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Simulations of supersonic flows using new kinetic scheme based on the free-molecular-type equation

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Abstract

We have devised a new simple lattice Boltzmann model which can simulate supersonic flows. This model is based on the free-molecular-type kinetic equation whose calculation system was constructed by Sone in 2002. Various numerical simulations are carried out to confirm that this model can compute supersonic flows and show that numerical results agree with the corresponding solutions of the compressible Navier-Stokes and Euler equations.

Introduction

The lattice Boltzmann method (LBM) [1-5] is often used recently to obtain numerical solutions of the fluid-dynamic-type equations. 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 kinetic-equation approach are the simple basic equation, the linear derivative terms, high resolution for capturing small oscillations like sound waves or discontinuities like shock waves.

The LBM for the compressible NS equations was first devised by Alexander *et al.* [3]. Their model includes the nonlinear deviation terms that are proportional to the third-order flow velocity. Later, Chen *et al.* [4] and Kataoka et al. [5] individually proposed the models without these nonlinear deviation terms. However, an important defect still remains, that is, the supersonic flow cannot be computed stably. When the flow speed exceeds the sound speed, numerical results based on the LBM are subjected to meaningless oscillations and diverge. Thus, computation of compressible flows using the LBM is very limited. In order to utilize the above-mentioned merits of the kinetic equation approach, especially high resolution for capturing discontinuities like shock waves, it is strongly desired that someone develops a kinetic scheme which can simulate supersonic flows stably.

In this study, therefore, we develop a new kinetic scheme which can simulate supersonic flows. The original idea is based on Sone [6]. He devised a simple way to construct a kinetic system of equation in such a way that some moments of the solution of the kinetic system satisfy the desired equations exactly. On the basis of this kinetic system, he discussed a much simpler numerical scheme which uses the free-molecular kinetic equation, but instead modifies the velocity distribution function completely to a certain equilibrium one at each time step. This modification makes this scheme free of errors proportional to Mach numbers inherent in the existing LBM. The error estimate of this scheme was also explained, and it was mentioned that the molecular velocity is not necessarily continuous.

In the present study therefore we make use of the above free-molecular kinetic system to construct the lattice Boltzmann model having a finite number of molecular velocities. The number and position of molecular velocities are dependent on the fluid-dynamic-type equations we want to solve, which are the compressible NS equations here. They are looked for under the constraint that some moments of velocity distribution function satisfy the prescribed relations (see (3a-c) and (7a,b) below). We then succeed in obtaining such model specifically and computation indicates that this new scheme can simulate supersonic flows stably.

Basic Equations (NS)

First, we write down the compressible NS equations (which include the compressible Euler equations) whose solution we want to get:

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

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

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

with

$$P_{\alpha\beta} = \rho RT \delta_{\alpha\beta} - \mu\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3}\frac{\partial u_\chi}{\partial x_\chi}\delta_{\alpha\beta}\right) - \mu_B \frac{\partial u_\chi}{\partial x_\chi}\delta_{\alpha\beta} , \tag{1d}$$

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

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

where t is the time, x_α 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 γ by

$$\gamma = \frac{b+2}{b} . \tag{2}$$

ρ, u_α, T, $P_{\alpha\beta}$, and Π_α are, respectively, the density, the flow velocity in the x_α direction, the temperature, the stress tensor, and the energy flux in the x_α direction of a gas. Three transport coefficients: $\mu(\rho,T)$ (the viscosity), $\mu_B(\rho,T)$ (the bulk viscosity), and $\lambda(\rho,T)$ (the thermal conductivity), are functions of ρ and T. The Euler equations are obtained by putting $\mu = \mu_B = \lambda = 0$. We use the subscripts α, β, and χ to represent the number of spatial coordinates and the summation convention is applied to these subscripts.

Lattice Boltzmann Model

New lattice Boltzmann model for the compressible NS equations (1) is as follows. Let $c_{\alpha i}$ ($\alpha = 1,\cdots,D$, $i = 0,1,\cdots,3I$) be the molecular velocities in the x_α 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 ρ , u_α , and T are defined as

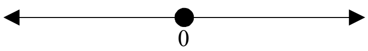
$$\rho = \sum_{i=0}^{3I} f_i \,, \tag{3a}$$

$$\rho u_\alpha = \sum_{i=0}^{3I} f_i c_{\alpha i} \,, \tag{3b}$$

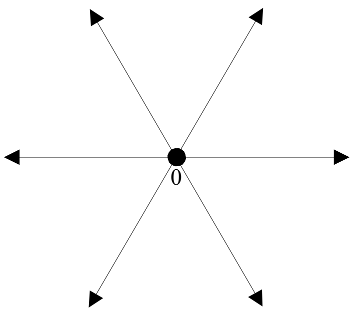
$$\rho\left(bRT + u_\beta^2\right) = f_0 v_0^2 + \sum_{i=0}^{3I} f_i c_{\beta i}^2 \,, \tag{3c}$$

with

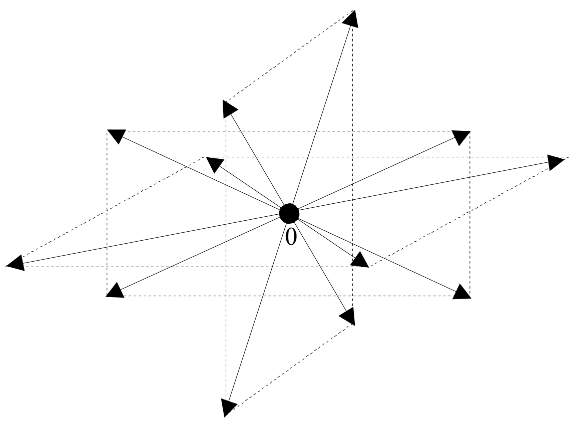
$$c_{\alpha i} = \begin{cases} 0 \quad \text{for } i = 0, \\ v_1 q_{\alpha i} \quad \text{for } i = 1,\cdots,I, \\ v_2 q_{\alpha\, i-I} \quad \text{for } i = I+1,\cdots,2I, \\ v_3 q_{\alpha\, i-2I} \quad \text{for } i = 2I+1,\cdots,3I, \end{cases} \tag{4a}$$



(a)



(b)



(c)

Figure 1. Distribution of the unit vector $q_{\alpha i}$ ($\alpha = 1,\cdots,D$; $i = 0,\cdots,I$): (a) one-dimensional model ($D=1$, $I=2$); (b) two-dimensional model ($D=2$, $I=6$); (c) three-dimensional model ($D=3$, $I=12$).

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

$$q_{\alpha i} = \begin{cases} \cos \pi i \ \ (D=1, I=2), \\ \left(\cos\dfrac{\pi i}{3}, \sin\dfrac{\pi i}{3}\right) \ (D=2, I=6), \\ cyc : \dfrac{1}{5^{1/4}}\left(0, \pm\sqrt{\dfrac{1+\sqrt{5}}{2}}, \pm\sqrt{\dfrac{2}{1+\sqrt{5}}}\right) \ (D=3, I=12). \end{cases} \tag{4b}$$

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

$$\frac{\partial f_i}{\partial t} + c_{\beta i}\frac{\partial f_i}{\partial x_\beta} = 0 \,, \tag{5}$$

in a continuous sequence of time intervals $(t_0, t_1]$, $(t_1, t_2]$, …. under the following initial condition for each interval $(t_m, t_{m+1}]$:

$$f_i = f_i^{\mathrm{Ini}}\left(\rho_{(m)}, u_{\alpha(m)}, T_{(m)}\right), \tag{6a}$$

where $\rho_{(m)}$, $u_{\alpha(m)}$, and $T_{(m)}$ are ρ , u_α , 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^{Ini} is defined as

$$f_i^{\mathrm{Ini}}(\rho, u_\alpha, T) = \begin{cases} \dfrac{\rho bRT - P_{\alpha\alpha}}{v_0^2} \quad \text{for } i = 0, \\ \dfrac{-(v_2^2+v_3^2)F_i(\rho,u_\alpha,T)}{v_1^2(v_1^2-v_2^2)(v_1^2-v_3^2)} \quad \text{for } i = 1,\cdots,I, \\ \dfrac{-(v_3^2+v_1^2)F_i(\rho,u_\alpha,T)}{v_2^2(v_2^2-v_3^2)(v_2^2-v_1^2)} \quad \text{for } i = I+1,\cdots,2I, \\ \dfrac{-(v_1^2+v_2^2)F_i(\rho,u_\alpha,T)}{v_3^2(v_3^2-v_1^2)(v_3^2-v_2^2)} \quad \text{for } i = 2I+1,\cdots,3I, \end{cases} \tag{6b}$$

where

$$\begin{aligned} &F_i(\rho, u_\alpha, T) \\ &= \frac{1}{D+1}\left\{ \rho u_\alpha c_{\alpha i} c_{\beta i}^2 + \frac{1}{D}\left(\rho - \frac{\rho bRT - P_{\beta\beta}}{v_0^2}\right) c_{\alpha i}^2 c_{\beta i}^2 + 2\Pi_\alpha c_{\alpha i} \right. \\ &\qquad \left. + \left[\frac{D+2}{2}(\rho u_\alpha u_\beta + P_{\alpha\beta}) - \frac{\rho u_\chi^2 + P_{\chi\chi}}{2}\delta_{\alpha\beta}\right] c_{\alpha i} c_{\beta i} \right\}. \end{aligned} \tag{6c}$$

Here the molecular velocities $c_{\alpha i}$ given by (4) and the distribution function $f_i^{\mathrm{Ini}}(\rho, u_\alpha, T)$ represented by (6) are determined under the constraint that they satisfy (3a-c) with f_i being replaced by $f_i^{\mathrm{Ini}}(\rho, u_\alpha, T)$ and the following relations:

$$\rho u_\alpha u_\beta + P_{\alpha\beta} = \sum_{i=0}^{3I} f_i^{\mathrm{Ini}}(\rho, u_\alpha, T) c_{\alpha i} c_{\beta i} \,, \tag{7a}$$

$$2\Pi_\alpha = \sum_{i=0}^{3I} f_i^{\mathrm{Ini}}(\rho, u_\alpha, T) c_{\alpha i} c_{\beta i}^2 \,. \tag{7b}$$

Then the macroscopic variables ρ , u_α , and T obtained from the solution f_i at an arbitrary time satisfy the compressible NS equations, or Eqs.(1) within the error of $O\left(\max(t_{m+1} - t_m)\right)$ which can be made sufficiently small irrespective of flow parameters (see Sone [6] for this derivation). In the next section, we will give numerical examples to show that the proposed scheme can compute supersonic flows stably.

Numerical Examples

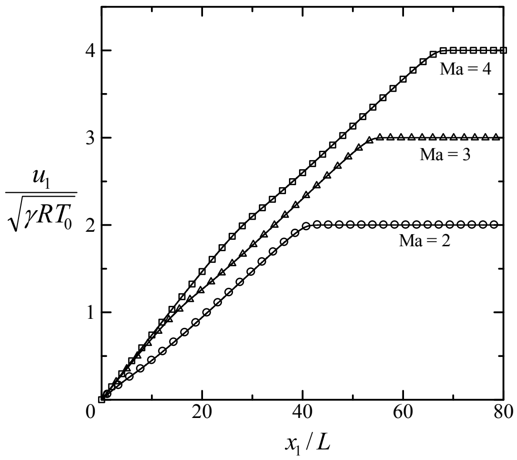
In this section we present various numerical examples. We solve the kinetic equation (5) by the following finite-difference scheme:

$$f_{i(m+1)} = f_{i(m)} - c_{\alpha i}\frac{\partial f_{i(m)}}{\partial x_\alpha}(t_{m+1} - t_m), \tag{8}$$

where $f_{i(m)}$ represents f_i at $t = t_m$, and $\partial f_{i(m)} / \partial x_\alpha$ 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

$$\rho = \rho_0, \quad u_1 = U \tanh(x_1 / L), \quad T = T_0, \tag{9}$$



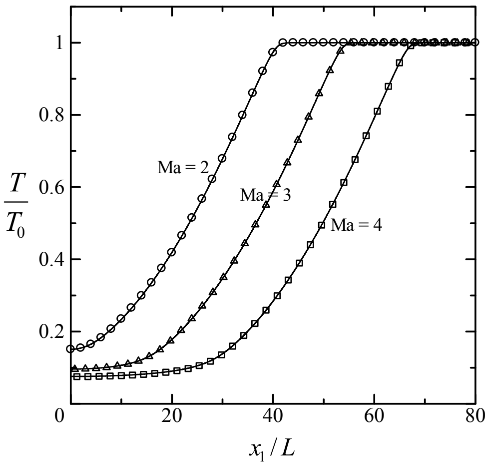


Figure 2. Numerical results $u_1 / \sqrt{\gamma R T_0}$ and T / T_0 at $\hat{t} = 10$ for the expansion-wave problem whose initial conditions are (9) with $\gamma = 5/3$ and three different values of Ma = 2, 3, and 4 ($\mu = \mu_B = \lambda = 0$). The symbols (○, Ma = 2; △, Ma = 3; □, Ma = 4) are the results by the proposed lattice Boltzmann scheme (3)-(6) with $D = 1$ and mesh interval $\Delta x_1 / L = 0.5$, 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 $x_1 = 0$, only the results for $x_1 > 0$ are shown.

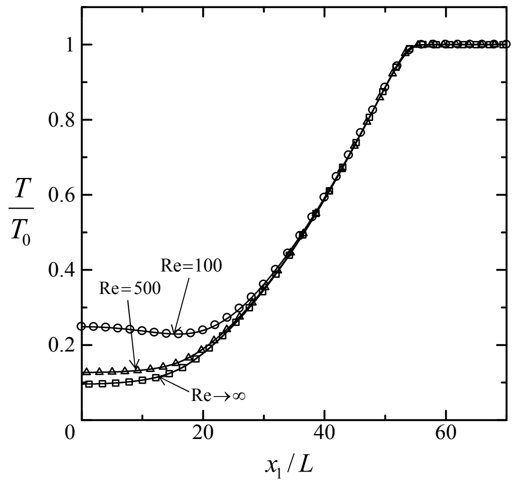


Figure 3. Temperature fields T / T_0 at $\hat{t} = 10$ for the expansion-wave problem whose initial conditions are (9) with $\gamma = 5/3$, $\mathrm{Ma} = 3$, $\mathrm{Pr} = 10$, and three different values of Re = 100, 500, and ∞ (μ and λ are constants). The symbols (○, Re = 100; △, Re = 500; □, $\mathrm{Re} = \infty$) are the results by the proposed lattice Boltzmann scheme (3)-(6) with $D = 1$ and mesh interval $\Delta x_1 / L = 0.5$, and the lines are the corresponding results of the NS equations solved by the MacCormack method with the sufficient number of meshes.

where ρ_0, U, L, and T_0 are given positive constants. When $\mu = \mu_B = \lambda = 0$, this problem is characterized by the specific-heat ratio γ defined by (2) and the Mach number $\mathrm{Ma} = U / \sqrt{\gamma R T_0}$. Numerical results at $\hat{t} \equiv t\sqrt{RT_0} / L = 10$ for $\gamma = 5/3$ and three different values of $\mathrm{Ma} = 2$, 3, and 4 are shown in figure 2. The symbols represent results by the proposed lattice Boltzmann scheme (3)-(6) with $D = 1$ while the solid lines are the corresponding numerical results of the Euler equations solved by the so-called MacCormack scheme [7] 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 characterized by the specific-heat ratio γ, the Mach number Ma, the Reynolds number Re, and the Prandtl number Pr defined by

$$\mathrm{Re} = \frac{UL}{\mu(\rho_0, T_0)}, \quad \mathrm{Pr} = \frac{bR\mu(\rho_0, T_0)}{2\lambda(\rho_0, T_0)}, \tag{10}$$

as well as the functional forms of $\mu(\rho, T)$ and $\lambda(\rho, T)$. Temperature fields at $\hat{t} = 10$ for $\gamma = 5/3$, $\mathrm{Ma} = 3$, $\mathrm{Pr} = 10$, and three different values of Re = 100, 500, and ∞ with μ and λ being constants (μ_B can be incorporated into μ for $D = 1$) are shown in figure 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 themselves (1) solved by the MacCormack scheme [7]. We find a good agreement between the two results for each case, or Re=100 and 500 (results for $\mathrm{Re} \to \infty$ are shown for the sake of comparison).

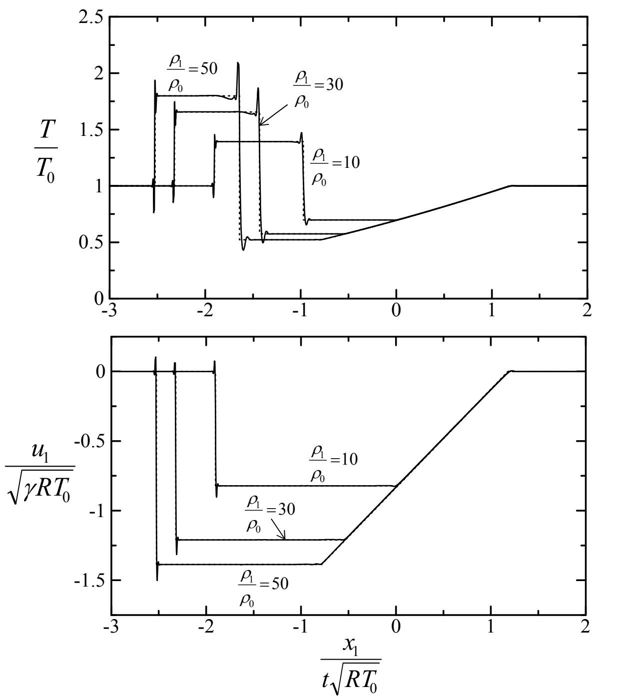


Figure 4. Numerical results T/T_0 and $u_1/\sqrt{\gamma RT_0}$ for the shock-tube problem whose initial conditions are (11) with $\gamma = 7/5$ and three different values of $\rho_1/\rho_0 = 10$, 30, and 50 ($\mu = \mu_B = \lambda = 0$). The solid lines are the results by the proposed lattice Boltzmann scheme (3)-(6) with $D = 1$ and mesh interval $\Delta x_1 / t\sqrt{RT_0} = 0.01$, and the dotted lines are the corresponding theoretical solutions.

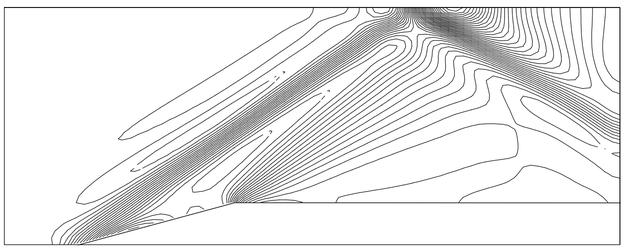


Figure 5. Isobaric lines of a supersonic flow (Mach number 4) past an array of wedges of half-angle 15° with after body. Results are obtained by the proposed lattice Boltzmann scheme (3)-(6) with $D = 2$. Only a half region between two neighbouring wedges is shown due to symmetry of the flow field. The flow velocity on the boundary of wedges is given such that its normal component vanishes.

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

$$\rho = \begin{cases} \rho_0 & \text{for } x_1 < 0 \\ \rho_1 & \text{for } x_1 > 0, \end{cases} \qquad u_1 = 0, \quad T = T_0, \tag{11}$$

where ρ_0, ρ_1, and T_0 are given positive constants. Here we treat the case of $\mu = \mu_B = \lambda = 0$, so that the problem is characterized by γ and ρ_1/ρ_0 . Numerical results for $\gamma = 7/5$ and three different values of $\rho_1/\rho_0 = 10$, 30, and 50 are shown in figure 4 by the symbols. The exact theoretical solutions are shown by the dotted lines. We find a good agreement between the two results for each value of ρ_1/ρ_0 . 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. We can say that the proposed scheme captures the discontinuities relatively well considering that no special fitting method is used.

Finally, a supersonic flow past an array of wedges after body is simulated. This flow is mainly characterized by the Mach number and the half-angle of each wedge. Figure 5 shows numerical result for Mach number 4 and the half-angle 15° obtained by the proposed kinetic system (3)-(6) with $D = 2$. Only a half region between two neighbouring wedges is shown due to symmetry of the flow field. We can see that the shock wave is clearly produced by the vertex of each wedge and crosses each other in the middle of two neighbouring wedges.

Conclusions

We have developed a new simple lattice Boltzmann scheme for the compressible NS and Euler equations which can simulate supersonic flows.

Acknowledgments

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