Gas-Flow Simulations by Novel Lattice Boltzmann Method

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We have developed a new lattice Boltzmann model which can simulate supersonic flows described by the compressible Euler and Navier-Stokes equations. The model is based on the free-molecular-type kinetic equation whose basic calculation system was devised by Sone in the year 2002. Our proposed scheme is superior to the existing lattice Boltzmann method (LBM) in the following two points: (I) supersonic flows can be simulated; (II) any transport coefficients can be chosen freely according to our convenience. Several numerical simulations are carried out to confirm the above merits of the scheme. Numerical results agree well with the corresponding solutions of the Euler and Navier-Stokes equations even for supersonic flows.

1. INTRODUCTION

Recently, the kinetic equation approach is extensively studied as an alternative numerical method to obtain solutions of the fluid-dynamic-type equations. The lattice Boltzmann method (LBM)\(^1\) is one of them, and it uses the molecular velocities of discrete type. Thus, the LBM solves the kinetic equation with a finite number of molecular velocities such that the macroscopic variables obtained from the solution satisfy the desired fluid-dynamic-type equations. The merits of this numerical method are the simple basic equation, the linear derivative terms, and high resolution for capturing discontinuities like shock waves without any special complicated treatment of the scheme, etc.

It is Alexander et al.\(^3\) who first devised the Lattice Boltzmann model for the compressible Navier-Stokes (NS) equations. His model includes several defects: an error proportional to the third-order flow velocities arises; the specific-heat ratio cannot be chosen freely, etc. Chen et al.\(^5\) removed the former defect and Kataoka & Tsutahara\(^7\) overcome the latter. The current LBM for the compressible flows then still has the following defects:

(i) Supersonic flows cannot be simulated stably.

(ii) Three transport coefficients, i.e. the viscosity, the bulk viscosity, and the thermal conductivity, cannot be chosen freely.

These demerits are, in fact, severe restriction as a numerical tool.

In the year 2002, Sone\(^8\) proposed a simple way to construct a kinetic system in such a way that some moments of the solution of the kinetic equation satisfy the Euler or NS set of equations exactly. On the basis of this kinetic system, he discussed a much simpler numerical scheme without collision term, but instead modifies the velocity distribution function at each time step. The error estimate of this scheme was also explained, and it was mentioned that the molecular velocity is not necessarily continuous. This scheme overcomes the above-mentioned defect (ii) of the current LBM.
Moreover in the kinetic system proposed by Sone, macroscopic variables can be calculated without velocity distribution function so that there is no need to store the velocity distribution function. In fact, Junk & Rao (9) (see also Inamuro (10)) devised such a discrete-velocity kinetic scheme for incompressible flows, but there is no model for compressible flows.

In the present study therefore we will make specific model for compressible flows on the basis of Sone’s kinetic system. The obtained kinetic scheme gives solution of the compressible Euler and NS equations even for supersonic flows so that the defect (i) is overcome in addition to (ii). Our proposed scheme thus becomes an efficient numerical tool for obtaining solution of the compressible Euler and NS equations.

2. LATTICE BOLTZMANN MODEL

First, we write down the compressible NS equations (which also include the compressible Euler equations):

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

\[
\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta}{\partial x_\beta} = -\frac{\partial P_{\alpha\beta}}{\partial x_\beta}, \tag{1b}
\]

\[
\frac{\partial \rho (bRT + u_\alpha^2)}{\partial t} + 2 \frac{\partial \Pi_\alpha}{\partial x_\alpha} = 0, \tag{1c}
\]

with

\[
P_{\alpha\beta} = \rho RT \delta_{\alpha\beta} - \mu \left( \frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3} \frac{\partial u_x}{\partial x_\alpha} \delta_{\alpha\beta} \right) - \mu_b \frac{\partial u_\alpha}{\partial x_\alpha} \delta_{\alpha\beta}, \tag{1d}
\]

\[
\Pi_\alpha = \frac{\rho}{2} \left( bRT + u_\alpha^2 \right) u_\alpha + P_{\alpha\beta} u_\beta - \lambda \frac{\partial T}{\partial x_\alpha}, \tag{1e}
\]

\[
(\alpha, \beta, \chi = 1, 2, \cdots, D)
\]

where \(t\) is the time, \(x_\alpha\) is the spatial coordinate, \(R\) is the specific gas constant, \(D\) is the number of dimensions, and \(b\) is a given constant related to the specific-heat ratio \(\gamma\) by

\[
\gamma = b + 2. \tag{2}
\]

\(\rho, u_\alpha, T, P_{\alpha\beta}, \) and \(\Pi_\alpha\) are, respectively, the density, the flow velocity in the \(x_\alpha\) direction, the temperature, the stress tensor, and the energy flux in the \(x_\alpha\) direction of a gas. There are three transport coefficients: \(\mu(\rho, T)\) (the viscosity), \(\mu_b(\rho, T)\) (the bulk viscosity), and \(\lambda(\rho, T)\) (the thermal conductivity), which are functions of \(\rho\) and \(T\). The Euler equations are obtained by putting \(\mu = \lambda = 0\). Note that, in the present study, the subscripts \(\alpha, \beta, \) and \(\chi\) represent the number of spatial coordinates and the summation convention is applied to these subscripts.

Now we present new lattice Boltzmann model that gives solution of the compressible Euler and NS equations (1). Let \(c_{\alpha i}(\alpha = 1, \cdots, D, \ i = 0, 1, \cdots, 3I)\) be the molecular velocities in the \(x_\alpha\) direction and \(f_i(t, x_\alpha)(\alpha = 1, \cdots, D, \ i = 0, 1, \cdots, 3I)\) be the velocity distribution function of the \(i\)th particle. The total number of discrete molecular velocities is \(3I + 1\). The macroscopic variables \(\rho, u_\alpha,\) and \(T\) are defined as

\[
\rho = \sum_{i=0}^{3I} f_i, \quad \rho u_\alpha = \sum_{i=0}^{3I} f_i c_{\alpha i}, \quad \rho (bRT + u_\alpha^2) = f_i v_i^2 + \sum_{i=0}^{3I} f_i c_{\alpha i}^2, \tag{3a-e}
\]

with
\[ c_{a_i} = \begin{cases} 0 & \text{for } i = 0, \\ v_i q_{a_0} & \text{for } i = 1, \cdots, I, \\ v_i q_{a_{i-1}} & \text{for } i = I + 1, \cdots, 2I, \\ v_i q_{a_{2I-1}} & \text{for } i = 2I + 1, \cdots, 3I, \end{cases} \quad (4a) \]

where \( v_0, v_1, v_2, \) and \( v_3 \) are given positive constants, and \( q_{a_i} \) (\( i = 1, \cdots, I \)) is the unit vector defined by (see Fig. 1)

\[ q_{a_i} = \begin{cases} \cos \frac{\pi}{D} (D = 1; I = 2), \left( \cos \frac{\pi}{3}, \sin \frac{\pi}{3} \right) (D = 2; I = 6), \\ \text{cyc:} \frac{1}{2^{1/4}} \left( 0, \pm \frac{1+\sqrt{5}}{2}, \pm \frac{2}{\sqrt{1+\sqrt{5}}} \right) (D = 3; I = 12). \end{cases} \quad (4b) \]

Here cyc represents cyclic permutation.

Consider the initial-value problem of the free-molecular-type kinetic equation:

\[ \frac{\partial f}{\partial t} + c_{a_i} \frac{\partial f}{\partial x_i} = 0, \quad (5) \]

in a continuous sequence of time intervals \((t_m, t_m'\)] under the following initial condition for each interval \((t_m, t_m']\):

\[ f_i = f_i^*(\rho_{(m)}, u_{a(m)}, T_{(m)}), \quad (6a) \]

where \( \rho_{(m)}, u_{a(m)}, \) and \( T_{(m)} \) are \( \rho, u_a, \) and \( T \) calculated from the solution \( f_i \) at \( t = t_m \) of (5) in the preceding interval \((t_{m-1}, t_m')\), and

\[ f_i^*(\rho, u_a, T) = \begin{cases} \frac{\rho bRT - P_{\text{max}}}{v_0^3} & \text{for } i = 0, \\ \frac{v_i^2 - v_{a_i}^2}{v_{a_i}^2 (v_i^2 - v_{a_i}^2)} F_i(\rho, u_a, T) & \text{for } i = 1, \cdots, I, \\ \frac{v_i^2 - v_{a_i}^2}{v_{a_i}^2 (v_i^2 - v_{a_i}^2)(v_i^2 - v_{a_i}^2)} F_i(\rho, u_a, T) & \text{for } i = I + 1, \cdots, 2I, \\ \frac{v_i^2 - v_{a_i}^2}{v_{a_i}^2 (v_i^2 - v_{a_i}^2)(v_i^2 - v_{a_i}^2)} F_i(\rho, u_a, T) & \text{for } i = 2I + 1, \cdots, 3I, \end{cases} \quad (6b) \]

with

Fig. 1 Distribution of the unit vector \( q_{a_i} \) (\( \alpha = 1, \cdots, D; \ i = 0, \cdots, I \)) (a) one-dimensional model \((D = 1, I = 2)\); (b) two-dimensional model \((D = 2, I = 6)\); (c) three-dimensional model \((D = 3, I = 12)\).
\begin{align}
F_i(\rho, u, T) &= \frac{1}{D+1} \left\{ \rho u_a c_\alpha c_\beta^2 + \frac{1}{D} \left( \rho - \frac{\rho b RT - P_{ij}}{v_i} \right) c_\alpha^2 c_\beta^2 + 2 \Pi_{ij} c_\alpha c_\beta^2 \right. \\
&\quad \left. + \left[ \frac{D+2}{2} (\rho u_a u_\beta + P_{ij} - \frac{\rho u_a^2 + P_{ij}}{2} \delta_{ij}) \right] c_\alpha c_\beta \right\}.
\end{align}
(6c)

Then the macroscopic variables \( \rho, \ u_a, \) and \( T \) obtained from the solution \( f_i \) at an arbitrary time satisfy the compressible NS equations (and Euler equations if we put \( \mu = \lambda = 0 \)), or (1), within the error of \( O(\max(t_{m+1} - t_n)) \). This error term can be made sufficiently small irrespective of flow parameters (see Sone\(^a\) for this derivation).

It is evident that the proposed lattice Boltzmann scheme (3)-(6) given above overcomes the defect (ii), since any transport coefficients \( \mu, \ \mu_g, \) and \( \lambda \) can be chosen freely. As for the defect (i), numerical examples in the next section show that the proposed scheme can compute supersonic flows stably. Thus, our proposed scheme can give solution of the compressible Euler and NS equations for any parameter sets including the Mach number greater than unity.

3. NUMERICAL EXAMPLES

Now we present several numerical examples. We will solve the kinetic equation (5) by the following finite-difference scheme:

\[ f_{i(m+1)} = f_{i(m)} - c_{\alpha} \frac{\partial f_{i(m)}}{\partial x_{\alpha}} (t_{m+1} - t_{m}), \]
(7)

where \( f_{i(m)} \) represents \( f_i \) at \( t = t_m \), and \( \frac{\partial f_{i(m)}}{\partial x_{\alpha}} \) is evaluated by the usual upwind finite-difference formula of third-order accuracy (so-called UTOPIA).

We first treat the expansion-wave problem whose initial macroscopic variables are given by
\[ \rho = \rho_0, \quad u = U \tanh(x/L), \quad T = T_0, \]
(8)

Fig. 2 Numerical results \( u_i/\sqrt{\gamma RT_0} \) and \( T/T_0 \) at \( \tilde{t} = 10 \) for the expansion-wave problem whose initial conditions are (8) with \( \gamma = 5/3 \) and three different values of \( Ma = 2, 3, \) and \( 4 \) (\( \mu = \lambda = 0 \)). The symbols (\( C, \ Ma = 2; \ \triangle, \ Ma = 3; \ \square, \ Ma = 4 \)) are the results by the proposed lattice Boltzmann scheme (3)-(6) with \( D = 1 \) and mesh interval \( \Delta x, \ l/L = 0.5 \), and the lines are the corresponding results of the Euler equations solved by the MacCormack method with the sufficient number of meshes. From the symmetry of the problem with respect to \( x_i = 0 \), only the results for \( x_i > 0 \) are shown.
where $\rho_0$, $U$, $L$, and $T_0$ are given positive constants. When $\mu = \lambda = 0$, this problem is simply characterized by the specific-heat ratio $\gamma$ defined by (2) and the Mach number $Ma = U/\sqrt{\gamma RT_0}$. Numerical results at $\tilde{t} = t/\sqrt{\gamma RT_0}/L = 10$ for $\gamma = 5/3$ and three different values of $Ma = 2, 3, $ and 4 are shown in Fig. 2. The symbols represent results by the proposed lattice Boltzmann scheme (3)-(6) with $D = 1$ ($v_0 = 0.6$, $v_1 = 0.3$, $v_2 = 1.2$, $v_3 = 60$ were chosen throughout this study) while the solid lines are the corresponding numerical results of the Euler equations solved by the so-called MacCormack scheme\textsuperscript{11}) with the sufficient number of meshes. We find a good agreement between the two results. Note that the existing lattice Boltzmann models can make calculation only for the Mach number smaller than unity.

Next, we consider the same problem when $\mu \neq 0$ and $\lambda \neq 0$. The problem is then characterized by the specific-heat ratio $\gamma$, the Mach number $Ma$, the Reynolds number $Re$, and the Prandtl number $Pr$ defined by

$$Re = \frac{UL}{\mu(\rho_0, T_0)}, \quad Pr = \frac{b\rho_0(\rho_0, T_0)}{2\lambda(\rho_0, T_0)},$$

as well as the functional forms of $\mu(\rho, T)$ and $\lambda(\rho, T)$. Numerical results at $\tilde{t} = 10$ for $\gamma = 5/3$, $Ma = 3$, $Pr = 10$, and three different values of $Re = 100, 500$, and $\infty$ with $\mu$ and $\lambda$ being constants ($\mu_0$ can be incorporated into $\mu$ for $D = 1$) are shown in Fig. 3. The symbols represent results by the proposed scheme (3)-(6) with $D = 1$ while the solid lines are the corresponding numerical results of the NS equations solved by the MacCormack scheme\textsuperscript{11}). We find a good agreement between the two results for each case, or $Re = 100$ and $500$ (results for $Re \to \infty$ are shown for the sake of comparison).

Thirdly, we treat the same problem when $\mu$ is not constant. Temperature fields at $\tilde{t} = 10$ calculated from the proposed scheme (3)-(6) with $D = 1$ are plotted in Fig. 4 by the symbols together with the corresponding results of the NS equations solved by the MacCormack scheme (represented by the solid line). We find a good agreement between the two results for each case, or $\mu(\rho, T)/\mu(\rho_0, T_0) = (T/T_0)^{1/2}$, $T/T_0$, and $(T/T_0)^{1/2}$ while $\lambda$ is constant. Note that the existing

![Fig 3 Numerical results $u_i/\sqrt{\gamma RT_0}$ and $T/T_0$ at $\tilde{t} = 10$ for the expansion-wave problem whose initial conditions are (8) with $\gamma = 5/3$, $Ma = 3$, $Pr = 10$, and three different values of $Re = 100, 500$, and $\infty$ ($\mu$ and $\lambda$ are constants). The symbols (O, $Re = 100$; $\triangledown$, $Re = 500$; $\square$, $Re = \infty$) are the results by the proposed one-dimensional lattice Boltzmann scheme with mesh interval $\Delta x_i/L = 0.5$, and the lines are the corresponding results of the NS equations solved by the MacCormack method with the sufficient number of meshes.](image-url)
lattice Boltzmann models can make calculation only for the same functional dependencies of $\mu$ and $\lambda$, or $\mu(\rho,T)/\mu(\rho_o,T_o) = \lambda(\rho,T)/\lambda(\rho_o,T_o)$, which corresponds to the defect (ii).

Finally, we consider the shock-tube problem in which the shock waves and contact discontinuities appear. The initial macroscopic variables are given by

$$\rho = \begin{cases} \rho_o & \text{for } x_i < 0 \\ \rho_i & \text{for } x_i > 0, \end{cases} \quad u_i = 0, \quad T = T_o,$$

where $\rho_o$, $\rho_i$, and $T_o$ are given positive constants. Here we treat the case of $\mu = \lambda = 0$, so that the problem is characterized simply by $\gamma$ and $\rho_i/\rho_o$. Numerical results for $\gamma = 7/5$ and three different values of $\rho_i/\rho_o = 10, 30,$ and $50$ are shown in Fig. 5 by the solid lines. The corresponding exact theoretical solutions are shown by the dotted lines. We find a good agreement between the two results.

![Fig. 4 Temperature fields $T/T_o$ at $t = 10$ for the expansion-wave problem whose initial conditions are (8) with $\gamma = 5/3$, Ma = 3, Re = 100, Pr = 10, and three different functional dependencies of $\mu(\rho,T)/\mu(\rho_o,T_o) = (T/T_o)^{3/2}$, $T/T_o$, and $(T/T_o)^{3/2} (\lambda$ is constant). The symbols (O), $\lambda(\rho,T)/\lambda(\rho_o,T_o) = (T/T_o)^{3/2}$; (O), $\lambda(\rho,T)/\lambda(\rho_o,T_o) = (T/T_o)^{3/2}$; (O), $T/T_o$; (O), $(T/T_o)^{3/2}$) are the results by the proposed one-dimensional lattice Boltzmann scheme with mesh interval $\Delta x_i/L = 0.5$, and the lines are those of the NS Equations solved by the MacCormack method.](image)

![Fig. 5 Numerical results $\rho/\rho_o$, $u_i/\sqrt{\gamma RT_o}$, and $T/T_o$ for the shock-tube problem whose initial conditions are (10) with $\gamma = 7/5$ and three different values of $\rho_i/\rho_o = 10, 30,$ and $50$ ($\mu = \lambda = 0$). The solid lines are the results by the proposed one-dimensional lattice Boltzmann scheme with mesh interval $\Delta x_i/L = 0.01$, and the dotted lines are the corresponding theoretical solutions.](image)
for each case of $\rho_i / \rho_j$. Numerical data near the shock waves and contact discontinuities deviate from the exact solution, but it is natural because we did not use a special complicated scheme like TVD schemes. Such an overshooting remains to occur even for $\mu > 0$ although its magnitude is reduced. We can say that the proposed scheme captures the discontinuities relatively well considering that no special fitting method is used.

4. CONCLUDING REMARKS

In conclusion, we have developed a simple lattice Boltzmann scheme which can simulate supersonic flows described by the compressible NS equations. This kinetic scheme is also superior to the existing LBM in that any transport coefficients can be chosen freely according to our convenience. Numerical examples and error estimates were also given to confirm the above statements.

Finally, we should mention one more advantage of our proposed scheme: the velocity distribution function does not need to be memorized because it can be recovered completely from the macroscopic variables using (6). The size of the computational memory is then considerably reduced from that for the existing lattice Boltzmann models in which the velocity distribution function must be memorized.

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