A coupled lattice Boltzmann model for thermal flows

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We present a coupled lattice Boltzmann method (LBM) for thermal viscous flows based on a two relaxation times kinetic model. The method is directly derived by projecting the coupled kinetic model equations for the distribution functions onto the tensor Hermite polynomials following Grad’s moment expansion method. By choosing a proper reference velocity, the coupling of lattice velocities and the local temperature is avoided and the resultant method is consistent with the original kinetic model. The intrinsic discrete nodes of the Gauss–Hermite quadrature provide the natural lattice velocities for the thermal LBM. Simulations of 2D natural convection flows are shown. The numerical results agree well with the previous benchmark data.

Keywords: thermal lattice Boltzmann; double distribution function; natural convection.

1. Introduction

In recent years, the lattice Boltzmann method (LBM) has achieved a great success in simulating fluid flow. However, the thermal LBM is still a challenge as reported in Lallemand & Luo (2003). The existing thermal LBMs can be classified into three categories. The first category is the passive-scalar approach (Shan, 1997) and the basic approach of this method is to assume that the viscous heat dissipation and the compression work done by the pressure can be neglected. As a consequence, the temperature can be simulated by a scalar density distribution function. The other two categories include the multi-speed distribution function approach (Alexander et al., 1993; Chen et al., 1994; Kataoka & Tsutahara, 2004) and the double distribution functions (DDF) approach (He et al., 1998; Peng et al., 2003; Shi et al., 2004; Guo et al., 2007), which comprise two distribution functions for describing flow field. A consistent LB model has been introduced (Ansumali & Karlin, 2005) with energy conservation on the standard lattices and the usual spurious bulk viscosity can be eliminated such that the Navier–Stokes and Fourier equations can be recovered. Later, this consistent LB method is extended (Prasianakis & Karlin, 2007) to allow thermal flow simulation on standard lattice, e.g., D2Q9 for 2D problems. This was done by finding out the deviations due to the lattice constraints D2Q9 model and correcting them in ‘forcing terms’ that are added in standard lattice Boltzmann–Bhatnagar-Gross-Krook (BGK) model. The multi-speed approach is achieved by increasing the numbers of discrete velocities, then, the compressible Navier–Stokes equations can be recovered by those increasing degrees of freedom. Although the multi-speed approach can reach a thermal LBM, but it suffers from severe numerical instability and a narrow range of temperature variation. Moreover, the Prandtl number is usually fixed at constant. On the other hand, the DDF approach utilizes two distribution functions, one is for describing the velocity field and the other for describing the internal energy or total energy. The DDF approach can achieve a better
numerical stability than the multi-speed approach. In He et al. (1998), an alternative thermal lattice Boltzmann equation model was proposed for low Mach number flows in the DDF framework. In the method, both viscous dissipation and compression work have been considered and good simulation results have been obtained, however, the energy equation is decoupled from the momentum equation due to the replacement of the local temperature by the constant reference temperature in the equilibrium distribution functions.

In this work, we derive a thermal LBM which is based on DDF method in which both the Maxwell equilibrium velocity distribution function and a total energy equilibrium distribution function are expanded on tensor Hermite polynomials according to Guo et al. (2007), Shan et al. (2006). By choosing a proper reference velocity, the coupling of lattice velocities and the local temperature is avoided and the uncoupling process between velocity field and temperature field as done in Guo et al. (2007) is not necessary. Thus, some limitations mentioned such as being valid only to small temperature variation and transport coefficients’ independence of temperature can be overcome. We also apply the Chapman–Enskog method to the present coupled thermal lattice Boltzmann–BGK equations to obtain the relations between the relaxation time and viscosity and thermal conductivity. Hydrodynamics based on moments up to third-order expansions are presented. Computational examples to illustrate the methods are given, and the results are carefully studied with the published result (Hortmann et al., 1990).

This paper is organized as follows. In Section 2, the two relaxation times kinetic model is briefly described. In Section 3, expansion of the two distribution functions using Grad’s method (Grad, 1949a,b) is derived. Then, the time discretization is shown in Section 4 and the boundary conditions are described in Section 5. Concluding remarks are given in Section 6. An Appendix on the mathematical details of Chapman–Enskog expansion of the present coupled thermal LBM is also provided.

2. Two relaxation times kinetic model

In this section, we briefly describe the coupled kinetic model equations based on DDFs for the later development of thermal LBM. We adopt the two relaxation times kinetic model equations proposed by He et al. (1998). The DDFs in terms of two relaxation times can be expressed as follows:

\[ \partial_t f + \vec{\xi} \cdot \vec{\nabla}_x f + \vec{a} \cdot \vec{\nabla}_\xi f = -\frac{1}{\tau_f} [f - f^{(0)}], \]

\[ \partial_t h + \vec{\xi} \cdot \vec{\nabla}_x h + \vec{a} \cdot \vec{\nabla}_\xi h = -\frac{1}{\tau_h} [h - h^{(0)}] + \frac{Z}{\tau_{hf}} [f - f^{(0)}] + f \vec{\xi} \cdot \vec{a}, \]

where \( f^{(0)} \) and \( h^{(0)} \) are equilibrium distribution functions and are given by

\[ f^{(0)} = \frac{\rho}{(2\pi RT)^{D/2}} \exp\left[-\frac{c^2}{2RT}\right], \]

\[ h^{(0)} = \frac{\rho \vec{\xi}^2}{2(2\pi RT)^{D/2}} \exp\left[-\frac{c^2}{2RT}\right]. \]

Here, \( f(\vec{\xi}, \vec{x}, t) \) is the usual velocity distribution function, \( h(\vec{\xi}, \vec{x}, t) = \vec{\xi}^2 f/2 \) is the total energy distribution function, \( \vec{\xi} \) is the particle velocity, \( \vec{u} \) the average velocity, \( \vec{c} = \vec{\xi} - \vec{u} \) the peculiar velocity, \( \vec{x} \) the
physical space position, \( \ddot{a} \) the acceleration due to external force and \( t \) is time. In (1) and (2), \( \tau_f \) and \( \tau_h \) are the relaxation times characterizing, respectively, the momentum change and internal energy change during particle collisions and \( \tau_f^{-1} = \tau_h^{-1} + \tau_f^{-1} \), \( Z = \ddot{x} \cdot \ddot{u} - u^2/2 \), where \( \ddot{u}(\dot{x}, t) \) is the mean velocity. In (3) and (4), \( \rho(\dot{x}, t) \) is the density, \( T \) the local temperature, \( R \) the gas constant and \( D \) is the space dimension.

Once the distribution functions \( f \) and \( h \) are known, the macroscopic quantities, e.g., the density \( \rho \) and mean velocity \( \dot{u} \) are defined by

\[
\rho(\dot{x}, t) = \int f \, d\ddot{x},
\]

\[
\rho \ddot{u}(\dot{x}, t) = \int \ddot{x} \, f \, d\ddot{x}.
\]

The internal energy density \( \rho \epsilon \), thus the temperature can be defined either from \( f \) as

\[
\rho \epsilon_f = \frac{1}{2} \int c^2 \, f \, d\ddot{x} , \quad \frac{1}{2} D \rho RT_f = \int f \, c^2 \, d\ddot{x} ,
\]

or from \( h \) as

\[
\frac{1}{2} D \rho RT_h = \rho \epsilon_h = \int h \, d\ddot{x} - \frac{\rho u^2}{2} .
\]

The temperature of the fluid is calculated as the average of \( T_f \) and \( T_h \), namely, \( T = (T_f + T_h)/2 \) and the fluid pressure is given by the equation of state, \( p = \rho RT \).

We note here that the temperature is obtained by taking average of \( T_f \) and \( T_h \) which allows some coupling of the momentum and energy transport and exhibits good numerical stability. We should make sure that the difference between the temperatures coming from two distribution functions is small and approaches zero when the steady state is achieved. We also note, in the past, recognizing that the momentum and energy should have different transport time scales during the collision process, two relaxation times were introduced into the non-equilibrium distribution function and adjustable physically correct Prandtl number can be obtained (Woods, 1993). Through the Chapman–Enskog expansion of the two relaxation time kinetic model equations, the thermal hydrodynamic equations at the compressible Navier–Stokes level can be obtained

\[
\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \dot{u}) = 0 ,
\]

\[
\frac{\partial}{\partial t} (\rho \dot{u}) + \nabla \cdot (\rho \ddot{u} \dot{u}) = -\nabla p + \nabla \cdot \ddot{\tau} + \rho \ddot{a} ,
\]

\[
\frac{\partial}{\partial t} (\rho E) + \nabla \cdot [(\rho + \rho E) \ddot{u}] = \nabla \cdot (\kappa \nabla T) + \nabla \cdot (\tau \cdot \ddot{u}) + \rho \ddot{u} \cdot \ddot{a} ,
\]

where \( \ddot{\tau} = \mu [\nabla u + (\nabla u)^\top] - (2/D)(\ddot{\tau}) \) \( \ddot{\tau} \) is the viscous stress tensor. The transport coefficients viscosity \( \mu \) and thermal conductivity \( \kappa \) are given, respectively, by

\[
\mu = \tau_f p , \quad \kappa = c_v \tau_h p ,
\]

where \( c_p = (D + 2)R/2 \) is the specific heat ratio at constant pressure. The Prandtl number of the kinetic system is \( \text{Pr} = \mu c_p / \kappa = \gamma \tau_f / \tau_h \) and can be made arbitrary by tuning the two relaxation times.
Introduce the characteristic (or reference) length $L$, time $t_0$ and velocity $c_0 = \sqrt{RT_0}$ scales, where $T_0$ is a reference temperature and with $t_0 = L/c_0$, we have the dimensionless quantities as follows:

\[
\begin{align*}
\hat{x} &= \frac{x}{L}, \quad (\hat{\zeta}, \hat{u}, \hat{c}) = \left( \frac{\zeta}{c_0}, \frac{u}{c_0}, \frac{c}{c_0} \right), \\
\hat{t} &= \frac{t}{(L/c_0)}, \quad (\hat{\tau}_f, \hat{\tau}_h) = \left( \frac{\tau_f}{L/c_0}, \frac{\tau_h}{L/c_0} \right),
\end{align*}
\]

(13)

Substituting the above dimensionless variables into the (1) and (2), it is straightforward to find that the resulting governing kinetic equations become dimensionless and remain unchanged in form and the equilibrium distribution functions, $\hat{f}^{(0)}$ and $\hat{h}^{(0)}$ are given by

\[
\hat{f}^{(0)} = \frac{\hat{\rho}}{(2\pi \hat{\theta})^{D/2}} \exp\left[-\frac{\hat{\zeta}^2}{2 \hat{\theta}}\right], \quad \hat{h}^{(0)} = \frac{\hat{\zeta}^2}{2} \hat{f}^{(0)},
\]

(14)

where $\theta \equiv RT$ and $\hat{\theta} \equiv RT/c_0^2$.

3. The lattice discrete velocity model

To derive a Lattice Boltzmann Equation (LBE) method for the above two relaxation times kinetic model, we first need a discrete velocity model (DVM) that discretizes the velocity space of the continuous kinetic equations into a set of discrete velocities and then the LBE method is obtained by discretizing the temporal and spatial derivations of the DVM, using standard numerical methods. The basic requirement for the derivation of discrete velocity set is that the DVM can match the original kinetic model with sufficient accuracy. In this section, we shall present a DVM for thermal flows based on the coupled kinetic model equations.

3.1 Expansions of the equilibrium distribution functions

Following the approach in Shan et al. (2006), we adopt the Grad’s moment expansion approach and seek solutions to (1) and (2) by expanding $f(\vec{x}, \vec{\zeta}, t)$ and $h(\vec{x}, \vec{\zeta}, t)$ in terms of Hermite polynomials,

\[
\begin{align*}
f(\vec{x}, \vec{\zeta}, t) &= \omega(\vec{\zeta}) \sum_{n=0}^{\infty} \frac{1}{n!} a^{(n)}(x, t) \mathcal{H}^{(n)}(\vec{\zeta}), \\
h(\vec{x}, \vec{\zeta}, t) &= \omega(\vec{\zeta}) \sum_{n=0}^{\infty} \frac{1}{n!} b^{(n)}(x, t) \mathcal{H}^{(n)}(\vec{\zeta}),
\end{align*}
\]

(15)

(16)

where

\[
\omega(\vec{\zeta}) = \frac{1}{(2\pi)^{D/2}} e^{-\vec{\zeta}^2/2}
\]

(17)

is the weighting function, $a^{(n)}$, $b^{(n)}$ and $\mathcal{H}^{(n)}(\vec{\zeta})$ are rank-$n$ tensors and the product on the right-hand side denotes full contraction. Here and throughout the manuscript, the shorthand notations of Grad (1949b)
for fully symmetric tensors have been adopted. The expansion coefficients \( a^{(n)}(x, t) \) and \( b^{(n)}(x, t) \) are given by

\[
a^{(n)} = \int f^{(n)}(\xi) d\xi, \quad b^{(n)} = \int h^{(n)}(\xi) d\xi.
\]

Similarly, the two equilibrium distribution functions \( f^{(0),M}(\xi, t) \) and \( h^{(0),N}(\xi, t) \) are also expanded to the same orders as follows:

\[
f^{(0),N}(\xi, t) = \omega(\xi) \sum_{n=0}^{N} \frac{1}{n!} a^{(n)}(x, t) H^{(n)}(\xi),
\]

\[
h^{(0),N}(\xi, t) = \omega(\xi) \sum_{n=0}^{N} \frac{1}{n!} b^{(n)}(x, t) H^{(n)}(\xi).
\]

The expansion coefficients \( a^{(n)}_{0}(x, t) \) and \( b^{(n)}_{0}(x, t) \) are given by

\[
a^{(n)}_{0} = \int f^{(0)} H^{(n)}(\xi) d\xi, \quad b^{(n)}_{0} = \int h^{(0)} H^{(n)}(\xi) d\xi.
\]

Note that with the weighting function, we have

\[
f^{(0)} = \frac{\rho}{(\theta)^{D/2}} \omega \left( \frac{c}{\sqrt{\theta}} \right).
\]

Without causing any confusion, all the \(^*\) signs will be taken off hereinafter and all the velocities should be considered as non-dimensional variables. After a change of variable \( \eta = \frac{c}{\sqrt{\theta}} \), we have

\[
a^{(n)}_{0} = \rho \int \omega(\eta) H^{(n)}(\sqrt{\theta} \eta + \tilde{u}) d\eta.
\]

The Hermite expansion coefficients \( a^{(n)}_{0} \) can be explicitly calculated as

\[
a^{(0)}_{0} = \rho,
\]

\[
a^{(1)}_{0} = \rho \tilde{u},
\]

\[
a^{(2)}_{0} = \rho [\tilde{u} \ddot{u} + (\theta - 1) \delta],
\]

\[
a^{(3)}_{0} = \rho [\tilde{u} \dddot{u} + (\theta - 1) \delta \ddot{u}].
\]

Similarly, the expansion coefficients \( b^{(n)}_{0} \) can be obtained as follows:

\[
b^{(0)}_{0} = \rho E,
\]

\[
b^{(1)}_{0} = (p + \rho E) \tilde{u},
\]

\[
b^{(2)}_{0} = (2p + \rho E) \ddot{u} + (p + \rho E(\theta - 1)) \delta.
\]
3.2 Discretization of velocity space

It is essential to realize that as a partial sum of Hermite series with finite terms, the truncated distribution function can be completely and uniquely determined by its values at a set of discrete abscissae. This is true because with $f$ (or $h$) truncated to order $N$, the integrands on the right-hand side of (15) can be written as

$$f^N(x, \xi, t) = \omega(\xi) p(x, \xi, t), \quad h^N(x, \xi, t) = \omega(\xi) q(x, \xi, t),$$

(26)

where $p(x, \xi, t)$ (or $q(x, \xi, t)$) is a polynomial in $\xi$ of a degree not $>2N$. Using the Gauss-Hermite quadrature, $a^{(n)}$ (or $b^{(n)}$) can be precisely expressed as a weighted sum of the functional values of $p(x, \xi, t)$ (or $q(x, \xi, t)$):

$$a^{(n)} = \int \omega(\xi) p(x, \xi, t) = \sum_{a=1}^{d} w_a p(x, \xi_a, t),$$

$$= \sum_{a=1}^{d} \frac{w_a}{\omega(\xi_a)} f^N(x, \xi_a, t) H^{(n)}(\xi_a),$$

(27)

where $w_a$ and $\xi_a$, $a = 1, 2, ..., d$, are, respectively, the weights and abscissae of a Gauss-Hermite quadrature of a degree $\geq 2N$. Similar expressions can be given for $b^{(n)}$ and $h^N(x, \xi_a, t)$. Hence, the set of discrete distribution function values $f^N(\xi_a)$ and $h^N(\xi_a)$ now serve as a new set of fundamental variables for defining the fluid system in place of the conventional thermohydrodynamic variables. For further details, see Shan et al. (2006). For the 2D problem, we can select the nine-point fifth degree Gauss-Hermite quadrature, which leads to the standard D2Q9 discrete velocities model (Shan et al., 2006). The D2Q9 velocity lattice $\xi_a$ and their corresponding weights $w_a$ are given by

<table>
<thead>
<tr>
<th>$\xi_a$</th>
<th>$w_a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0, 0)</td>
<td>4/9</td>
</tr>
<tr>
<td>$(\sqrt{3}, 0)_{fs}$</td>
<td>1/9</td>
</tr>
<tr>
<td>$(\pm \sqrt{3}, \pm \sqrt{3})$</td>
<td>1/36</td>
</tr>
</tbody>
</table>

Here, the subscript $fs$ denotes a fully symmetric set of points.

After obtaining $a^{(n)}$ and $b^{(n)}$, we can calculate $f_a^{(0),N}$ and $h_a^{(0),N}$ from (19) and (20). For $N = 3$ in velocity distribution function and $N = 2$ in total energy distribution function, we get the explicit Hermite expansion of these two distribution functions at the discrete velocities $\xi_a$ as follows:

$$f_a^{(0),3} = \omega_a \rho \left[ 1 + u_a + \frac{u_a^2}{2} - \frac{u^2}{2} + (\theta - 1) \frac{(\xi_a^2 - D)}{2} \right. \left. + \frac{\rho u_a}{6} \left[ u_a^2 - 3u^2 + 3(\theta - 1)(\xi_a^2 - D) - 2 \right] \right],$$

(28)
\[ h_a^{(0),2} = \omega_a \rho \left\{ E + \left( \frac{p}{\rho} + E \right) u_a + \left( \frac{p + E}{2} \right) (u_a^2 - u^2) + \frac{p}{2\rho} (\dot{\xi}_a^2 - D) + \frac{E}{2} (\theta - 1)(\dot{\xi}_a^2 - D) \right\} \]

\[ = \omega_a \rho \left[ u_a + u_a^2 - u^2 + \frac{1}{2}(\dot{\xi}_a^2 - D) \right] + Ef^{(0),2}, \quad (29) \]

where \( u_a = \dot{\xi}_a \cdot \hat{u}, \) \( D = \delta_{ii} \) and \( f^{(0),2} \) are the expansion of \( f^{(0)} \) to \( N = 2 \) order,

\[ f_a^{(0),2} = \omega_a \rho \left\{ 1 + u_a + \frac{u_a^2 - u^2}{2} + \frac{1}{2}(\dot{\xi}_a^2 - D) \right\}. \quad (30) \]

The governing equations for the coupled lattice Boltzmann–BGK method are

\[ \dot{c}_t f_a + \ddot{\xi}_a \cdot \nabla \hat{x}_a f_a = -\frac{1}{\tau_f} [f_a - f_a^{(0),3}] + F_a, \quad (31) \]

\[ \dot{c}_t h_a + \ddot{\xi}_a \cdot \nabla \hat{x}_a h_a = -\frac{1}{\tau_h} [h_a - h_a^{(0),2}] + \frac{Z_a}{\tau_{hf}} [f_a - f_a^{(0),3}] + q_a, \quad (32) \]

where \( F_a \) and \( q_a \) are given respectively, by

\[ F_a = \omega_a \rho (\ddot{\xi} \cdot \hat{a} + (\ddot{\xi}_a \cdot \hat{a})(\ddot{\xi}_a \cdot \hat{u}) - \ddot{\xi} \cdot \ddot{u}), \quad (33) \]

\[ q_a = \omega_a \rho \left[ \frac{E}{2} \dot{\xi}_a \cdot \hat{a} + f_a \ddot{\xi}_a \cdot \hat{a} \right], \quad (34) \]

come from the similar procedures expanding the forcing terms onto Hermite polynomials.

At this stage, some notes are in order. First, we note that the above development follows closely the works presented in Shan et al. (2006). The model presented here is a coupled LBM, that is, the local temperature \( \theta = RT \) appears in both equilibrium velocity distribution function \( f_a^{(0),3} \) and equilibrium total energy distribution function \( h_a^{(0),2} \), as also mentioned in Shan et al. (2006) and Philippi et al. (2006), by choosing a proper reference velocity \( c_0 = \sqrt{\Omega_0} \), the particle velocity \( \ddot{\xi} \) depends on a constant \( c_0 \) but not on the local temperature \( \theta \) and the resultant DVM is consistent with the original kinetic model where the particle velocity, \( \ddot{\xi}, \hat{x} \) and \( \hat{t} \) are independent variables. Second, in Guo et al. (2007), the zeroth- and first-order moments of \( f^{(eq),2}(T_0) \) and the zeroth-order moment of \( h^{(eq),2}(T_0) \) in their (36a) and (36b) are the same as those of the equilibrium distribution functions with local temperature \( T \), however, the higher-order moments required in the derivation of the thermal Navier–Stokes equations are different when one replaces the local temperature \( T \) by \( T_0 \) in their (36a) and (36b). Third, with our formulation, the conventional lattice Boltzmann scheme still can be used, and we do not need to uncouple (28) and (29) as described in Guo et al. (2007).

4. Time and spatial discretizations

The detailed descriptions of the time discretization of thermal LBM based on DDF can be found in Guo et al. (2007). First, integrating the (31) along the characteristic line, one has

\[ f_a(x + c_a b\xi, t + \delta t) - f_a(x, t) = \int_0^{\delta t} \left[ \Omega f(x + c_a b\xi', t + t') + F_a(x + c_a b\xi', t + t') \right] \, dt', \quad (35) \]
where $\delta_t$ is the time step and $\Omega_f = (f_a^{(0),3} - f_a)/\tau_f$. Then, applying trapezoidal rule to the integral, one leads to

$$f_a(x + c_a\delta_t, t + \delta_t) - f_a(x, t) = \frac{\delta_t}{2} [\Omega_f(x + c_a\delta_t, t + \delta_t) + F_a(x + c_a\delta_t, t + \delta_t)]$$

$$+ \frac{\delta_t}{2} [\Omega_f(x, t) + F_a(x, t)]. \quad (36)$$

Introduce the following distribution function:

$$\bar{f}_a = f_a - \frac{\delta_t}{2} (\Omega_f + F_a). \quad (37)$$

Then, one can get

$$f_a - f_a^{(0),3} = \frac{\bar{f}_a - f_a^{(0),3} + \frac{\delta_t}{2} F_a}{1 + \frac{\delta_t}{2\tau_f}}, \quad (38)$$

$$\bar{f}_a - f_a = -\frac{\delta_t}{2} (\Omega_f + F_a). \quad (39)$$

From above equations, one obtains the governing equation of distribution function with time discretization,

$$\bar{f}_a(x + c_a\delta_t, t + \delta_t) - \bar{f}_a(x, t) = -\omega_f [\bar{f}_a(x, t) - f_a^{(0),3}(x, t)]$$

$$+ \delta_t \left( 1 - \frac{\omega_f}{2} \right) F_a, \quad (40)$$

where $\omega_f = \frac{1}{\tau_f}$. The macroscopic density $\rho$ and velocity $\bar{u}$ are determined by

$$\rho = \sum_a \bar{f}_a, \quad (41)$$

$$\rho \bar{u} = \sum_a c_a \bar{f}_a + \frac{\delta_t}{2} \rho \bar{a}, \quad (42)$$

$$\frac{D}{2} \rho RT_f = \sum_a c_a^2 \bar{f}_a. \quad (43)$$

By the similar procedures, the governing equation of total energy distribution function with time discretization is shown as following together with the determination of the total energy. Similar to (40), we have

$$\bar{h}_a(x + c_a\delta_t, t + \delta_t) - \bar{h}_a(x, t) = -\omega_h [\bar{h}_a(x, t) - h_a^{(0),2}(x, t)] + \delta_t \left( 1 - \frac{\omega_h}{2} \right) q_a$$

$$+ (\omega_h - \omega_f) Z_a \left( \bar{f}_a(x, t) - f_a^{(0),2}(x, t) + \frac{\delta_t}{2} F_a \right), \quad (44)$$

where $\omega_h = \frac{1}{\tau_h}$ can be calculated from Prandtl number as $Pr = \gamma \frac{\tau_f - 0.5}{\tau_h - 0.5}$ once $\tau_f$ has been determined as described in Appendix. Also note that

$$\bar{h}_a = h_a - \frac{\delta_t}{2} (\Omega_h + F_a). \quad (45)$$
The determination of $T_h$ can be found by
\[
\frac{D}{2} \rho RT_h = \sum_a \bar{h}_a + \frac{\delta_t}{2} \rho \bar{u} \cdot \bar{a}.
\] (46)

With $T_f$ and $T_h$, we determine the temperature $T = (T_f + T_h)/2$ and the pressure $p = \rho RT$ and return these values back to (28)–(30).

After the time is discretized, we now come to the discretization of space. For the 2D case and with D2Q9 model, we can employ the existing standard LBE method and the lattice spacing is chosen to be $\delta_x = c \delta_t$, where $c = \sqrt{RT_0}$.

A comparison is made here between the present coupled thermal method and the decoupled method of Guo et al. (2007). First, we note that both models share many similar features, e.g., to have the same kinetic model equations with two relaxation time concept and to allow variable Prandtl number. Second, the differences between the two models are also apparent, namely, in their model, the local temperature $T$ in the truncated equilibrium distribution functions are replaced by a reference constant temperature $T_0$ resulting in a decoupled set of kinetic equations, while our model is a coupled set and the coupling of lattice velocity and temperature is avoided by choosing a proper reference velocity. As a consequence, our model is not limited by the Boussinesq assumption.

5. Boundary conditions and Buoyancy force

The required wall boundary conditions in this case include isothermal walls, adiabatic walls and no-slip boundary conditions. In order to transform macroscopic variables’ boundary conditions to that of the distribution functions, we apply non-equilibrium boundary condition as described in Guo et al. (2007). In this method, the distribution function is separated into equilibrium and non-equilibrium parts, where the equilibrium part is determined by the macroscopic variables, and the non-equilibrium part is determined by that of the distribution function at the nearest neighbour node in the fluid region. According to this approach, the distribution function $f_a(x_b)$ can be assigned new values by setting $u_b = 0$, and for an adiabatic wall, $\theta_b = \theta_f$, for an isothermal wall, $\theta_b = \theta_H$ or $\theta_b = \theta_L$. Here, $\theta_H$ means the high temperature at the isothermal wall and $\theta_L$ means the low temperature one. Finally, the distribution functions on the boundary points are calculated as follows:

\[
\begin{align*}
  f_a(x_b) &= f_a^{(0),3}(x_b, u_b, \theta_b) + [f_a(x_f) - f_a^{(0),3}(x_f)], \\
  h_a(x_b) &= h_a^{(0),2}(x_b, u_b, \theta_b) + [h_a(x_f) - h_a^{(0),2}(x_f)],
\end{align*}
\]

where $\rho_b, \theta_b$ and $u_b$ denote the hydrodynamic variables at the boundary points and $\rho_f, \theta_f$ and $u_f$ denote the corresponding ones at the nearest neighbourhood. In natural convection flows, the buoyancy force is an important mechanism that drives the flow movement. The Boussinesq approximation assumes that the temperature difference between two isothermal sides is small in comparison with the average temperature ($\theta_H + \theta_L)/2$ such that the density is changing with temperature variations via $\rho = \rho_0[1 - \beta(T - T_0)]$. Multiplying $\rho$ by the gravity acceleration $\bar{g}$, we get $\rho \bar{g} = \rho_0 \bar{g} - \rho_0 \bar{g} \beta(T - T_0)$. After absorbing the constant part $\rho_0 \bar{g}$ into the pressure, the external force becomes

\[
\rho \bar{a} = -\rho_0 \bar{g} \beta(T - T_0).
\]
It is noted that the pressure now is the dynamic part \( \tilde{\rho} = p - \rho_0 g y \), with \( g \) being the magnitude of gravity and \( y \) the coordinate opposite to the gravity force.

6. Results and discussion

In this section, we apply the present thermal LBE method to natural convection flows in a square cavity and Rayleigh–Benard convection. Before doing the simulations, we note that the local temperature \( \theta = RT \) is coupled in both the equilibrium velocity distribution function \( f^{(0)} \) and the equilibrium total energy distribution function \( h^{(0)} \), since the numerical case is low speed flow, we can average the local temperature computed from velocity distribution function and the total energy distribution function, respectively.

6.1 Natural convection in a square cavity

First, we carried out the simulation for a natural convection in a 2D square cavity with sidewalls maintained at different temperatures. The temperature difference between the walls induces a temperature gradient in the fluid and the consequent density variations induce the fluid motion. A boundary treatment using the non-equilibrium exploration boundary conditions proposed in Guo et al. (2007) is applied. On the left and right sides of the cavity, the isothermal boundary conditions with \( \theta_{\text{left}} = \theta_H \), \( \theta_{\text{right}} = \theta_L \) are applied. On the top and bottom sides of the cavity, the adiabatic boundary conditions are applied. No-slip conditions \( \vec{u} = 0 \) are set on the four sides. The convection flow induced by the temperature difference is characterized by the Prandtl number \( Pr = \frac{c_p \mu}{\kappa} \) and Rayleigh number \( Ra = \frac{g \beta \Delta T H^3 Pr}{\nu^2} \), where \( \Delta T = T_H - T_L \) is the temperature difference or we can represent \( Ra \) number as \( Ra = \frac{g \beta \Delta T H^3 Pr}{T_0 \nu^2} = \frac{g \hat{\beta} \Delta \theta H^3 Pr}{\theta_0 \nu^2} \), where \( T_0 \) is the reference temperature and \( \hat{\beta} = T_0 \beta \). The grid system used is 129 x 129 for \( Ra = 10^3 \) and \( Ra = 10^4 \) and 257 x 257 for \( Ra = 10^5 \). We set \( \theta_H = 1.04 \) and \( \theta_L = 1.0 \). The initial temperature is set at \( (\theta_H + \theta_L)/2 \) and initial density is \( \rho = 1.0 \). Note that there are three unknowns \( \tau_f \), \( \tau_h \) and \( \beta \) relating to two parameters \( Pr \) and \( Ra \). We set \( \frac{1}{\tau_f} = 1.5 \) in all cases, then the \( \tau_h \) and \( \beta \) can be determined once the Prandtl number and Rayleigh number are specified. Here, we set \( Pr = 0.71 \). The streamline patterns for several Rayleigh numbers are shown in Fig. 1. With the increase of the Rayleigh number, the fluid motion becomes stronger because of the larger buoyancy. The heat is transferred mainly by conduction at small Rayleigh number and by convection at large Rayleigh number. For low Rayleigh number, a vortex appears at the centre. As Rayleigh number increases, the vortex tends to become elliptic and breaks up into two vortices at \( Ra = 10^5 \). Similarly, the results for isothermal lines are shown in Fig. 2. The isothermal lines are nearly vertical at small Rayleigh number and become horizontal at large Rayleigh number. To quantify the results, we define the average Nusselt

\[
\text{Fig. 1. Streamlines of natural convection for different Rayleigh numbers. (a) } Ra = 10^3, \text{ (b) } Ra = 10^4 \text{ and (c) } Ra = 10^5.
\]
784 L.-H. HUNG AND J.-Y. YANG

Fig. 2. Isotherms of natural convection for different Rayleigh numbers. (a) $Ra = 10^3$, (b) $Ra = 10^4$ and (c) $Ra = 10^5$.

TABLE 1 Comparisons of the average Nusselt number and the maximum velocity components across the cavity centre. The data in parentheses are the locations of the maxima.

<table>
<thead>
<tr>
<th>Ra</th>
<th>Nu ave</th>
<th>$u_{\text{max}}(y)$</th>
<th>$v_{\text{max}}(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>Present</td>
<td>1.1194</td>
<td>3.5519 (0.8203)</td>
</tr>
<tr>
<td></td>
<td>Guo et al. (2002)</td>
<td>1.1168</td>
<td>3.6554 (0.8125)</td>
</tr>
<tr>
<td>$10^4$</td>
<td>Present</td>
<td>2.2015</td>
<td>15.7489 (0.8203)</td>
</tr>
<tr>
<td></td>
<td>Hortmann et al. (1990)</td>
<td>2.2442</td>
<td>16.1802 (0.8265)</td>
</tr>
<tr>
<td>$10^5$</td>
<td>Present</td>
<td>4.5327</td>
<td>34.4184 (0.8477)</td>
</tr>
<tr>
<td></td>
<td>Hortmann et al. (1990)</td>
<td>4.5216</td>
<td>34.7399 (0.8558)</td>
</tr>
</tbody>
</table>

number as $Nu_{\text{ave}} = 1 + < u_x T > \frac{H}{\chi(T_H - T_L)} = 1 + < u_x \theta > \frac{H}{\chi(\theta_H - \theta_L)}$, where $< \cdot >$ means the system average, and $\chi = \frac{\kappa}{\rho c_p}$ is the thermal diffusivity. We also calculate the maximum velocities along the horizontal and vertical lines through the cavity centre. The results are listed in Table 1 together with previous data. Our present simulations are able to illustrate and explore the manifestation of the effect of thermal Navier–Stokes flows. All these results are in good agreement with those reported in Guo et al. (2007).

6.2 Rayleigh–Bénard thermal convection

Next, we also consider the Rayleigh–Bénard convection flow which is a classical benchmark on thermal LB models. The calculation of Rayleigh–Bénard convection is similar to the natural convection case. The fluid is enclosed between two parallel stationary walls with hot (bottom) and cold (top) temperatures and subjected to the gravitational force. Density variations induced by the temperature difference will drive the flow and the viscous force will counteract to balance it. The calculation domain is set as 200 × 100 lattices, the top and bottom sides are set at the isothermal boundary conditions that are $\theta_L$ and $\theta_H$ corresponding to low temperature and high temperature accordingly. The $x$-direction is set with periodical boundary conditions. The simulations correspond to three different $Ra$ number which are $Ra = 4000$, $Ra = 1000$ and $Ra = 50000$. We set $\theta_H = 1.04$ and $\theta_L = 1.0$. The initial temperature is set at $(\theta_H + \theta_L)/2$ and initial density is $\rho = 1.0$. We set $\frac{1}{\tau_f} = 1.5$ and $Pr = 0.71$ in all cases, then the $\tau_h$ and $\beta$ can be determined once the Prandtl number and Rayleigh number are specified just as described above. Top and bottom walls are applied by isothermal boundary condition, and left and right walls are applied by periodical boundary conditions. The streamlines and isotherms patterns for several Rayleigh numbers are shown in Fig. 3. With the increase of the Rayleigh number, the fluid motion becomes
stronger because of the larger buoyancy. The heat is transferred mainly by conduction at small Rayleigh number and by convection at large Rayleigh number.

7. Concluding remarks

To conclude, a new coupled thermal LBM based on DDFs with two relaxation times is derived for thermohydrodynamic Navier–Stokes equations. The method is obtained by first projecting the governing two relaxation time kinetic model equations onto the Hermite polynomial basis as pioneered by Shan et al. (2006) and Guo et al. (2007). The approximate lattice equilibrium distribution functions of lattice Boltzmann equations for simulating thermal viscous flows are derived through expanding both the equilibrium velocity distribution and the equilibrium total energy distribution onto Hermite polynomial basis which is done in an a priori manner and is freedom of usual ad hoc parameter matching. The present work can be considered as an extension and generalization of the work of Shan et al. (2006) and Guo et al. (2007) for simulating thermal viscous flows and shares equally many desirable properties such as free of drawbacks in conventional higher-order hydrodynamic formulations and variable Prandtl number. Moreover, by choosing a proper reference velocity, the coupling of lattice velocities and local temperature can be avoided and our development is derived without limitations in the work of Guo et al. (2007). Several 2D natural convection flows have been simulated and the results are accurate and stable and are in good agreement with the published results. Lastly, the present development of thermal LBM provides a coupled framework for simulating thermohydrodynamic flows.

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Appendix A. The thermohydrodynamic equations of the DVM

Although the development of this Appendix is similar to Appendix B of Guo et al. (2007), there are several key differences in the resulting equations in various places due to the difference between the decoupling approach of Guo et al. (2007) and the present coupling one. We give the detailed derivations below and point out the difference when it is appropriate.

We compute all the following summations by the Maxwell equilibrium distribution function (28) and total energy distribution function (29).

\[ \sum_a f_a^{(0),3} = \rho, \]  

(A.1)
\[
\sum_a \varepsilon_a f_a^{(0),3} = \rho \ddot{u}, \quad (A.2)
\]
\[
\sum_a \varepsilon_a \varepsilon_a f_a^{(0),3} = p \ddot{\delta} + \rho \ddot{u}, \quad (A.3)
\]
\[
\sum_a \varepsilon_a \varepsilon_a \varepsilon_a f_a^{(0),3} = p [\ddot{u} t]_s \quad (A.4)
\]
\[
\sum_a \varepsilon_a h_a^{(0),2} = (p + \rho E) \ddot{u}, \quad (A.5)
\]
\[
\sum_a \varepsilon_a \varepsilon_a h_a^{(0),2} = p (1 + E) \ddot{\delta} + (2p + \rho E) \ddot{u}, \quad (A.6)
\]

where \( \delta \) is the Kronecker delta with two indices. It is noted that the pressure \( p \) is not constant as that in Guo et al. (2007). Also due to the difference in \( \sum_a \varepsilon_a \varepsilon_a h_a^{(0),2} \), in the following, where this term appears will cause difference.

Introduce the following expansions:

\[
f_a \simeq f_a^{(0)} + \varepsilon f_a^{(1)} + \varepsilon^2 f_a^{(2)} + \cdots
\]
\[
h_a \simeq h_a^{(0)} + \varepsilon h_a^{(1)} + \varepsilon^2 h_a^{(2)} + \cdots
\]
\[
F_a = \varepsilon F_a^{(1)}, \quad q_a = \varepsilon q_a^{(1)} + \varepsilon^2 q_a^{(2)} + \cdots
\]
\[
t_1 = t \varepsilon, \quad t_2 = t \varepsilon^2, \quad r_1 = r \varepsilon,
\]

such that the time and space derivative are expressed as

\[
\tilde{\varepsilon}_t = \varepsilon \tilde{\varepsilon}_t + \varepsilon^2 \tilde{\varepsilon}_t,
\]
\[
\ddot{\varepsilon} = \varepsilon \ddot{\varepsilon}_1.
\]

The above expressions of the derivatives are substituted into (31) and (32), and terms involving different orders of \( \varepsilon \) are separated as

\[
\varepsilon^0: f_a^{(0)} = f_a^{(0),3}, \quad (A.7)
\]
\[
\varepsilon^1: \tilde{\varepsilon}_t f_a^{(0)} + \varepsilon \tilde{\varepsilon}_t V_1 f_a^{(0)} = -\frac{1}{\tau f} f_a^{(1)} + F_a^{(1)}, \quad (A.8)
\]
\[
\varepsilon^2: \tilde{\varepsilon}_t f_a^{(0)} + \varepsilon \tilde{\varepsilon}_t f_a^{(1)} + \varepsilon \tilde{\varepsilon}_t V_1 f_a^{(1)} = -\frac{1}{\tau f} f_a^{(2)}, \quad (A.9)
\]

and

\[
\varepsilon^0: h_a^{(0)} = h_a^{(0),2}, \quad (A.10)
\]
\[
\varepsilon^1: \tilde{\varepsilon}_t h_a^{(0)} + \varepsilon \tilde{\varepsilon}_t V_1 h_a^{(0)} = -\frac{1}{\tau h} h_a^{(1)} + \frac{Z a}{\tau_{hf}} f_a^{(1)} + q_a^{(1)}, \quad (A.11)
\]
\[
\varepsilon^2: \tilde{\varepsilon}_t h_a^{(0)} + \varepsilon \tilde{\varepsilon}_t h_a^{(1)} + \varepsilon \tilde{\varepsilon}_t V_1 h_a^{(1)} = -\frac{1}{\tau h} h_a^{(2)} + \frac{Z a}{\tau_{hf}} f_a^{(2)} + q_a^{(2)}. \quad (A.12)
\]
From the above equations, we have
\[ f_a^{(0)} = f_a^{(0)3}, \quad h_a^{(0)} = h_a^{(0)2}, \]
\[ \sum_a F_a = 0, \quad \sum_a \tilde{\zeta} a F_a = \rho \tilde{a}, \quad \sum_a \tilde{\zeta} a \tilde{\zeta} a F_a = \rho [\tilde{a} \bar{u}]_s, \]
\[ \sum_a q_a = \rho \tilde{u} \cdot \tilde{a}, \quad \sum_a \tilde{\zeta} a q_a = (\rho E \tilde{I} + \tilde{I}^2) \cdot \tilde{a}, \]
\[ \sum_a f_a^{(l)} = 0, \quad \sum_a f_a^{(l) \tilde{z} a} = 0, \quad (l \geq 1), \]
\[ \sum_a h_a^{(l)} = 0, \quad \sum_a h_a^{(l) \tilde{z} a} = 0, \quad (l \geq 1), \]
where \( \tilde{I} = \sum a \tilde{z} a \tilde{z} a f_a. \)

From (A.8) and (A.11), we obtain the following first-order thermal hydrodynamic equations:
\[ \partial_t \rho + \tilde{V}_1 \cdot (\rho \tilde{u}) = 0, \quad (A.13) \]
\[ \partial_t (\rho \tilde{u}) + \tilde{V}_1 \cdot (\rho \tilde{u}\tilde{u} + \rho \tilde{I}) = \rho \tilde{a}_1, \quad (A.14) \]
\[ \partial_t (\rho E) + \tilde{V}_1 \cdot ((\rho + E)\tilde{u}) = \rho \tilde{u} \cdot \tilde{a}_1. \quad (A.15) \]

From (A.9) and (A.12), we get the following second-order thermal hydrodynamic equations:
\[ \partial_{t_2} \rho = 0, \quad (A.16) \]
\[ \partial_{t_2} (\rho \tilde{u}) + \tilde{V}_1 \cdot \tilde{I}^{(1)} = 0, \quad (A.17) \]
\[ \partial_{t_2} (\rho E) + \tilde{V}_1 \cdot \tilde{Q}^{(1)} = 0, \quad (A.18) \]
wherein, \( \tilde{I}^{(1)} = \sum a \tilde{z} a \tilde{z} a f_a^{(1)} \), and \( \tilde{Q}^{(1)} = \sum a \tilde{z} a h_a^{(1)}. \) To calculate \( \tilde{I}^{(1)} \), we use (A.8) to get
\[ -\frac{1}{\tau_f} \tilde{I}^{(1)} = \partial_t \tilde{I}^{(0)} + \tilde{V}_1 \cdot \sum a \tilde{z} a \tilde{z} a f_a^{(0)} - \sum a \tilde{z} a \tilde{z} a F_a^{(1)}. \quad (A.19) \]

With the aid of (A.1), from (A.13), (A.14) and (A.15), we have
\[ \partial_t (\rho \tilde{u}\tilde{u}) = -[\tilde{u} \tilde{V}_1 p]_s - \tilde{V}_1 (\rho \tilde{u}\tilde{u}\tilde{u}) + \rho \tilde{a}\tilde{u}, \quad (A.20) \]
\[ \partial_t p = -\tilde{V}_1 (p\tilde{u}) - \frac{2}{D} p \tilde{V}_1 \cdot \tilde{u}, \quad (A.21) \]

note that the \( \rho \tilde{u}\tilde{u}\tilde{u} \) term could be neglected due to the low velocity flow. Such that,
\[ \tilde{I}^{(1)} = -\tau_f p \left( \tilde{s}_1 - \frac{2}{D} (\tilde{V}_1 \cdot \tilde{u}) \tilde{I} \right), \quad (A.22) \]
where \( \tilde{s}_1 = [\tilde{V}_1 u]_s. \) And, to calculate \( Q^{(1)} \), we use (A.11), and can get
\[ -\frac{1}{\tau_h} \tilde{Q}^{(1)} + \frac{1}{\tau_{hf}} \tilde{I}^{(1)} \cdot \tilde{u} + \tilde{I}^{(0)} \cdot \tilde{a} = \partial_t \tilde{Q}^{(0)} + \tilde{V}_1 \cdot \sum a \tilde{z} a \tilde{z} a h_a^{(0)} + \tilde{a}_1 \cdot \sum a \tilde{z} a q_a^{(1)} \]
\[ = \tilde{I}^{(0)} \cdot \tilde{a}_1 + p \left( -\frac{2}{D} \tilde{u} (\tilde{V}_1 \cdot \tilde{u}) + \tilde{u} \cdot \tilde{V}_1 \tilde{u} + \tilde{V}_1 E \right) \]
\[ = \tilde{I}^{(0)} \cdot \tilde{a}_1 + \frac{D}{2} p \tilde{V}_1 \theta - \frac{1}{\tau_f} \tilde{I}^{(1)} \cdot \tilde{u}, \quad (A.23) \]
Then, we can get

\[
\tilde{\mathcal{Q}}^{(1)} = - \frac{D}{2} \tau_h p \tilde{\mathbf{V}}_1 \theta + \tilde{\Pi}^{(1)} \cdot \tilde{u}. \tag{A.24}
\]

In deriving above equation, we need the following equations derived from (A.13), (A.14) and (A.15):

\[
\begin{align*}
\partial_t (\rho E \tilde{u}) &= - \tilde{\mathbf{V}}_1 [(p + \rho E) \tilde{u} \tilde{u}] + \rho \tilde{u} (\tilde{u} \cdot \tilde{a}_1) \\
&\quad + \rho E \tilde{a}_1 - E \tilde{\mathbf{V}} p + p \tilde{u} \cdot \tilde{\mathbf{V}} \tilde{u}, \quad \tag{A.25} \\
\partial_t (p \tilde{u}) &= - \tilde{\mathbf{V}}_1 (p \tilde{u} \tilde{u}) - \theta \tilde{\mathbf{V}}_1 p + p \tilde{a}_1 - \frac{2}{D} (\tilde{\mathbf{V}}_1 \cdot \tilde{u}) p \tilde{u}. \quad \tag{A.26}
\end{align*}
\]

Finally, based on equations from (A.13) to (A.18), together with (A.22) and (A.23), we obtain the thermal hydrodynamic equations at the Navier–Stokes level as expressed in (8)–(11). We note that the discrete effect should be considered in the LBM, that is, \( \mu = (\tau_f - 1/2) p \) and \( \kappa = c_v (\tau_h - 1/2) p \). Then, the Prandtl number becomes 

\[
Pr = \frac{\mu}{\kappa} = \frac{\gamma (\tau_f - 1/2)}{\tau_h - 1/2},
\]

where \( \gamma = c_p / c_v \) is the heat capacity ratio and \( c_v = DR/2 \).

We also note that the pressure \( p \) in the final thermal hydrodynamic equations is not constant \( p_0 \) as that in Guo et al. (2007) due to the present coupling approach. Comparing to Guo’s model, the problem of variable velocities depending on local temperature is avoided at the beginning of deriving the present model. Such that, it does not have to replace local temperature with reference temperature in equilibrium distribution functions, in which there is no clear physical meaning.