Decoupled scheme based on the Hermite expansion to construct lattice Boltzmann models for the compressible Navier-Stokes equations with arbitrary specific heat ratio

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A decoupled scheme based on the Hermite expansion to construct lattice Boltzmann models for the compressible Navier-Stokes equations with arbitrary specific heat ratio is proposed. The local equilibrium distribution function including the rotational velocity of particle is decoupled into two parts, i.e., the local equilibrium distribution function of the translational velocity of particle and that of the rotational velocity of particle. From these two local equilibrium functions, two lattice Boltzmann models are derived via the Hermite expansion, namely one is in relation to the translational velocity and the other is connected with the rotational velocity. Accordingly, the distribution function is also decoupled. After this, the evolution equation is decoupled into the evolution equation of the translational velocity and that of the rotational velocity. The two evolution equations evolve separately. The lattice Boltzmann models used in the scheme proposed by this work are constructed via the Hermite expansion, so it is easy to construct new schemes of higher-order accuracy. To validate the proposed scheme, a one-dimensional shock tube simulation is performed. The numerical results agree with the analytical solutions very well.

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I. INTRODUCTION

The lattice Boltzmann method (LBM) has been successfully applied to isothermal fluids [1,2]. However, when it is applied to thermal fluids, the LBM encounters some difficulties. One of them is that the specific heat ratio γ in the macroscopic equations derived from the Bhatnager-Gross-Krook (BGK) equation via the Chapman-Enskog expansion is fixed, in other words, the specific heat ratio γ is not realistic. Several lattice Boltzmann (LB) schemes with flexible specific heat ratio have been proposed [3–6]. These LB schemes are derived in a similar way. The discrete velocities and the local equilibrium distribution function are determined by a set of constraints which makes sure the macroscopic equations match the thermohydrodynamic equations with certain accuracy. Since 2006, a new way to construct LB models has been developed [7–17]. Contrary to the previous way, the new way derives the discrete velocities and the equilibrium distribution function via the Hermite quadrature and the Hermite expansion. It is easy to construct LB models of higher order via the Hermite expansion.

In this work, we apply the new way to constructing LB schemes for the compressible Navier-Stokes equations with flexible specific heat ratio.

The local equilibrium distribution function including the rotational velocity of particle is decoupled into two parts—one is in relation to the translational velocity and the other is connected with the rotational velocity. The distribution function is also decoupled into two parts accordingly. Two LB models are derived via the Hermite expansion. One is for the distribution function of the translational velocity and the other is for that of the rotational velocity. After this, we decouple the evolution equation into the evolution equation of the translational velocity and that of the rotational velocity. The two evolution equations evolve separately. The decoupled scheme given above is validated by a shock tube simulation. The results of simulation agree with the analytical solutions very well.

II. DECOUPLING THE LOCAL EQUILIBRIUM DISTRIBUTION FUNCTION $f^{eq}(\boldsymbol{\xi},\eta)$ AND THE DISTRIBUTION FUNCTION $f(\boldsymbol{\xi},\eta)$

We begin with the local equilibrium distribution function. The origin that the specific heat ratio is fixed is that gases are supposed to be monatomic, so there is only the translational free degree and the rotational free degree is limited. To describe diatomic gases or polyatomic gases, the rotational velocity of particle should be introduced. The local equilibrium distribution function including the rotational velocity of particle is [5,18]

$$f^{eq}(\boldsymbol{\xi},\eta) = \rho \frac{1}{(2\pi R_g T)^{\frac{D}{2}}} \frac{1}{(2n\pi R_g T)^{\frac{1}{2}}} \times \exp\left[-\frac{(\boldsymbol{\xi}-\boldsymbol{u})^2}{2R_g T} - \frac{\eta^2}{2nR_g T}\right], \quad (1)$$

where ρ is the density, T is the absolute temperature, $\boldsymbol{u}$ is the macroscopic velocity, $\boldsymbol{\xi}$ is the translational velocity of particle, η is the rotational velocity of particle, n is the free degree of the rotational velocity of particle, D is the dimension, and R_g is the universal gas constant.

The dimensionless local equilibrium distribution function is

$$\tilde{f}^{eq}(\tilde{\boldsymbol{\xi}},\tilde{\eta}) = \frac{\tilde{\rho}}{(2\pi\tilde{\theta})^{\frac{D}{2}}} \frac{1}{(2\pi\tilde{\theta})^{\frac{1}{2}}} \exp\left(-\frac{|\tilde{\boldsymbol{\xi}}-\tilde{\boldsymbol{u}}|^2}{2\tilde{\theta}}\right) \exp\left(-\frac{\tilde{\eta}^2}{2\tilde{\theta}}\right), \quad (2)$$

where

$$\begin{aligned} &\tilde{f}^{eq} = f^{eq}\theta_0^{N/2}(n\theta_0)^{1/2}, && \theta = R_g T,\\ &\tilde{\rho} = \rho/\rho_0, && \tilde{\boldsymbol{\xi}} = \boldsymbol{\xi}/\sqrt{\theta_0},\\ &\tilde{\eta} = \eta/n\sqrt{\theta_0}, && \tilde{\boldsymbol{u}} = \boldsymbol{u}/\sqrt{\theta_0},\\ &\tilde{\theta} = \tilde{T} = \theta/\theta_0, && \theta_0 = R_g T_0. \end{aligned}$$

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Omitting the tildes on ρ, $\boldsymbol{\xi}$, η, $\boldsymbol{u}$, and $\theta(T)$, we simplify Eq. (2),

$$f^{\mathrm{eq}}(\boldsymbol{\xi},\eta) = \frac{\rho}{(2\pi\theta)^{\frac{D}{2}}}\frac{1}{(2\pi\theta)^{\frac{1}{2}}}\exp\left(-\frac{|\boldsymbol{\xi}-\boldsymbol{u}|^2}{2\theta}\right)\exp\left(-\frac{\eta^2}{2\theta}\right). \tag{3}$$

The dimensionless local equilibrium distribution function can be decoupled into the local equilibrium distribution function of $\boldsymbol{\xi}$ and that of η,

$$f^{\mathrm{eq}}(\boldsymbol{\xi},\eta) = g^{\mathrm{eq}}(\boldsymbol{\xi})h^{\mathrm{eq}}(\eta), \tag{4}$$

where

$$g^{\mathrm{eq}}(\boldsymbol{\xi}) = \frac{\rho}{(2\pi\theta)^{\frac{D}{2}}}\exp\left(-\frac{|\boldsymbol{\xi}-\boldsymbol{u}|^2}{2\theta}\right),$$

$$h^{\mathrm{eq}}(\eta) = \frac{1}{(2\pi\theta)^{\frac{1}{2}}}\exp\left(-\frac{\eta^2}{2\theta}\right).$$

Taking the moment integrals of $f^{\mathrm{eq}}(\boldsymbol{\xi})$, we obtain

$$\rho = \int g^{\mathrm{eq}}(\boldsymbol{\xi})d\boldsymbol{\xi}, \tag{5a}$$

$$\rho\boldsymbol{u} = \int g^{\mathrm{eq}}(\boldsymbol{\xi})\boldsymbol{\xi}d\boldsymbol{\xi}, \tag{5b}$$

$$\rho\left(e_t + \frac{1}{2}u^2\right) = \int g^{\mathrm{eq}}(\boldsymbol{\xi})\frac{1}{2}\xi^2 d\boldsymbol{\xi}, \tag{5c}$$

where $e_t = \frac{D}{2}T$ is the translational internal energy.

Taking the moment integrals of $f^{\mathrm{eq}}(\eta)$, we get

$$1 = \int h^{\mathrm{eq}}(\eta)d\eta, \tag{6a}$$

$$e_r = \int h^{\mathrm{eq}}(\eta)\frac{n}{2}\eta^2 d\eta, \tag{6b}$$

where $e_r = \frac{n}{2}T = \frac{n}{D}e_t$ is the rotational internal energy.

Taking the moment integrals of the local equilibrium distribution function $f^{\mathrm{eq}}(\boldsymbol{\xi},\eta)$, we obtain

$$\rho = \iint f^{\mathrm{eq}}(\boldsymbol{\xi},\eta)d\boldsymbol{\xi}d\eta, \tag{7a}$$

$$\rho\boldsymbol{u} = \iint f^{\mathrm{eq}}(\boldsymbol{\xi},\eta)\boldsymbol{\xi}d\boldsymbol{\xi}d\eta, \tag{7b}$$

$$\rho\left(E + \frac{1}{2}u^2\right) = \iint f^{\mathrm{eq}}(\boldsymbol{\xi},\eta)\left(\frac{1}{2}\xi^2 + \frac{n}{2}\eta^2\right)d\boldsymbol{\xi}d\eta, \tag{7c}$$

where $E = \frac{D+n}{2}T = \frac{D+n}{D}e_t$ is the internal energy. It is the sum of the translational energy e_t and the rotational energy e_r.

According to the kinetic theory, we get

$$\rho = \iint f(\boldsymbol{\xi},\eta)d\boldsymbol{\xi}d\eta, \tag{8a}$$

$$\rho\boldsymbol{u} = \iint f(\boldsymbol{\xi},\eta)\boldsymbol{\xi}d\boldsymbol{\xi}d\eta, \tag{8b}$$

$$\rho\left(E + \frac{1}{2}u^2\right) = \iint f(\boldsymbol{\xi},\eta)\left(\frac{1}{2}\xi^2 + \frac{n}{2}\eta^2\right)d\boldsymbol{\xi}d\eta. \tag{8c}$$

Now we assume that the translational velocity of particle $\boldsymbol{\xi}$ is independent of the rotational velocity of particle, so the distribution function $f(\boldsymbol{\xi},\eta)$ can be decoupled into $g(\boldsymbol{\xi})$ and $h(\eta)$,

$$f(\boldsymbol{\xi},\eta) = g(\boldsymbol{\xi})h(\eta), \tag{9}$$

where we define

$$f(\boldsymbol{\xi},\eta) = \rho b(\boldsymbol{\xi},\eta) = \rho b_1(\boldsymbol{\xi})h(\eta), \tag{10a}$$

$$g(\boldsymbol{\xi}) = \int f(\boldsymbol{\xi},\eta)d\eta, \tag{10b}$$

$$h(\eta) = \int b(\boldsymbol{\xi},\eta)d\boldsymbol{\xi}. \tag{10c}$$

Section III will discuss the reasonableness of this assumption.

It should be noted that $b(\boldsymbol{\xi},\eta)$ is a joint probability distribution, $b_1(\boldsymbol{\xi})$ and $h(\eta)$ are marginal probability distributions, and $g(\boldsymbol{\xi})$ is the product of ρ and a marginal probability distribution.

According to Eqs. (8) and (10), the moments of the distribution function $g(\boldsymbol{\xi})$ are

$$\int g(\boldsymbol{\xi})d\boldsymbol{\xi} = \iint f(\boldsymbol{\xi},\eta)d\boldsymbol{\xi}d\eta = \rho, \tag{11a}$$

$$\int g(\boldsymbol{\xi})\boldsymbol{\xi}d\boldsymbol{\xi} = \iint f(\boldsymbol{\xi},\eta)\boldsymbol{\xi}d\boldsymbol{\xi}d\eta = \rho\boldsymbol{u}, \tag{11b}$$

$$\int g(\boldsymbol{\xi})\frac{1}{2}\xi^2 d\boldsymbol{\xi} = \iint f(\boldsymbol{\xi},\eta)\frac{1}{2}\xi^2 d\boldsymbol{\xi}d\eta = \rho\left(e_t + \frac{1}{2}u^2\right). \tag{11c}$$

Similarly to (11), the moments of the distribution function $h(\eta)$ are

$$\int h(\eta)d\eta = \iint b(\boldsymbol{\xi},\eta)d\boldsymbol{\xi}d\eta = 1, \tag{12a}$$

$$\int h(\eta)\frac{n}{2}\eta^2 d\eta = \iint b(\boldsymbol{\xi},\eta)\frac{n}{2}\eta^2 d\boldsymbol{\xi}d\eta = e_r. \tag{12b}$$

III. DECOUPLING THE EVOLUTION EQUATION

We have decoupled the equilibrium distribution function $f^{\mathrm{eq}}(\boldsymbol{\xi},\eta)$ and the distribution function $f(\boldsymbol{\xi},\eta)$ in Sec. II,

$$f^{\mathrm{eq}}(\boldsymbol{\xi},\eta) = g^{\mathrm{eq}}(\boldsymbol{\xi})h^{\mathrm{eq}}(\eta),$$
$$f(\boldsymbol{\xi},\eta) = g(\boldsymbol{\xi})h(\eta).$$

After decoupling $f^{\mathrm{eq}}(\boldsymbol{\xi},\eta)$ and $f(\boldsymbol{\xi},\eta)$, we can decouple the evolution equation of $f(\boldsymbol{\xi},\eta)$. The evolution equation of $f(\boldsymbol{\xi},\eta)$ can be expressed as

$$\frac{\partial f(\boldsymbol{\xi},\eta)}{\partial t} + \boldsymbol{\xi}\cdot\nabla f(\boldsymbol{\xi},\eta) = -\frac{1}{\tau}[f(\boldsymbol{\xi},\eta) - f^{\mathrm{eq}}(\boldsymbol{\xi},\eta)], \tag{13}$$

where τ is the relaxation time.

Integrating (13) on η, and substituting (10b) into it, we obtain the evolution equation of $g(\boldsymbol{\xi})$,

$$\frac{\partial g(\boldsymbol{\xi})}{\partial t} + \boldsymbol{\xi}\cdot\nabla g(\boldsymbol{\xi}) = -\frac{1}{\tau}[g(\boldsymbol{\xi}) - g(\boldsymbol{\xi})^{\mathrm{eq}}]. \tag{14}$$

Substituting Eq. (4) and Eq. (9) into Eq. (13), we obtain

$$\frac{\partial g(\boldsymbol{\xi})h(\eta)}{\partial t} + \boldsymbol{\xi}\cdot\nabla g(\boldsymbol{\xi})h(\eta) = -\frac{1}{\tau}[g(\boldsymbol{\xi})h(\eta) - g^{\mathrm{eq}}(\boldsymbol{\xi})h^{\mathrm{eq}}(\eta)]. \tag{15}$$

Expanding Eq. (15) and simplifying it, we obtain

$$h(\eta)\left[\frac{\partial g(\boldsymbol{\xi})}{\partial t} + \boldsymbol{\xi}\cdot\nabla g(\boldsymbol{\xi})\right] + g(\boldsymbol{\xi})\left[\frac{\partial h(\eta)}{\partial t} + \boldsymbol{\xi}\cdot\nabla h(\eta)\right] = -\frac{1}{\tau}[g(\boldsymbol{\xi})h(\eta) - g^{\mathrm{eq}}(\boldsymbol{\xi})h^{\mathrm{eq}}(\eta)]. \tag{16}$$

Substituting Eq. (14) into Eq. (16), integrating on $\boldsymbol{\xi}$, and simplifying it, we obtain the evolution equation of $h(\eta)$,

$$\frac{\partial h(\eta)}{\partial t} + \boldsymbol{u}\cdot\nabla h(\eta) = -\frac{1}{\tau}[h(\eta) - h(\eta)^{\mathrm{eq}}]. \tag{17}$$

Discretizing the evolution equation of $g(\boldsymbol{\xi})$ and $h(\eta)$ in the discrete velocity space, we obtain the discrete evolution equations of g_i and h_j,

$$\frac{\partial g_i}{\partial t} + \boldsymbol{\xi}_i\cdot\nabla g_i = -\frac{1}{\tau}\left(g_i - g_i^{\mathrm{eq}}\right), \tag{18a}$$

$$\frac{\partial h_j}{\partial t} + \boldsymbol{u}\cdot\nabla h_j = -\frac{1}{\tau}\left(h_j - h_j^{\mathrm{eq}}\right), \tag{18b}$$

where g_i and h_j are the discrete form of $g(\boldsymbol{\xi})$ and $h(\eta)$. Equation (18a) is the evolution equation of the discrete translational velocity $\boldsymbol{\xi}_i$ and Eq. (18b) is the evolution equation of the discrete rotational velocity η_j. It should be noted that Eq. (18a) is independent of η_j and Eq. (18b) is indirectly connected to Eq. (18a) via the macroscopic velocity $\boldsymbol{u}$.

From the two evolution equations of g_i and h_j, i.e., Eqs. (18a) and (18b), the Navier-Stokes equations with flexible specific heat ratio via the Chapman-Enskog expansion can be derived,

$$\frac{\partial}{\partial t}\rho + \nabla\cdot\rho\boldsymbol{u} = 0, \tag{19a}$$

$$\frac{\partial}{\partial t}\rho\boldsymbol{u} + \nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u} + P\boldsymbol{\delta}) = \nabla\cdot\mu\left[(\nabla\boldsymbol{u} + \boldsymbol{u}\nabla) - \frac{2}{D+n}\nabla\cdot\boldsymbol{u}\boldsymbol{\delta}\right], \tag{19b}$$

$$\frac{\partial}{\partial t}\rho\left(E + \frac{1}{2}u^2\right) + \nabla\cdot\rho\boldsymbol{u}\left(E + \frac{1}{2}u^2 + \frac{P}{\rho}\right) = \nabla\cdot\mu\boldsymbol{u}\left(\nabla\boldsymbol{u} + \boldsymbol{u}\nabla - \frac{2}{D+n}\nabla\cdot\boldsymbol{u}\delta\right) + \nabla\cdot\kappa\nabla E, \tag{19c}$$

where $P = \frac{2}{D}\rho e_t$ is the pressure, $\mu = \frac{2}{D}\rho e_t\tau$ is the dynamic viscosity coefficient, $\kappa = \frac{2(D+n+2)}{D(D+n)}\rho e_t\tau$ is the heat conductivity, and the specific heat ratio γ is defined as

$$\gamma = \frac{D+n+2}{D+n}. \tag{20}$$

The derivation shows that it is reasonable to assume the distribution function $f(\boldsymbol{\xi},\eta)$ can be decoupled into $g(\boldsymbol{\xi})$ and $h(\eta)$.

The Appendix will give the derivation in details.

IV. LB MODELS FOR THE TRANSLATIONAL VELOCITY AND THE ROTATIONAL VELOCITY

In this section, we derive LB models from $g^{\mathrm{eq}}(\boldsymbol{\xi})$ and $h^{\mathrm{eq}}(\eta)$, respectively, via the Hermite expansion. The process of deriving LB models via the Hermite expansion has been discussed intensively by X. Shan [9,19], C. Philippi [7,8,10], and J. W. Shim [12,13].

In this work, we only discuss two-dimensional fluids. The case of three dimensions is similar. Employing the Hermite expansion, we construct a two-dimensional LB model of fourth-order accuracy, i.e., D2Q37, from $g^{\mathrm{eq}}(\boldsymbol{\xi})$. The discrete particle velocities $\boldsymbol{\xi}_i$ and the weights ω_i of D2Q37 are showed in Table I. The discrete equilibrium distribution function $g_i^{\mathrm{eq}}(\boldsymbol{\xi})$ of D2Q37 is

$$g_i^{\mathrm{eq}}(\boldsymbol{\xi}) = \omega_i\rho\sum_{k=0}^{4}\frac{1}{k!}\boldsymbol{a}^{(k)}\cdot\boldsymbol{H}^{(k)}, \tag{21}$$

where

$$\begin{aligned}
\boldsymbol{a}^{(0)}\cdot\boldsymbol{H}^{(0)} &= 1,\\
\boldsymbol{a}^{(1)}\cdot\boldsymbol{H}^{(1)} &= \boldsymbol{\xi}\cdot\boldsymbol{u},\\
\boldsymbol{a}^{(2)}\cdot\boldsymbol{H}^{(2)} &= (\boldsymbol{\xi}\cdot\boldsymbol{u})^2 + (\theta-1)(\theta^2-D) - u^2,\\
\boldsymbol{a}^{(3)}\cdot\boldsymbol{H}^{(3)} &= (\boldsymbol{\xi}\cdot\boldsymbol{u})[(\boldsymbol{\xi}\cdot\boldsymbol{u})^2 - 3u^2\\
&\quad + 3(\theta-1)(u^2-D-2)],\\
\boldsymbol{a}^{(4)}\cdot\boldsymbol{H}^{(4)} &= (\boldsymbol{\xi}\cdot\boldsymbol{u})^4 - 6(\boldsymbol{\xi}\cdot\boldsymbol{u})^2u^2 + 3u^4\\
&\quad + 6(\theta-1)[(\boldsymbol{\xi}\cdot\boldsymbol{u})^2(u^2-D-4)\\
&\quad + (D+2-u^2)\xi^2]\\
&\quad + 3(\theta-1)^2[u^4 - 2(D+2)u^2 + D(D+2)],
\end{aligned}$$

and $D = 2$.

TABLE I. Discrete velocities and weights of D2Q37. Perm denotes permutation and k denotes the number of discrete velocities included in each group. The scaling factor is $r = 1.1969797752$.

k	$\boldsymbol{\xi}_i$	ω_i
1	(0,0)	$2.03916918 \times 10^{-1}$
4	Perm(r,0)	$1.27544846 \times 10^{-1}$
4	Perm(r,r)	$4.37537182 \times 10^{-2}$
4	Perm(2r,0)	$8.13659044 \times 10^{-3}$
4	Perm(2r,r)	$9.40079914 \times 10^{-3}$
4	Perm(3r,0)	$6.95051049 \times 10^{-4}$
4	Perm(3r,r)	$3.04298494 \times 10^{-5}$
4	Perm(3r,3r)	$2.81093762 \times 10^{-5}$

TABLE II. Discrete velocities and weights of D1Q7. k denotes the number of discrete velocities included in each group. The scaling factor is $r = 1.1969797752$.

k	η_j	ω_j
1	0	$4.766698882 \times 10^{-1}$
2	$\pm r$	$2.339147370 \times 10^{-1}$
2	$\pm 2r$	$2.693818936 \times 10^{-2}$
2	$\pm 3r$	$8.121295330 \times 10^{-4}$

It should be noted that the LB model given above differs from the LB model given by Ref. [7].

In a similar way, a one-dimensional LB model of fourth-order accuarcy can be derived from $h^{\mathrm{eq}}(\eta)$. Here, we adopt the D1Q7 model proposed by J. W. Shim [13]. The discrete velocities η_j and the weights ω_j are shown in Table II. The discrete equilibrium distribution function is

$$h_j^{\mathrm{eq}}(\eta) = \omega_j \sum_{j=0}^{4} \frac{1}{j!} \boldsymbol{a}^{(j)} \cdot \boldsymbol{H}^{(j)}, \tag{22}$$

where

$$\begin{aligned}
\boldsymbol{a}^{(0)} \cdot \boldsymbol{H}^{(0)} &= 1,\\
\boldsymbol{a}^{(1)} \cdot \boldsymbol{H}^{(1)} &= 0,\\
\boldsymbol{a}^{(2)} \cdot \boldsymbol{H}^{(2)} &= (\theta - 1)(\theta^2 - D),\\
\boldsymbol{a}^{(3)} \cdot \boldsymbol{H}^{(3)} &= 0,\\
\boldsymbol{a}^{(4)} \cdot \boldsymbol{H}^{(4)} &= 3(\theta - 1)^2[\eta^4 - 2(D+2)\eta^2 + D(D+2)],
\end{aligned}$$

and $D = 1$.

D2Q37 and D1Q7 are both models of fourth-order accuracy, so the scheme given above is of fourth-order accuracy. In this way, the higher-order of accuracy can be achieved easily.

We can also construct or adopt other LB models. But it should be noticed that the scaling factors r of LB models derived form $g^{\mathrm{eq}}(\boldsymbol{\xi})$ and $h^{\mathrm{eq}}(\eta)$ should be equal or else interpolation is necessary.

V. CALCULATION PROCEDURE

In this section, we first discretize the evolution equations of $g(\boldsymbol{\xi})$ and $h(\eta)$ in time and space, then we give the computational algorithm.

A. Discretized the evolution equation in space and time

Now we discretize the discrete evolution equations of $\boldsymbol{\xi}_i$ and η_j in time and space. The first-order difference is employed for the time discretization and the convection term is performed by the third-order upwind scheme. The discretized form of Eq. (18a) is

$$g_i(\boldsymbol{x},t+\Delta t) = g_i(\boldsymbol{x},t) - \Delta t \boldsymbol{\xi}_i \cdot \nabla g_i - \frac{\Delta t}{\tau}\left[g_i(\boldsymbol{x},t) - g_i^{\mathrm{eq}}(\boldsymbol{x},t)\right], \tag{23}$$

where Δt is the time increment, and the convection term along the coordinate x is

$$\begin{aligned}
\xi_{ix}\frac{\partial g_i}{\partial x} =& \frac{1}{2}\frac{\xi_{i,x} + |\xi_{i,x}|}{6\Delta x}[g_i(x-2\Delta x) - 6g_i(x-\Delta x)\\
&+ 3g_i(x) + 2g_i(x+\Delta x)]\\
&+ \frac{1}{2}\frac{\xi_{i,x} - |\xi_{i,x}|}{6\Delta x}[-g_i(x+2\Delta x) + 6g_i(x+\Delta x)\\
&- 3g_i(x) - 2g_i(x-\Delta x)],
\end{aligned}$$

and Δx is the space increment. The convection term along the y coordinate is similar. In a similar way, the discretized form of the discrete evolution equation of η_j, i.e., Eq. (18b), is

$$h_j(\boldsymbol{x},t+\Delta t) = h_j(\boldsymbol{x},t) - \Delta t \boldsymbol{u} \cdot \nabla h_j - \frac{\Delta t}{\tau}\left[h_j(\boldsymbol{x},t) - h_j^{\mathrm{eq}}(\boldsymbol{x},t)\right], \tag{24}$$

where the convection term is similar with that of Eq. (18a),

$$\begin{aligned}
u_x\frac{\partial h_j}{\partial x} =& \frac{1}{2}\frac{u_x + |u_x|}{6\Delta x}[h_j(x-2\Delta x) - 6h_j(x-\Delta x)\\
&+ 3h_j(x) + 2h_j(x+\Delta x)]\\
&+ \frac{1}{2}\frac{u_x - |u_x|}{6\Delta x}[-h_j(x+2\Delta x) + 6h_j(x+\Delta x)\\
&- 3h_j(x) - 2h_j(x-\Delta x)].
\end{aligned}$$

The convection term along the y coordinate is similar.

B. Computational algorithm

The computational algorithm is as follows:

(1) Update g_i by Eq. (23);

(2) Update h_j by Eq. (24);

(3) Calculate the density ρ, the macroscopic velocity $\boldsymbol{u}$ and the translational internal energy e_t,

$$\rho = \sum_i g_i, \tag{25a}$$

$$\rho \boldsymbol{u} = \sum_i g_i \boldsymbol{\xi}_i, \tag{25b}$$

$$\frac{1}{2}\rho u^2 + \rho e_t = \sum_i g_i \frac{1}{2}\xi_i^2, \tag{25c}$$

where the translational internal energy e_t is

$$e_t = \frac{D}{2}T. \tag{26}$$

The pressure is defined as $P = \frac{2}{D}\rho e_t$.

(4) Calculate the rotational internal energy e_r,

$$e_r = \sum_j \frac{n}{2} h_j \eta_j^2, \tag{27}$$

and combine Eq. (27) with (25c); we then obtain

$$\frac{1}{2}\rho u^2 + \rho E = \sum_i g_i \frac{1}{2}\xi_i^2 + \rho \sum_j h_j \frac{n}{2}\eta_j^2. \tag{28}$$

As defined above, the internal energy E is the sum of the translational internal energy e_t and the rotational internal

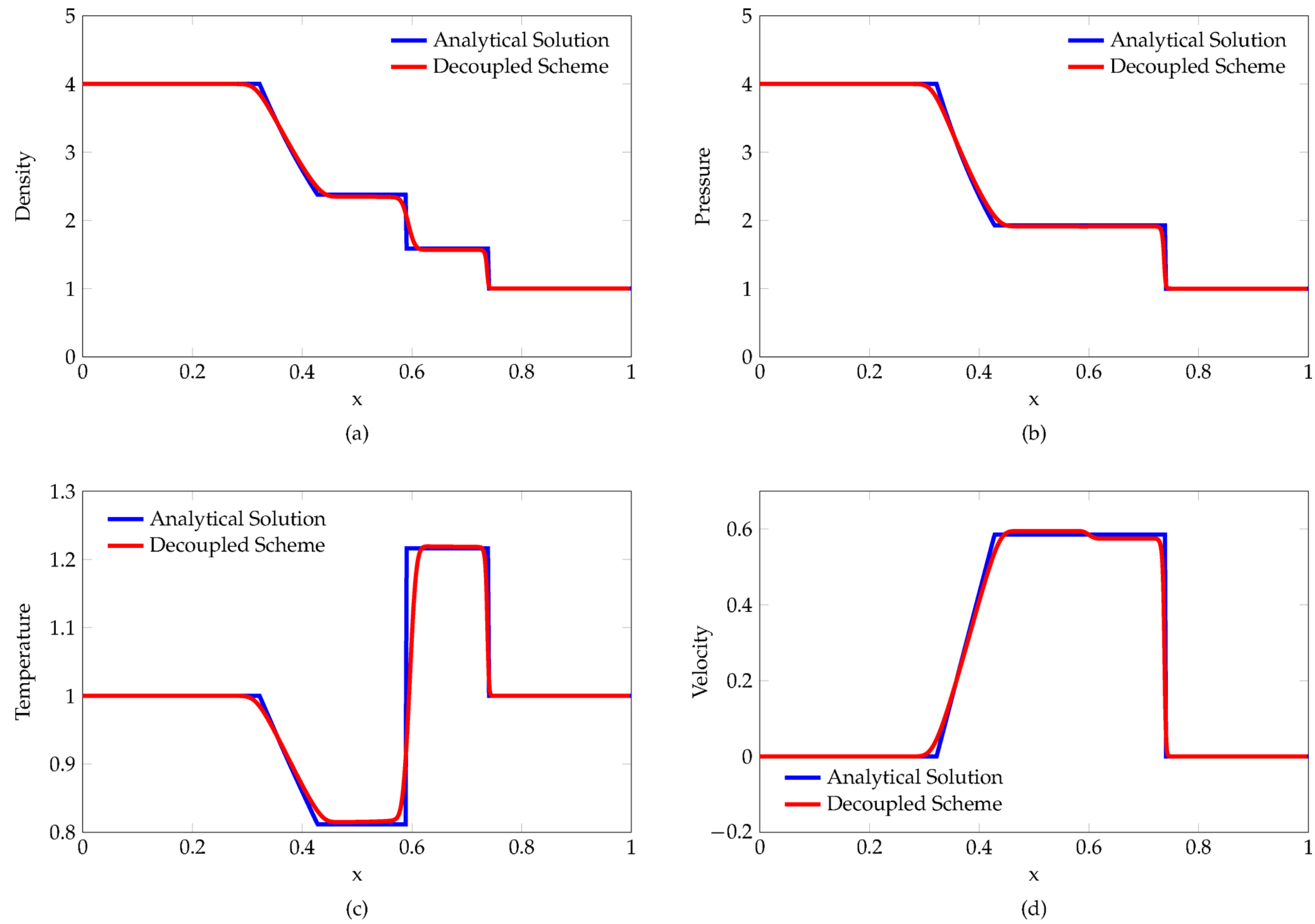

FIG. 1. The density, pressure, temperature, and velocity profiles of the shock tube are drawn. The red lines are the numerical results of simulation and the blue lines are the analytical resolutions. These are the results at the 180th step, i.e., the time $t = 0.1504$. The specific heat ratio is $\gamma = 1.4$ and the relaxation time is $\tau = 2/3$.

energy e_r,

$$E = e_t + e_r = \frac{D+n}{D} e_t. \tag{29}$$

Substituting Eq. (29) into (28) we obtain the internal energy E,

$$E = \frac{\sum_i g_i \frac{1}{2}\xi_i^2 + \rho \sum_j \frac{n}{2} h_j \eta_j^2 - \rho \frac{1}{2} u^2}{\rho}. \tag{30}$$

Substituting Eq. (26) and (29) into (30), we obtain the absolute temperature T,

$$T = \frac{2}{D+n} \frac{\sum_i g_i \frac{1}{2}\xi_i^2 + \rho \sum_j \frac{n}{2} h_j \eta_j^2 - \rho \frac{1}{2} u^2}{\rho}. \tag{31}$$

(5) Implement the boundary conditions.

VI. NUMERICAL VALIDATION

In this section, we apply the decoupled scheme given above to simulating a shock tube. The grid is $X \times Y = 1000 \times 16$. The initial condition of the left tube is $\rho = 4$, $T = 1$, $\boldsymbol{u} = 0$ and that of the right tube is $\rho = 1$, $T = 1$, $\boldsymbol{u} = 0$. The specific heat ratio is $\gamma = 1.4$, the rotational free degree is $n = 3$, and the relaxation time is $\tau = 2/3$. All of these macroscopic variables are dimensionless. The periodic boundary condition is employed for the up and down boundaries and the open boundary condition is employed for the left and right boundaries.

Figure 1 gives the results of simulation employing the decoupled scheme given above at step = 180, i.e., time

$$t = \frac{\text{step}}{Xr} = \frac{180}{1000 \times 1.1969797752} = 0.1504.$$

The analytical solutions [20] at the same time are also given. The red lines show the numerical results and the blue lines show the analytical resolutions. It can be seen from Fig. 1 that the numerical simulation results agree with the analytical resolutions very well.

Table III gives the relative error of density ρ, pressure p, absolute temperature T, and the velocity u. The relative error

TABLE III. Relative error of the numerical solutions.

	ρ	p	T	u_x
Error	0.0077	0.0055	0.0064	0.0242

is defined as

$$\text{Error} = \frac{\sum_i |x_{\text{nume},i} - x_{\text{anal},i}|}{\sum_i |x_{\text{anal},i}|}, \tag{32}$$

where x_{nume} is the numerical solutions, x_{anal} is the analytical solutions, and $i = X + 1$. Table III shows that the maximum of relative error is 2.42%. This relative error is acceptable.

VII. CONCLUSION

This work proposes a way based on the Hermite expansion to construct LB schemes for the compressible Navier-Stokes equations with arbitrary specific heat ratio. The equilibrium distribution function $f^{\text{eq}}(\boldsymbol{\xi},\eta)$, the distribution function $f(\boldsymbol{\xi},\eta)$, and the evolution function are decoupled into two parts, namely one is in relation to the translational velocity $\boldsymbol{\xi}$ and the other is connected with the rotational velocity η. The two evolution equations evolve separately. The translational velocity $\boldsymbol{\xi}$ is discretized in a two- or three-dimensional LB model and the rotational velocity η is discretized in another one-dimensional LB model. The Hermite expansion is applied to deriving these two LB models. The correct flexible specific heat ratio is obtained and the correct relation between the temperature T and the internal energy E is derived via the Chapman-Enskog expansion. The decoupled scheme is validated by a shock tube simulation. The simulation results agree with the analytical resolutions very well.

The LB models used in the decoupled scheme are the same as the ones used in the schemes with fixed specific heat ratio. It is not necessary for the decoupled scheme to construct new LB models specifically. The models with fixed specific heat ratio can applied to the decoupled scheme without any recommendation. This differs from the existing schemes which construct new models in order to adjust the specific heat ratio.

The decoupled scheme proposed by this work can make use of the models constructed via the Hermite expansion, so the process of constructing new schemes is simple and higher-order accuracy can be achieved easily.

APPENDIX: DERIVATION OF THE NAVIER-STOKES EQUATIONS FROM THE EVOLUTION EQUATIONS OF $g(\boldsymbol{\xi})$ AND $h(\eta)$ VIA THE CHAPMAN-ENSKOG EXPANSION

In this Appendix, we derive the Navier-Stokes equations with flexible specific heat ratio from the evolution equations of $g(\boldsymbol{\xi})$ and $h(\eta)$ via the Chapman-Enskog expansion.

Expanding the distribution functions g_i and h_j, the derivatives of the time t, and the space in terms of the Kundsen number ϵ, we obtain

$$\boldsymbol{\nabla} = \epsilon \boldsymbol{\nabla}_1, \tag{A1a}$$

$$\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2}, \tag{A1b}$$

$$g_i = g_i^{(0)} + \epsilon g_i^{(1)} + \epsilon^2 g_i^{(2)} + \cdots, \tag{A1c}$$

$$h_j = h_j^{(0)} + \epsilon h_j^{(1)} + \epsilon^2 h_j^{(2)} + \cdots. \tag{A1d}$$

Substituting Eq. (A1c) into the evolution equation of the translational velocity, i.e., Eq. (18a), and comparing the order of ϵ we obtain

$$g_i^{(0)} = g_i^{(\text{eq})}, \tag{A2a}$$

$$\left(\frac{\partial}{\partial t_1} + \boldsymbol{\xi}_i \cdot \boldsymbol{\nabla}_1\right) g_i^{(0)} + \frac{1}{\tau} g_i^{(1)} = 0, \tag{A2b}$$

$$\frac{\partial g_i^{(0)}}{\partial t_2} + \left(\frac{\partial}{\partial t_1} + \boldsymbol{\xi}_i \cdot \boldsymbol{\nabla}_1\right) g_i^{(1)} + \frac{1}{\tau} g_i^{(2)} = 0. \tag{A2c}$$

Considering the discrete form of Eq. (11) in the discrete velocity space,

$$\sum_i g_i = \sum_i g_i^{\text{eq}} = \rho, \tag{A3a}$$

$$\sum_i g_i = \sum_i g_i^{\text{eq}} = \rho \boldsymbol{u}, \tag{A3b}$$

$$\sum_i g_i \frac{1}{2}\xi_i^2 = \sum_i g_i^{\text{eq}} \frac{1}{2}\xi_i^2 = \rho\left(\frac{1}{2}u^2 + e_t\right), \tag{A3c}$$

we obtain

$$\sum_i g_i^{(n)} = 0, \quad \sum_i g_i^{(n)} \boldsymbol{\xi}_i = 0,$$

$$\sum_i g_i^{(n)} \frac{1}{2}\xi_i^2 = 0, \quad n = 1,2,\ldots. \tag{A4}$$

Substituting Eq. (A1d) into the evolution equation of the rotational velocity, i.e. Eq. (18b), and comparing the order of ϵ we obtain

$$h_j^{(0)} = h_j^{(\text{eq})}, \tag{A5a}$$

$$\left(\frac{\partial}{\partial t_1} + \boldsymbol{u} \cdot \boldsymbol{\nabla}_1\right) h_j^{(0)} + \frac{1}{\tau} h_j^{(1)} = 0, \tag{A5b}$$

$$\frac{\partial h_j^{(0)}}{\partial t_2} + \left(\frac{\partial}{\partial t_1} + \boldsymbol{u} \cdot \boldsymbol{\nabla}_1\right) h_j^{(1)} + \frac{1}{\tau} h_j^{(2)} = 0. \tag{A5c}$$

Considering the discrete form of Eq. (12) in the discrete velocity space,

$$\sum_j h_j = \sum_j h_j^{\text{eq}} = 1, \tag{A6a}$$

$$\sum_j h_j \frac{n}{2}\eta_j^2 = \sum_j h_j^{\text{eq}} \frac{n}{2}\eta_j^2 = e_r, \tag{A6b}$$

we obtain

$$\sum_j h_j^{(n)} = 0, \quad \sum_j h_j^{(n)} \frac{n}{2}\eta_j^2 = 0, \quad n = 1,2,\ldots. \tag{A7}$$

Some velocity moments of g_i and h_j will be used in the derivation of the Navier-Stokes equations and we list them as follows:

$$\sum_i g_i^{\text{eq}} = \rho, \tag{A8a}$$

$$\sum_i g_i^{\text{eq}} \boldsymbol{\xi}_i = \rho \boldsymbol{u}, \tag{A8b}$$

$$\sum_i g_i^{eq} \boldsymbol{\xi}_i \boldsymbol{\xi}_i = \rho \boldsymbol{u}\boldsymbol{u} + P\boldsymbol{\delta}, \tag{A8c}$$

$$\sum_i g_i^{eq} \boldsymbol{\xi}_i \boldsymbol{\xi}_i \boldsymbol{\xi}_i = \rho \boldsymbol{u}\boldsymbol{u}\boldsymbol{u} + P\boldsymbol{u}\boldsymbol{\delta}, \tag{A8d}$$

$$\sum_i g_i^{eq} \frac{1}{2}\xi_i^2 = \rho\left(\frac{1}{2}u^2 + e_t\right), \tag{A8e}$$

$$\sum_i g_i^{eq} \frac{1}{2}\xi_i^2 \boldsymbol{\xi}_i = \rho\left(\frac{1}{2}u^2 + e_t\right)\boldsymbol{u}, \tag{A8f}$$

$$\sum_i g_i^{eq} \frac{1}{2}\xi_i^2 \boldsymbol{\xi}_i \boldsymbol{\xi}_i = P\left(\frac{2}{D}e_t + \frac{1}{2}u^2 + e_t\right)\boldsymbol{\delta}, + \left(2P + \frac{1}{2}\rho u^2 + \rho e_t\right)\boldsymbol{u}\boldsymbol{u}, \tag{A8g}$$

where $P\boldsymbol{u}\boldsymbol{\delta} = P(u_r\delta_{st} + u_s\delta_{tr} + u_t\delta_{rs})$. Here, the Grad notes are used [21].

Two velocity moments of h_j will be used in the following parts:

$$\sum_j h_j^{eq} = 1, \tag{A9a}$$

$$\sum_j h_j^{eq} \frac{n}{2}\eta^2 = e_r. \tag{A9b}$$

1. Derivation of the continuity equation

Taking the zeroth-order moment of Eq. (A2b), we obtain

$$\sum_i \left(\frac{\partial}{\partial t_1} + \boldsymbol{\xi}_i \cdot \nabla_1\right) g_i^{(0)} + \frac{1}{\tau}\sum_i g_i^{(1)} = 0. \tag{A10}$$

Substituting Eq. (A4) and (A8) into (A10), the continuity equation of the first order is obtained,

$$\frac{\partial}{\partial t_1}\rho + \nabla_1 \cdot \rho\boldsymbol{u} = 0. \tag{A11}$$

Taking the zeroth-order moment of Eq. (A2c), we obtain

$$\frac{\partial \sum_i g_i^{(0)}}{\partial t_2} + \sum_i \left(\frac{\partial}{\partial t_1} + \boldsymbol{\xi}_i \cdot \nabla_1\right) g_i^{(1)} + \frac{1}{\tau}\sum_i g_i^{(2)} = 0. \tag{A12}$$

Substituting Eq. (A4) and (A8) into (A12), and then summing on i, we obtain the continuity equation of the second order,

$$\frac{\partial \rho}{\partial t_2} = 0. \tag{A13}$$

Making use of Eq. (A1b) and combining the continuity equation of the first and second orders, i.e., Eq. (A11) and (A13), the continuity equation is obtained,

$$\frac{\partial}{\partial t}\rho + \nabla \cdot \rho\boldsymbol{u} = 0. \tag{A14}$$

2. Derivation of the momentum conservation equation

Taking the first-order moment of Eq. (A2b),

$$\sum_i \left(\frac{\partial}{\partial t_1} + \boldsymbol{\xi}_i \cdot \nabla_1\right) g_i^{(0)}\boldsymbol{\xi}_i + \frac{1}{\tau}\sum_i g_i^{(1)}\boldsymbol{\xi}_i = 0, \tag{A15}$$

and inserting Eqs. (A4) and (A8), we get the conservation momentum equation of the first order,

$$\frac{\partial}{\partial t_1}\rho\boldsymbol{u} + \nabla_1 \cdot (\rho\boldsymbol{u}\boldsymbol{u} + P\boldsymbol{\delta}) = 0. \tag{A16}$$

Taking the first-order moment of Eq. (A2c),

$$\frac{\partial \sum_i g_i^{(0)}\boldsymbol{\xi}_i}{\partial t_2} + \sum_i \left(\frac{\partial}{\partial t_1} + \boldsymbol{\xi}_i \cdot \nabla_1\right) g_i^{(1)}\boldsymbol{\xi}_i + \frac{1}{\tau}\sum_i g_i^{(2)}\boldsymbol{\xi}_i = 0, \tag{A17}$$

substituting Eq. (A2b) into Eq. (A17), and simplifying, we obtain

$$\frac{\partial \sum_i g_i^{(0)}\boldsymbol{\xi}_i}{\partial t_2} - \tau\nabla_1 \cdot \left(\frac{\partial}{\partial t_1}\sum_i \boldsymbol{\xi}_i\boldsymbol{\xi}_i g_i^{(0)} + \nabla_1 \cdot \sum_i \boldsymbol{\xi}_i\boldsymbol{\xi}_i\boldsymbol{\xi}_i g_i^{(1)}\right) = 0. \tag{A18}$$

Inserting the moments of g_i, i.e., Eq. (A8), into Eq. (A18) we obtain

$$\frac{\partial \rho\boldsymbol{u}}{\partial t_2} - \tau\nabla_1 \cdot \left[\frac{\partial}{\partial t_1}(\rho\boldsymbol{u}\boldsymbol{u} + P\boldsymbol{\delta}) + \nabla_1 \cdot \sum_i \boldsymbol{\xi}_i\boldsymbol{\xi}_i\boldsymbol{\xi}_i g_i^{(1)}\right] = 0, \tag{A19}$$

where $\frac{\partial P}{\partial t_1}$ is a difficult point to simplify. To simplify $\frac{\partial P}{\partial t_1}$, we should obtain the energy conservation equation of the first-order first.

Multiplying $\frac{1}{2}\xi_i^2$ to Eq. (A2b) and summing on i we obtain

$$\sum_i \left(\frac{\partial}{\partial t_1} + \boldsymbol{\xi}_i \cdot \nabla_1\right) g_i^{(0)}\frac{1}{2}\xi_i^2 + \frac{1}{\tau}\sum_i g_i^{(1)}\frac{1}{2}\xi_i^2 = 0. \tag{A20}$$

Substituting the moments of $\boldsymbol{\xi}_i$, i.e., Eq. (A8), into Eq. (A20), we obtain the translational internal energy conversation equation of the first order,

$$\frac{\partial}{\partial t_1}\left(\frac{1}{2}\rho u^2 + \rho e_t\right) + \nabla_1 \cdot \left(\frac{1}{2}\rho u^2 + \rho e_t + P\right)\boldsymbol{u} = 0. \tag{A21}$$

Multiplying $\frac{1}{2}\eta^2$ to Eq. (A5b), summing on j, and inserting the moments of h_j, i.e., Eq. (A9), we obtain the rotational internal energy conversation equation of the first order in nonconservation form,

$$\frac{\partial}{\partial t_1}e_r + \boldsymbol{u} \cdot \nabla_1 e_r = 0. \tag{A22}$$

Multiplying ρ to Eq. (A22) and multiplying e_r to Eq. (A11), and then adding, we obtain

$$\rho\left(\frac{\partial}{\partial t_1}e_r + \boldsymbol{u} \cdot \nabla_1 e_r\right) + e_r\left(\frac{\partial}{\partial t_1}\rho + \nabla_1 \cdot \rho\boldsymbol{u}\right) = 0. \tag{A23}$$

Simplifying Eq. (A23), we obtain the rotational internal conversation energy equation of the first order in conservation form,

$$\frac{\partial}{\partial t_1}\rho e_r + \nabla_1 \cdot \rho \boldsymbol{u} e_r = 0. \tag{A24}$$

Combining the translational internal energy conversation equation of the first order, i.e., Eq. (A21), and the rotational internal energy conversation equation of the first order, i.e., Eq. (A24), we obtain the energy conversation equation of the first order,

$$\frac{\partial}{\partial t_1}\left(\frac{1}{2}\rho u^2 + \rho E\right) + \nabla_1 \cdot \left(\frac{1}{2}\rho u^2 + \rho E + P\right)\boldsymbol{u} = 0. \tag{A25}$$

Substituting $P = \frac{2}{D+n}\rho E$ into Eq. (A25) we obtain

$$\frac{\partial}{\partial t_1}\left(\frac{1}{2}\rho u^2 + \frac{D+n}{D}P\right) + \nabla_1 \cdot \left(\frac{1}{2}\rho u^2 + \frac{D+n+2}{D}P\right)\boldsymbol{u} = 0. \tag{A26}$$

Expanding Eq. (A26), and substituting Eqs. (A11) and (A16) into it, after some algebra, we obtain

$$\frac{\partial P}{\partial t_1} = -\nabla_1 \cdot P\boldsymbol{u} - \frac{2}{D+n}P\nabla_1 \cdot \boldsymbol{u}. \tag{A27}$$

Substituting Eq. (A27) into Eq. (A19), after some algebra, we obtain the momentum conversation equation of the second order,

$$\frac{\partial}{\partial t_2}\rho\boldsymbol{u} = \nabla_1 \cdot \frac{2}{D}\rho e_t \tau\left[(\nabla_1 \boldsymbol{u} + \boldsymbol{u}\nabla_1) - \frac{2}{D+n}\nabla_1 \cdot \boldsymbol{u}\boldsymbol{\delta}\right]. \tag{A28}$$

Combining the momentum equation of the first order and second order, we obtain the moment conversation equation

$$\frac{\partial}{\partial t}\rho\boldsymbol{u} + \nabla \cdot (\rho\boldsymbol{u}\boldsymbol{u} + P\boldsymbol{\delta}) = \nabla \cdot \mu\left[(\nabla \boldsymbol{u} + \boldsymbol{u}\nabla) - \frac{2}{D+n}\nabla \cdot \boldsymbol{u}\boldsymbol{\delta}\right], \tag{A29}$$

where $\mu = \frac{2}{D}\rho e_t \tau$ is the dynamic viscosity coefficient.

3. Derivation of the energy conversation equation

We have obtained the energy conversation equation of the first order, i.e., Eq. (A25),

$$\frac{\partial}{\partial t_1}\left(\frac{1}{2}\rho u^2 + \rho E\right) + \nabla_1 \cdot \left(\frac{1}{2}\rho u^2 + \rho E + P\right)\boldsymbol{u} = 0.$$

Now we derive the energy conversation equation of the second order.

Multiplying $\frac{1}{2}\xi_i^2$ to Eq. (A2c), substituting (A2b) into it, and summing on i, we obtain

$$\frac{\partial}{\partial t_2}\sum_i g_i^{(0)}\frac{1}{2}\xi_i^2 = \nabla_1 \cdot \tau\left(\frac{\partial}{\partial t_1}\sum_i g_i^{(0)}\frac{1}{2}\xi_i^2\boldsymbol{\xi}_i + \nabla_1 \cdot g_i^{(0)}\boldsymbol{\xi}_i\boldsymbol{\xi}_i\frac{1}{2}\xi_i^2\right). \tag{A30}$$

Substituting the moments of g_i into Eq. (A30), we obtain

$$\frac{\partial}{\partial t_2}\left(\frac{1}{2}\rho u^2 + e_t\right) = \nabla_1 \cdot \tau\left[\frac{\partial}{\partial t_1}\left(\frac{1}{2}\rho u^2 + e_t + P\right)\boldsymbol{u} + \nabla_1 \cdot P\left(\frac{2}{D}e_t + \frac{1}{2}u^2 + e_t\right)\boldsymbol{\delta} + \left(2P + \frac{1}{2}\rho u^2 + e_t\right)\boldsymbol{u}\boldsymbol{u}\right]. \tag{A31}$$

Inserting Eq. (A11), (A16), (A26), and (A27) into Eq. (A31), after some algebra, we get the translational internal energy conversation equation of the second order

$$\frac{\partial}{\partial t_2}\left(\frac{1}{2}\rho u^2 + e_t\right) = \nabla_1 \cdot \tau P\boldsymbol{u}\left[(\nabla_1 \boldsymbol{u} + \boldsymbol{u}\nabla_1) - \frac{2}{D+n}\nabla_1 \boldsymbol{u}\boldsymbol{\delta}\right] + \nabla_1 \cdot \tau P\frac{D+2}{D}\nabla_1 e_t. \tag{A32}$$

Multiplying $h_j^{(0)}$ to Eq. (A2c), multiplying $g_i^{(0)}$ to Eq. (A5c), and adding them yields

$$\frac{\partial}{\partial t_2}g_i^{(0)}h_j^{(0)} + \left(\frac{\partial}{\partial t_1} + \xi \cdot \nabla_1\right)g_i^{(1)}h_j^{(0)} + \left(\frac{\partial}{\partial t_1} + \boldsymbol{u} \cdot \nabla_1\right)g_i^{(0)}h_j^{(1)} + \frac{1}{\tau}\left(g_i^{(2)}h_j^{(0)} + g_i^{(0)}h_j^{(2)}\right) = 0, \tag{A33}$$

and substituting Eq. (A2b) into Eq. (A33), we get

$$\frac{\partial}{\partial t_2}g_i^{(0)}h_j^{(0)} - \nabla_1 \cdot \tau\left(\frac{\partial}{\partial t_1}\boldsymbol{\xi}_i g_i^{(0)}h_j^{(0)} + \nabla_1 \cdot \boldsymbol{\xi}_i\boldsymbol{\xi}_i g_i^{(0)}h_j^{(0)}\right) + \left(\frac{\partial}{\partial t_1} + \boldsymbol{u} \cdot \nabla_1\right)g_i^{(0)}h_j^{(1)} + \frac{1}{\tau}(g_i^{(2)}h_j^{(0)} + g_i^{(0)}h_j^{(2)}) = 0. \tag{A34}$$

Multiplying $\frac{n}{2}\eta^2$ to Eq. (A34) and summing on i and j we obtain

$$\frac{\partial}{\partial t_2}\rho e_r = \nabla_1 \cdot \tau\left[\frac{\partial}{\partial t_1}\rho\boldsymbol{u}e_r + \nabla_1 \cdot (\rho\boldsymbol{u}\boldsymbol{u} + P\boldsymbol{\delta})e_r\right]. \tag{A35}$$

Inserting Eqs. (A16) and (A24) into Eq. (A35), after some algebra, we obtain the rotational internal energy conversation equation of the second order,

$$\frac{\partial}{\partial t_2}\rho e_r = \nabla_1 \cdot \tau\rho e_t\frac{n}{D}\nabla_1 e_r. \tag{A36}$$

Combining the rotational internal energy conversation equation of the second order, i.e., Eq. (A36), with the translational internal conversation energy of the second order, i.e., Eq. (A32), we obtain the energy conversation equation of the second order,

$$\frac{\partial}{\partial t_2}\left(\frac{1}{2}\rho u^2+\rho E\right) = \nabla_1\cdot\tau P\boldsymbol{u}\left[(\nabla_1\boldsymbol{u}+\boldsymbol{u}\nabla_1)-\frac{2}{D+n}\nabla_1\boldsymbol{u}\boldsymbol{\delta}\right] + \nabla_1\cdot\frac{D+n+2}{D}\tau\rho e_t\nabla_1 e_t. \tag{A37}$$

Combining the energy conversation equation of the second order, i.e., Eq. (A37), with the energy conversation equation of the first order, i.e., Eq. (A25), we obtain the energy conversation equation

$$\frac{\partial}{\partial t}\rho\left(E+\frac{1}{2}u^2\right)+\nabla\cdot\rho\boldsymbol{u}\left(E+\frac{1}{2}u^2+\frac{P}{\rho}\right) = \nabla\cdot\mu\boldsymbol{u}\left(\nabla\boldsymbol{u}+\boldsymbol{u}\nabla-\frac{2}{D+n}\nabla\cdot\boldsymbol{u}\delta\right)+\nabla\cdot\kappa\nabla E, \tag{A38}$$

where

$$P=\frac{2}{D}\rho e_t,\quad \mu=\frac{2}{D}\rho e_t\tau,\quad \kappa=\frac{2(D+n+2)}{D(D+n)}\rho e_t\tau.$$

Equation (A38) is the energy conversation equation with flexible specific heat ratio and the specific heat ratio γ is

$$\gamma=\frac{D+n+2}{D+n}.$$

The specific heat ratio γ can be adjusted by changing the free degree of the rotational velocity n.

[1] S. Chen, Z. Wang, X. Shan, and G. D. Doolen, J. Stat. Phys. **68**, 379 (1992).
[2] S. Chen and G. D. Doolen, Annu. Rev. Fluid Mech. **30**, 329 (1998).
[3] W. Shi, W. Shyy, and R. Mei, Numer. Heat Transfer, Part B **40**, 1 (2001).
[4] T. Kataoka and M. Tsutahara, Phys. Rev. E **69**, 035701 (2004).
[5] M. Watari, Physica A **382**, 502 (2007).
[6] M. Tsutahara, T. Kataoka, K. Shikata, and N. Takada, Comput. Fluids **37**, 79 (2008).
[7] P. C. Philippi, L. A. Hegele, Jr., L. O. E. dos Santos, and R. Surmas, Phys. Rev. E **73**, 056702 (2006).
[8] P. Philippi, D. Siebert, L. Hegele, Jr., and K. Mattila, J. Braz. Soc. Mech. Sci. Eng. **38**, 1401 (2016).
[9] X. Shan, X.-F. Yuan, and H. Chen, J. Fluid Mech. **550**, 413 (2006).
[10] K. K. Mattila, L. A. Hegele Júnior, and P. C. Philippi, Sci. World J. **2014**, 142907 (2014).
[11] J. W. Shim and R. Gatignol, Phys. Rev. E **83**, 046710 (2011).
[12] J. W. Shim, Phys. Rev. E **88**, 053310 (2013).
[13] J. W. Shim, Phys. Rev. E **87**, 013312 (2013).
[14] S. Ansumali, I. V. Karlin, and H. C. Öttinger, Europhys. Lett. **63**, 798 (2003).
[15] S. S. Chikatamarla and I. V. Karlin, Phys. Rev. Lett. **97**, 190601 (2006).
[16] S. S. Chikatamarla and I. V. Karlin, Phys. Rev. E **79**, 046701 (2009).
[17] W. P. Yudistiawan, S. K. Kwak, D. V. Patil, and S. Ansumali, Phys. Rev. E **82**, 046701 (2010).
[18] A. Xu, G. Zhang, Y. Li, and H. Li, Prog. Phys. **34** (2014).
[19] X. Shan, Phys. Rev. E **81**, 036702 (2010).
[20] G. A. Sod, J. Comput. Phys. **27**, 1 (1978).
[21] H. Grad, Commun. Pure Appl. Math. **2**, 325 (1949).