Entropy and weak solutions in the lattice Bhatnagar–Gross–Krook model*

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We derive the entropy functions whose local equilibria are suitable to recover the Euler-like equations in the framework of the lattice Boltzmann method. Numerical examples are also given, which are consistent with the above theoretical arguments. In all cases, we observe a negative entropy range existing near the shock, while numerical oscillations are captured.

Keywords: lattice Boltzmann method, entropy, weak solution

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1. Introduction

In recent years, the lattice Boltzmann method (LBM) and the lattice Bhatnagar–Gross–Krook (LBGK) model have aroused considerable interest for the simulation of complex hydrodynamic phenomena, and has been proved successful in simulating nearly incompressible and isothermal fluid flows, for which it is a viable alternative to conventional numerical methods.[1−4] However, applications to flows with substantial temperature fluctuations have been proved problematic. Many schemes are subjected to instabilities,[5] often attributed to the use of polynomial approximations for the equilibrium distributions. These equilibria may become negative, which violates the assumptions of a discrete H-theorem and may permit instability.[6] This has spurred recent work on constructing non-polynomial equilibria which remain positive, and often arises from some existing entropy functions.[7] To date, there are still several directions where the LBM theory calls for substantial progress and upgrades, the Galilean invariance and the thermohydrodynamics of LBM.[8−12] One of the most interesting problems is the H theorem in LBGK model.

Another interpretation of the lattice Boltzmann approach is as a discretized version of the continuum Boltzmann equation. The governing equations of gasdynamics are expressions of conservation and the second law of thermodynamics. Conservation requires that the three fundamental quantities, mass, momentum, and energy, are neither created nor destroyed but are only redistributed or, excepting mass, converted from one form to another. A companion principle to conservation, known as the second law of thermodynamics, requires that a fourth fundamental quantity called entropy should never decrease. The second law of thermodynamics restricts the redistributions and conversions of conserved quantities otherwise allowed by the conservation laws. As another supplement to conservation, the equations of state and the second law of thermo dynamics collectively constitute the Euler equations. An interesting problem we encounter is how to realize this counterparts in LBGK model.

2. BGK Boltzmann equation and its hydrodynamics

We begin with the Bhatnagar–Gross–Krook (BGK)[13] Boltzmann equation, which is a model kinetic equation widely studied

$$\partial_t f + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} f = -\omega(f - g), \tag{1}$$

where the single particle distribution function $f \equiv f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ is a time-dependent function of particle coordinate $\boldsymbol{x}$ and velocity $\boldsymbol{\xi}$, ω is the relaxation parameter which characterizes the typical collision process, and g is the local Maxwellian equilibrium distribution function defined by

$$g(\rho, \boldsymbol{u}, \theta) = \rho(2\pi\theta)^{-D/2} \exp\left[-(\boldsymbol{\xi} - \boldsymbol{u})^2/2\theta\right], \tag{2}$$

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where D is the dimension of the velocity space $\boldsymbol{\xi}$, ρ, $\boldsymbol{u}$ and $\theta = k_{\rm B}T/m$ are the mass density, macroscopic velocity and normalized temperature per unit mass, respectively, $k_{\rm B}, T$ and m are the Boltzmann constant, temperature and particle mass respectively. The mass density ρ, velocity $\boldsymbol{u}$ and temperature θ (or internal energy density) are the hydrodynamic moments of f or g[14]

$$\rho = \int {\rm d}\xi f = \int {\rm d}\xi g, \tag{3}$$

$$\rho \boldsymbol{u} = \int {\rm d}\xi\xi f = \int {\rm d}\xi\xi g, \tag{4}$$

$$\frac{D}{2}\rho\theta = \int {\rm d}\xi \frac{1}{2}(\xi - u)^2 f = \int {\rm d}\xi \frac{1}{2}(\xi - u)^2 g. \tag{5}$$

At equilibrium $f = g$, the Boltzmann equation (1) becomes

$$D_t g = 0, \tag{6}$$

where

$$D_t \equiv \partial_t + \boldsymbol{\xi}\cdot\boldsymbol{\nabla}. \tag{7}$$

The Euler equation can be easily derived from the above equation by evaluating its hydrodynamic moments

$$\partial_t \rho + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{u}) = 0, \tag{8}$$

$$\partial_t(\rho\boldsymbol{u}) + \boldsymbol{\nabla}(\rho\boldsymbol{u}\boldsymbol{u} + \rho\theta) = 0, \tag{9}$$

$$\partial_t\left(\frac{D}{2}\rho\theta + \frac{1}{2}\rho u^2\right) + \boldsymbol{\nabla}\cdot\left(\frac{D+2}{2}\rho\theta\boldsymbol{u} + \frac{1}{2}\rho u^2\boldsymbol{u}\right) = 0, \tag{10}$$

where $\boldsymbol{u}\boldsymbol{u}$ denotes a second rank tensor $u_\alpha u_\beta$ and $u^2 = \boldsymbol{u}\cdot\boldsymbol{u}$. The momentum equation can also be rewritten as

$$\rho\partial_t\boldsymbol{u} + \rho\boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u} = -\boldsymbol{\nabla}P, \tag{11}$$

where

$$P = \rho\theta \tag{12}$$

is the equation of state for ideal gas.

3. Lattice Boltzmann equation and its hydrodynamics

The lattice Boltzmann equation can be derived by discretizing the continuous BGK equation in both time and phase space. The obtained lattice Boltzmann equation is

$$f_i(t+1, \boldsymbol{x}+\boldsymbol{c}_i) - f_i(t,\boldsymbol{x}) = -\omega[f_i(t,\boldsymbol{x}) - f_i^{\rm eq}(t,\boldsymbol{x})], \tag{13}$$

where $f_i^{\rm eq}$ is the discretized equilibrium function and $\{\boldsymbol{c}_i\}$ is the discrete velocity set.

For the sake of explicitness, we use the nine-bit lattice Boltzmann equation in two-dimensional space in what follows, and the equilibrium distribution function of the nine-bit model is

$$f_i^{\rm eq} = w_i\rho\left[1 + \frac{3(\boldsymbol{c}_i\cdot\boldsymbol{u})}{c^2} + \frac{9(\boldsymbol{c}_i\cdot\boldsymbol{u})^2}{2c^4} - \frac{3u^2}{2c^2}\right], \tag{14}$$

where

$$w_i = \begin{cases} 4/9, & i = 0, \\ 1/9, & i = 1,\ldots,4, \\ 1/36, & i = 5,\ldots,8, \end{cases} \tag{15}$$

and

$$c_i = \begin{cases} (0,0), & i = 0, \\ (\cos((i-1)\pi/2), \sin((i-1)\pi/2)) & i = 1,\ldots,4, \\ (\cos((i-5)\pi/2), \sin((i-5)\pi/2)) & i = 5,\ldots,8, \end{cases} \tag{16}$$

are the associated weight coefficient and discrete velocity set respectively. The hydrodynamics moments of the lattice Boltzmann equation are given by

$$\rho = \sum_i f_i = \sum_i f_i^{\rm eq}, \tag{17}$$

$$\rho\boldsymbol{u} = \sum_i \boldsymbol{c}_i f_i = \sum_i \boldsymbol{c}_i f_i^{\rm eq}, \tag{18}$$

$$\frac{D}{2}\rho\theta = \sum_i \frac{1}{2}(\boldsymbol{c}_i - \boldsymbol{u})^2 f_i = \sum_i \frac{1}{2}(\boldsymbol{c}_i - \boldsymbol{u})^2 f_i^{\rm eq}. \tag{19}$$

Through the Chapman-Enskog[15] analysis (see Appendix A),

$$D_t f_i^{\rm eq} = -\omega f_i^{(1)}, \tag{20}$$

the moments of the zeroth order of Eq. (20) in the discrete momentum space lead to the Euler equations

$$\partial_t \rho + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{u}) = 0, \tag{21}$$

$$\partial_t(\rho\boldsymbol{u}) + \boldsymbol{\nabla}(\rho\boldsymbol{u}\boldsymbol{u} + \rho\theta) = 0, \tag{22}$$

$$\partial_t\left(\frac{D}{2}\rho\theta + \frac{1}{2}\rho u^2\right) + \boldsymbol{\nabla}\cdot\left(\frac{D+2}{2}\rho\theta\boldsymbol{u}\right) = 0. \tag{23}$$

Note that equation (23) differs from its counterpart Eq. (10), which is derived from the continuous BGK Boltzmann equation.[13] The energy flux $\frac{1}{2}\rho u^2\boldsymbol{u}$ due to the advection of fluid is missing. Thus, shock waves across which the entropy of fluid particles decreases may occur in the numerical results. However, we believe that such shock waves will not consistent with the real physical solutions.

4. The derivation of the entropy equation

The derivation of the entropy equation from Eqs. (21)–(23) in the one-dimensional problem is as follows. Rewrite Eqs. (21)–(23) as

$$\partial_t\rho + \partial_x(\rho u) = 0, \tag{24}$$

$$\partial_t(\rho u) + \partial_x\left(\rho u^2 + P\right) = 0, \tag{25}$$

$$\partial_t(\rho E) + \partial_x(pu + \rho E u) = \partial_x\left(\frac{1}{2}\rho u^3\right), \tag{26}$$

where

$$E = e + \frac{1}{2}\rho u^2. \tag{27}$$

From Eqs. (24) and (26), we have

$$\rho\partial_t E + \rho u\partial_x E + \partial_x(Pu) = \partial_x\left(\frac{1}{2}\rho u^3\right). \tag{28}$$

Then substituting Eq. (27) into Eq. (28), we have

$$\partial_t e + u\partial_x e = \frac{1}{\rho}\Big[\partial_x\Big(\frac{1}{2}\rho u^3\Big) - \rho\partial_t\Big(\frac{1}{2}u^2\Big) - \rho u\partial_x\Big(\frac{1}{2}u^2\Big) - \partial_x(Pu)\Big]. \tag{29}$$

Based on the definition of entropy

$$\mathrm{d}S = \mathrm{d}Q/T, \tag{30}$$

and the well known equation

$$\mathrm{d}e = \mathrm{d}Q + \frac{P}{\rho^2}\mathrm{d}\rho, \tag{31}$$

we obtain

$$T\,\mathrm{d}S = \mathrm{d}e - \frac{P}{\rho^2}\mathrm{d}\rho. \tag{32}$$

At this stage, we have

$$\partial_t S + u\partial_x S = \frac{1}{T}\Big[(\partial_t e + u\partial_x e) - \frac{P}{\rho^2}(\partial_t\rho + u\partial_x\rho)\Big]. \tag{33}$$

Substituting Eq. (24) into Eq. (33), we obtain

$$\partial_t S + u\partial_x S = \frac{1}{T}\left(\partial_t e + u\partial_x e + \frac{P}{\rho}\partial_x u\right). \tag{34}$$

At last, we could deduce the entropy equation as follows:

$$\begin{aligned}
\partial_t S + u\partial_x S &= \frac{1}{\rho T}\Big[\partial_x\Big(\frac{1}{2}\rho u^3\Big) - \rho\partial_t\Big(\frac{1}{2}u^2\Big) - \rho u\partial_x\Big(\frac{1}{2}u^2\Big) - \partial_x(Pu) + P\partial_x u\Big] \\
&= \frac{1}{\rho T}\Big[\partial_x\Big(\frac{1}{2}\rho u^3\Big) - \rho u\partial_t u - \rho u^2\partial_x u - u\partial_x P\Big] \\
&= \frac{1}{\rho T}\Big[\partial_x\Big(\frac{1}{2}\rho u^3\Big) - u(\rho\partial_t u) - \rho u^2\partial_x u - u\partial_x P\Big] \\
&= \frac{1}{\rho T}\Big\{\partial_x\Big(\frac{1}{2}\rho u^3\Big) - u[-\partial_x P - \partial_x(\rho u^2) - u\partial_t\rho] - \rho u^2\partial_x u - u\partial_x P\Big\} \\
&= \frac{1}{\rho T}\Big\{\partial_x\Big(\frac{1}{2}\rho u^3\Big) - u[-\partial_x P - \partial_x\Big(\rho u^2\Big) + u\partial_x(\rho u)] - \rho u^2\partial_x u - u\partial_x P\Big\} \\
&= \frac{1}{\rho T}\Big\{\partial_x\Big(\frac{1}{2}\rho u^3\Big) + u\partial_x P + u\partial_x(\rho u^2) - u^2\partial_x(\rho u) - \rho u^2\partial_x u - u\partial_x P\Big\} \\
&= \frac{1}{\rho T}\Big\{\partial_x\Big(\frac{1}{2}\rho u^3\Big) + u\partial_x(\rho u^2) - u^2\partial_x(\rho u) - \rho u^2\partial_x u\Big\} \\
&= \frac{1}{\rho T}\Big\{\partial_x\Big(\frac{1}{2}\rho u^3\Big) + u^2\partial_x(\rho u) + \rho u^2\partial_x u - u^2\partial_x(\rho u) - \rho u^2\partial_x u\Big\} \\
&= \frac{1}{\rho T}\partial_x\Big(\frac{1}{2}\rho u^3\Big),
\end{aligned} \tag{35}$$

$$\partial_t S + u\partial_x S = \frac{1}{2\rho T}(u^3\partial_x\rho + 3\rho u^2\partial_x u). \tag{36}$$

Now we could compute

$$C = u^3\partial_x\rho + 3\rho u^2\partial_x u$$

to demonstrate the entropy preservation condition in the LBGK calculation.

We use the one-dimensional three and five velocity model (D1Q3, D1Q5) to numerically study the entropy in LBGK calculation. In Figs. 1 and 2, the entropy profiles are presented at different times for D1Q3 and D1Q5, and different ω ranging from 1.2 to 1.5. In all cases, we observe a negative entropy range existing near the shock, while oscillations are captured.

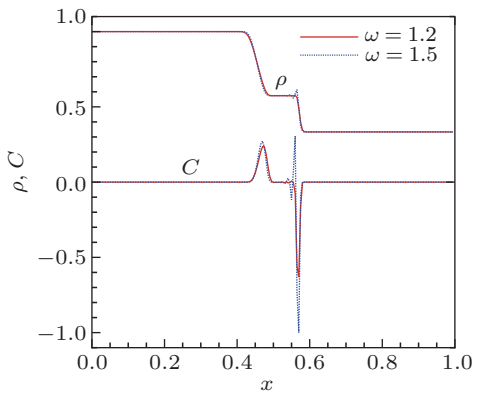


Fig. 1. The density and entropy profiles with different values of relaxation parameter for D1Q3 model.

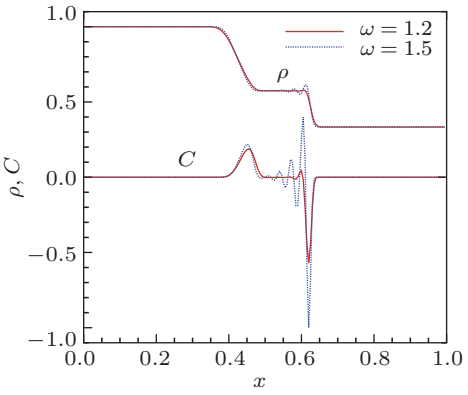


Fig. 2. The density and entropy profiles with different values of relaxation parameter for D1Q5 model.

5. Conclusions

We reported in this paper the entropy calculation in LBGK model. Great care has been paid to the links between the oscillation solution and the negative entropy. An explicit relation is obtained and confirmed by the numerical simulation, which must be in accordance with the second law of thermodynamics. The entropy condition for general LBGK method is a quite interesting and debatable question.

Appendix A Chapman–Enskog procedure

A1. Taylor expansion for the LBGK equation

The Chapman–Enskog method is the standard procedure used in statistical mechanics to solve an equation such as Eq. (13) with a perturbation parameter

$$f_i(t+1, \boldsymbol{x}+\boldsymbol{c}_i) - f_i(t, \boldsymbol{x}) = -\omega[f_i(t, \boldsymbol{x}) - f_i^{\mathrm{eq}}(t, \boldsymbol{x})].$$

Equation (13) can be Taylor expanded up to the second order. A straightforward calculation gives

$$(\partial_t + c_{i\alpha}\partial_\alpha) f_i + \frac{1}{2}(\partial_t + c_{i\alpha}\partial_\alpha)^2 f_i = \omega\left(f_i^{\mathrm{eq}} - f_i\right). \tag{A1}$$

A2. Multiscale expansion

Introduce two time scales $t_1 = \varepsilon t$, $t_2 = \varepsilon^2 t$ and one spatial scale $\boldsymbol{x}_1 = \varepsilon \boldsymbol{x}$, and expand in the multiscale for time, spatial and f_i,[15]

$$\begin{aligned}
\partial_t &= \varepsilon\partial_{t_1} + \varepsilon^2\partial_{t_2},\\
\partial_\alpha &= \varepsilon\partial_{1\alpha},\\
f_i &= f_i^{\mathrm{eq}} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \cdots.
\end{aligned}$$

Substituting them into Eq. (A1), we obtain

$$\begin{aligned}
&(\varepsilon\partial_{t_1} + \varepsilon^2\partial_{t_2} + \varepsilon c_{i\alpha}\partial_{1\alpha})(f_i^{\mathrm{eq}} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \cdots) + \frac{1}{2}\left(\varepsilon\partial_{t_1} + \varepsilon^2\partial_{t_2} + \varepsilon c_{i\alpha}\partial_{1\alpha}\right)^2\left(f_i^{\mathrm{eq}} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \cdots\right)\\
&\quad = \omega\left(f_i^{\mathrm{eq}} - f_i^{\mathrm{eq}} - \varepsilon f_i^{(1)} - \varepsilon^2 f_i^{(2)} - \cdots\right) \varepsilon\left(\partial_{t_1} + c_{i\alpha}\partial_{1\alpha}\right) f_i^{\mathrm{eq}} + \varepsilon^2\left[\partial_{t_2} f_i^{\mathrm{eq}} + \left(\partial_{t_1} + c_{i\alpha}\partial_{1\alpha}\right) f_i^{(1)}\right]\\
&\quad\quad + \varepsilon^2\frac{1}{2}\left(\partial_{t_1} + c_{i\alpha}\partial_{1\alpha}\right)^2 f_i^{\mathrm{eq}} + o\left(\varepsilon^2\right) = \omega\left(f_i^{\mathrm{eq}} - f_i^{\mathrm{eq}} - \varepsilon f_i^{(1)} - \varepsilon^2 f_i^{(2)} - \cdots\right).
\end{aligned}$$

Comparing the coefficients, we obtain

$$\begin{aligned}
\varepsilon^1 :&\quad \left(\partial_{t_1} + c_{i\alpha}\partial_{1\alpha}\right) f_i^{\mathrm{eq}} = -\omega f_i^{(2)},\\
\varepsilon^2 :&\quad \partial_{t_2} f_i^{\mathrm{eq}} + \frac{1}{2}\left(\partial_{t_1} + c_{i\alpha}\partial_{1\alpha}\right)^2 f_i^{\mathrm{eq}} + \left(\partial_{t_1} + c_{i\alpha}\partial_{1\alpha}\right) f_i^{(1)} = -\omega f_i^{(2)}.
\end{aligned}$$

A3. The derivation of Eq. (23)

For the derivation of Euler equation, only ε^1 scale is studied,

$$\left(\partial_{t_1} + c_{i\alpha}\partial_{1\alpha}\right) f_i^{\mathrm{eq}} = -\omega f_i^{(1)}. \tag{A2}$$

Based on Eqs. (17), (18), and (19), we obtain

$$\begin{aligned}
&\frac{D}{2}\rho\theta = \sum_i \frac{1}{2}\left(\boldsymbol{c}_i - \boldsymbol{u}\right)^2 f_i = \sum_i \frac{1}{2}\left(\boldsymbol{c}_i - \boldsymbol{u}\right)^2 f_i^{\mathrm{eq}},\\
&\frac{D}{2}\rho\theta = \sum_i \frac{1}{2}c_i^2 f_i - \sum_i u_\alpha c_{i\alpha} f_i + \sum_i \frac{1}{2}u^2 f_i = \sum_i \frac{1}{2}c_i^2 f_i^{\mathrm{eq}} - \sum_i u_\alpha c_{i\alpha} f_i^{\mathrm{eq}} + \sum_i \frac{1}{2}u^2 f_i^{\mathrm{eq}},\\
&\frac{D}{2}\rho\theta = \sum_i \frac{1}{2}c_i^2 f_i - u_\alpha \sum_i c_{i\alpha} f_i + \frac{1}{2}u^2 \sum_i f_i = \sum_i \frac{1}{2}c_i^2 f_i^{\mathrm{eq}} - u_\alpha \sum_i c_{i\alpha} f_i^{\mathrm{eq}} + \frac{1}{2}u^2 \sum_i f_i^{\mathrm{eq}},
\end{aligned}$$

$$\frac{D}{2}\rho\theta = \sum_i \frac{1}{2}c_i^2 f_i - u_\alpha \sum_i \boldsymbol{c}_{i\alpha} f_i + \frac{1}{2}u^2 \sum_i f_i = \sum_i \frac{1}{2}c_i^2 f_i^{\rm eq} - u_\alpha \sum_i c_{i\alpha} f_i^{\rm eq} + \frac{1}{2}u^2 \sum_i f_i^{\rm eq},$$
$$\frac{D}{2}\rho\theta = \sum_i \frac{1}{2}c_i^2 f_i - \rho u^2 + \frac{1}{2}\rho u^2 = \sum_i \frac{1}{2}c_i^2 f_i^{\rm eq} - \rho u^2 + \frac{1}{2}\rho u^2,$$
$$\frac{D}{2}\rho\theta = \sum_i \frac{1}{2}c_i^2 f_i - \frac{1}{2}\rho u^2 = \sum_i \frac{1}{2}c_i^2 f_i^{\rm eq} - \frac{1}{2}\rho u^2.$$

Then we obtain

$$\frac{D}{2}\rho\theta + \frac{1}{2}\rho u^2 = \sum_i \frac{1}{2}c_i^2 f_i = \sum_i \frac{1}{2}c_i^2 f_i^{\rm eq}, \tag{A3}$$

$$0 = \sum_i \frac{1}{2}c_i^2 f_i^{(1)}. \tag{A4}$$

Take the D2Q9 model for example, based on Eq. (14), we obtain

$$f_i^{\rm eq} = w_i\rho\left[1 + \frac{3\left(\boldsymbol{c}_i\cdot\boldsymbol{u}\right)}{c^2} + \frac{9\left(\boldsymbol{c}_i\cdot\boldsymbol{u}\right)^2}{2c^4} - \frac{3u^2}{2c^2}\right].$$

Then the calculation is as follows:

$$\begin{aligned}\sum_i c_{i\alpha}c_{i\beta}c_{i\gamma}f_i^{\rm eq} &= \sum_i c^3 e_{i\alpha}e_{i\beta}e_{i\gamma}f_i^{\rm eq} = \sum_i 3\rho c^2 w_i e_{i\alpha}e_{i\beta}e_{i\gamma}e_{i\theta}u_\theta = 3c^2\rho\sum_i w_i e_{i\alpha}e_{i\beta}e_{i\gamma}e_{i\theta}u_\theta \\ &= 3c^2\rho\Big[\frac{1}{9}\times 2\delta_{\alpha\beta\gamma\theta}u_\theta + \frac{1}{36}\times 4\left(\delta_{\alpha\beta}\delta_{\gamma\theta}+\delta_{\alpha\gamma}\delta_{\beta\theta}+\delta_{\alpha\theta}\delta_{\gamma\beta}\right)u_\theta - \frac{1}{36}\times 8\delta_{\alpha\beta\gamma\theta}u_\theta\Big] \\ &= \frac{1}{3}c^2\rho\left(\delta_{\alpha\beta}\delta_{\gamma\theta}+\delta_{\alpha\gamma}\delta_{\beta\theta}+\delta_{\alpha\theta}\delta_{\gamma\beta}\right)u_\theta = \rho\theta\left(u_\alpha\delta_{\beta\gamma}+u_\beta\delta_{\gamma\alpha}+u_\gamma\delta_{\alpha\beta}\right).\end{aligned}$$

Then we obtain

$$\sum_i c_i^2 c_{i\alpha} f_i^{\rm eq} = \sum_i c_{i\alpha}c_{i\beta}c_{i\beta}f_i^{\rm eq} = (D+2)\,\rho\theta u_\alpha. \tag{A5}$$

Based on Eq. (A1), we obtain

$$\begin{aligned}&\left(\partial_t + c_{i\alpha}\partial_\alpha\right) f_i^{\rm eq} = -\omega f_i^{(1)}, \\ &\partial_t\left(\sum_i \frac{1}{2}c_i^2 f_i^{\rm eq}\right) + \partial_\alpha\left(\sum_i \frac{1}{2}c_i^2 c_{i\alpha} f_i^{\rm eq}\right) \\ &\quad = -\omega\sum_i \frac{1}{2}c_i^2 f_i^{(1)}.\end{aligned}$$

Based on Eqs. (A3), (A4), (A5), we obtain

$$\partial_{t_1}\left(\frac{D}{2}\rho\theta + \frac{1}{2}\rho u^2\right) + \partial_{1\alpha}\left(\frac{D+2}{2}\rho\theta u_\alpha\right) = 0. \tag{A6}$$

Multiplying Eq. (A6) by ε, we can obtain Eq. (23).

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