crank-Nicolson scheme:

$$f_i|_{t+\Delta t}=f_i|_t-\frac{c_{i\alpha}\Delta t}{2}\left(\left.\frac{\partial f_i}{\partial x_\alpha}\right|_t+\left.\frac{\partial f_i}{\partial x_\alpha}\right|_{t+\Delta t}\right) +\left.\frac{f_i^{\mathrm{eq}}(\rho,u_\alpha,T)-f_i}{\phi(\rho,T)}\right|_t\Delta t, \tag{9}$$

where the quantities with $|_t$ are evaluated at time t. Δt is the time step, Δx is the grid step, and $\partial f_i/\partial x_\alpha$ is the usual second-order upstream finite difference given by

$$\frac{\partial f_i}{\partial x_\alpha}=\begin{cases}[3f_i(x_\alpha)-4f_i(x_\alpha-\Delta x)+f_i(x_\alpha-2\Delta x)]/2\Delta x & \text{for } c_{i\alpha}>0\\ [-3f_i(x_\alpha)+4f_i(x_\alpha+\Delta x)-f_i(x_\alpha+2\Delta x)]/2\Delta x & \text{for } c_{i\alpha}<0,\end{cases} \tag{10}$$

where $f_i(x_\alpha)$ is evaluated at space x_α. Although the collision term, or the last term on the right-hand side of Eq. (9) is evaluated at time t, we can easily find that scheme (9) with $\Delta t \sim \phi(\rho_0,T_0)$ and $\Delta x \sim (\rho_0,T_0)\sqrt{RT_0}$ achieves second-order accuracy in ε, and can describe the solution of the compressible NS equations (1a)–(1c) appropriately.

A stable calculation of scheme (9) with the large Courant number $|c_{i\alpha}|\Delta t/\Delta x$ is possible. Moreover, it can be solved from the upstream side of $c_{i\alpha}$ successively without using an iterative method, because $\partial f_i/\partial x_\alpha|_{t+\Delta t}$ can be evaluated by the already calculated values of $f_i|_{t+\Delta t}$ on the upstream side.

Now several numerical examples are presented. First, consider the Riemann problem whose initial macroscopic variables are given by

$$\hat{\rho}=\hat{T}=1, \quad \hat{u}_1=\begin{cases}-U & \text{for } \hat{x}_1<0\\ U & \text{for } \hat{x}_1>0,\end{cases} \tag{11}$$

where U is a given constant. This problem is characterized by U, ε, $\hat{\phi}(\hat{\rho},\hat{T})\equiv\phi(\rho,T)/\phi(\rho_0,T_0)$, and γ. The numerical results with $U=0.5$, $\varepsilon=0.001$, and $\hat{\phi}=1/\hat{\rho}$ are shown for three different values of γ=5/3, 7/5, and 9/7 (or $b=3$, 5, and 7) in Fig. 2 by the plots. There is no characteristic length in the initial condition so that the dimension of the length is nondimensionalized by $t_0\sqrt{RT_0}$, where the presented results are those at $t=t_0$. The corresponding numerical results of the NS equations themselves [Eqs. (1a)–(1c)], solved by the so-called MacCormack scheme [13] with the sufficient number of meshes, are shown by the lines. We find a good agreement between the two results for each value of γ.

Next, we consider the shock-tube problem. The initial macroscopic variables are given by

$$\hat{\rho}=\begin{cases}1 & \text{for } \hat{x}_1<0\\ P & \text{for } \hat{x}_1>0,\end{cases} \quad \hat{u}_1=0, \quad \hat{T}=1, \tag{12}$$

where P is a given constant. This problem is characterized by the four parameters P, ε, $\hat{\phi}(\hat{\rho},\hat{T})$, and γ. The numerical results with $P=2$, ε=0.001, and $\hat{\phi}=1/\hat{\rho}$ are shown for three different values of γ=5/3, 7/5, and 9/7 in Fig. 3 by the plots together with the corresponding numerical results of the NS equations solved by the MacCormack scheme (represented by the lines). We find a good agreement between the two results for each value of γ.

Finally, we show the results of the two-dimensional steady Couette flow. The boundary conditions are

$$\hat{u}_1=-U, \quad \hat{T}=1 \quad \text{at } \hat{x}_2=0, \tag{13a}$$

$$\hat{u}_1=U, \quad \hat{T}=1 \quad \text{at } \hat{x}_2=1, \tag{13b}$$

where U is a given constant. This problem is characterized by the four parameters U, ε, $\hat{\phi}(\hat{\rho},\hat{T})$, and γ. The numerical results with $U=0.5$, $\varepsilon=0.002$, and $\hat{\phi}=1/\hat{\rho}$ are shown for three different values of γ=5/3, 7/5, and 9/7 in Fig. 4 by the plots together with the corresponding numerical results of the NS equations solved by the MacCormack scheme (represented by the lines). We find a good agreement between the two results for each value of γ.

TABLE I. The coefficients $a_{0i},\ldots,e_i$ ($i=1,2,\ldots,16$) in the local equilibrium distribution function f_i^{eq} given by Eq. (8).

i	1–4	5–8	9–12	13–16
a_{0i}	0	1/96	81/160	$-4/15$
a_{1i}	$\frac{b-2}{25}$	$\frac{-121b-408}{86400}$	$\frac{-229b+8}{3200}$	$\frac{89b+222}{2700}$
a_{2i}	0	$\frac{b+2}{1728}$	$\frac{b+2}{320}$	$\frac{-b-2}{270}$
a_{3i}	$-36/115$	$-799/397440$	$-117/640$	13/135
a_{4i}	$\frac{b+4}{115}$	$\frac{19b+306}{397440}$	$\frac{9b+38}{640}$	$\frac{-2b-9}{270}$
a_{5i}	1/115	19/397440	9/640	$-1/135$
b_{0i}	0	0	9/40	$-2/45$
b_{1i}	$\frac{2(b-2)}{25}$	$\frac{-2b+29}{32400}$	$\frac{-14b+3}{400}$	$\frac{2(7b+11)}{2025}$
b_{2i}	0	$-1/2592$	1/80	$-7/810$
d_{0i}	72/115	$-29/298080$	9/160	$-2/405$
d_{1i}	$\frac{-2(b+4)}{115}$	$\frac{b+4}{74520}$	$\frac{-b-4}{160}$	$\frac{b+4}{810}$
d_{2i}	$-2/115$	1/74520	$-1/160$	1/810
e_i	0	1/46656	$-3/320$	8/3645

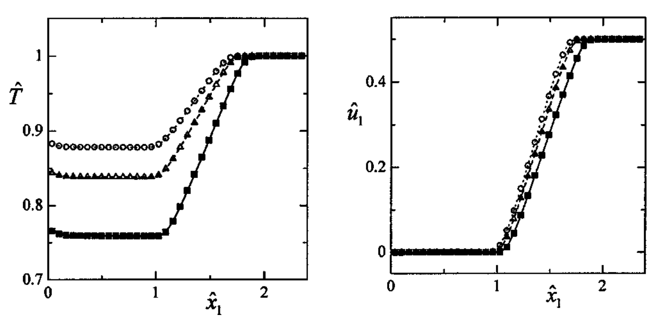

FIG. 2. The profiles of $\hat{T}$ and $\hat{u}_1$ for the Riemann problem whose initial condition is Eq. (11) with $U=0.5$, $\varepsilon=0.001$, and $\hat{\phi}=1/\hat{\rho}$. The plots are the results by the LBM: ■, γ=5/3; △, γ=7/5; ○, γ=9/7. The lines represent the corresponding results by the MacCormack method with the sufficient number of meshes: γ=5/3 (solid lines), 7/5 (dashed lines), and 9/7 (dotted lines).

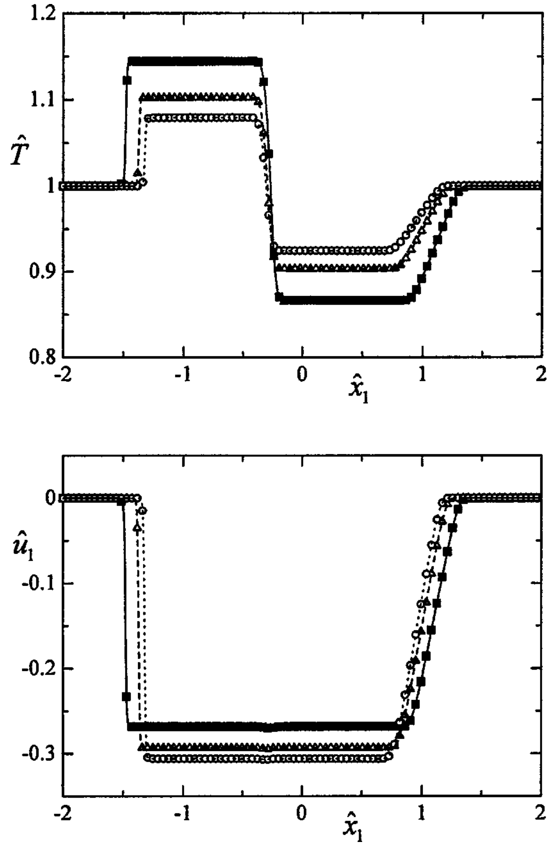

FIG. 3. The profiles of $\hat{T}$ and $\hat{u}_1$ for the shock-tube problem whose initial condition is Eq. (12) with $P=2$, $\varepsilon=0.001$, and $\hat{\phi}=1/\hat{\rho}$. See the caption of Fig. 2 for the representation of the symbols ■, △, ○, and the lines.

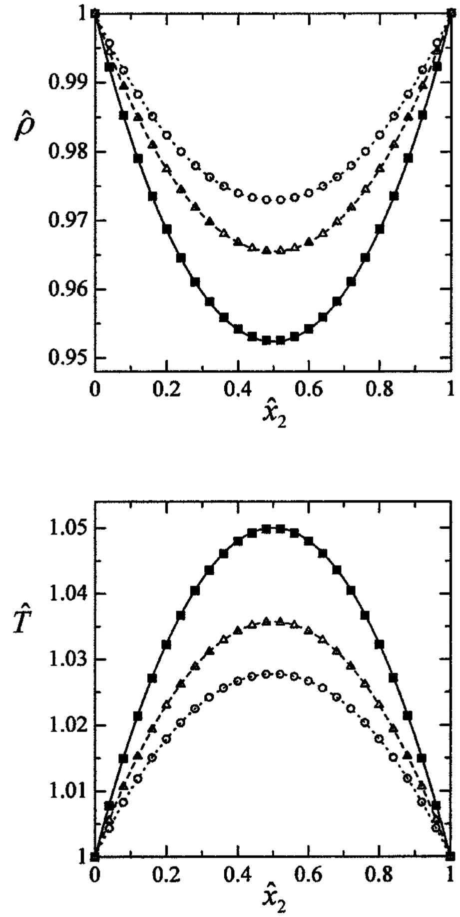

FIG. 4. The profiles of $\hat{\rho}$ and $\hat{T}$ for the two-dimensional steady Couette flow whose boundary conditions are Eqs. (13a) and (13b) with $U=0.5$, $\varepsilon=0.002$, and $\hat{\phi}=1/\hat{\rho}$. See the caption of Fig. 2 for the representation of the symbols ■, △, ○, and the lines.

In conclusion, we have developed a lattice Boltzmann model for the compressible NS equations with a flexible specific-heat ratio. Several numerical results are presented and they agree well with the corresponding solutions of the compressible NS equations solved by the MacCormack scheme. Thus, the validity of our model has been strongly confirmed. The explicit finite-difference scheme is also proposed for the numerical calculation of the LBM. This scheme can make a stable calculation with large Courant number so that it can be a new merit of the LBM. According to our numerical tests, it can make stable calculation with the Courant number of up to 100 if the solution is smooth and $\Delta t < 2\phi(\rho,T)$ is satisfied.

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