Lattice Boltzmann method for thermal flow simulation on standard lattices

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The recently introduced consistent lattice Boltzmann model with energy conservation [S. Ansumali, I.V. Karlin, Phys. Rev. Lett. 95, 260605 (2005)] is extended to the simulation of thermal flows on standard lattices. The two-dimensional thermal model on the standard square lattice with nine velocities is developed and validated in the thermal Couette and Rayleigh-Bénard natural convection problems.

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I. INTRODUCTION

The lattice Boltzmann (LB) method is a powerful approach to hydrodynamics, with applications ranging from large Reynolds number flows to flows at a micron scale, porous media and multi-phase flows [1]. The LB method solves a fully discrete kinetic equation for populations \( f_i(x, t) \), designed in a way that it reproduces the target equations of continuum mechanics in the hydrodynamic limit. Populations correspond to discrete velocities \( c_i, i = 1, \ldots, N \), which fit into a regular spatial lattice with the nodes \( x \). This enables a simple and efficient ‘stream-along-links-and-equilibrate-at-nodes’ realization of the LB algorithm.

In the case of incompressible flows, where the target equations are Navier-Stokes equations at low Mach number, the LB method proves to be competitive to conventional methods of computational fluid dynamics [2]. In that case, the LB models on the so-called standard lattices with a relatively small number of velocities \( (N = 9 \text{ in two dimensions, see Fig. } 1\text{ and } N = 15, 19, 27 \text{ in three}) \) are available and most commonly used. In this paper, we will follow the usual nomenclature and indicate the models as \( DMQN \) where \( M = 2, 3 \) is the spatial dimension and \( N \) the number of the discrete velocities of the model.

However, situation is quite different with LB models for compressible thermal flows. In spite of a number of recent suggestions, a commonly accepted LB model for thermal flows has not yet been established, to the best of our knowledge. A reason for such a difference between the isothermal and thermal cases is mainly because it is not straightforward to incorporate the temperature into the lattice equilibrium when using the standard lattices, and simultaneously to satisfy a number of conditions for recovering the Navier-Stokes and Fourier equations for compressible flows [3]. At present, two major approaches to constructing thermal LB models can be distinguished. In the first approach, lattices with a larger number of discrete velocities or off-lattice velocity sets are considered to enable local energy conservation and isotropy [4, 5]. In the second approach, two copies of the standard lattices are considered, one of which is designed to treat the density and momentum and the other - the energy density. The standard isothermal LB model on the first lattice is considered, and the coupling between the lattices is enhanced by introducing force terms in order to recover viscous heat dissipation [6]. However, both these approaches inevitably deal with more discrete speeds than the standard single-lattice LB models which leads to reducing efficiency.

Recently, a so-called consistent LB model has been introduced in Ref. [7]. It has been shown that it is possible to construct the LB model with energy conservation on the standard lattices in such a way that the spurious bulk viscosity of isothermal LB models is eliminated, and that the Navier-Stokes and Fourier equations are recovered once the temperature is varied in a small neighborhood of a reference temperature. However, the consistent LB model is limited to weakly compressible flows, and is not yet sufficient to simulate thermal flows. The reason for that is the low symmetry of the standard lattices which leads to accumulation of deviations of the resulting hydrodynamic equations from their Navier-Stokes and Fourier counterparts. It should be noted, however, that the consistent LB model with energy conservation on standard lattices should be considered as a better and more natural starting point for a development of the thermal LB model as compared to the isothermal model.

In this paper, we complete the program of constructing the thermal LB model on standard lattices as an extension of the consistent LB model [7]. A new thermal lattice Boltzmann model is derived on the most commonly used \( D2Q9 \) lattice as follows: In section III we revisit the derivation of the local equilibrium of the thermal model, using the method of guided equilibrium [8]. This enables to enhance Galilean invariance of the consistent LB method for large temperature variations. We shall also identify the remaining deviations in the higher-order moments due to the lattice constraints. In section IV the impact of these deviations on the hydrodynamic equations is identified (algebraic details of the derivation are presented in the Appendix. In section V additional terms are introduced in the Boltzmann equation in

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such a way that all the deviations of the hydrodynamic
equations from their Navier-Stokes and Fourier counter-
parts are eliminated. In addition, further terms are in-
troduced to represent external forces, as well as to tune
the Prandtl number of the model. In section IV the dis-
cretization in time and space of the kinetic equation of
the Prandtl number of the model. In section V, the dis-


tropy function (2) under constraints provided by
the consistent lattice Boltzmann model shows de-
viations of the order of $u^2 \Delta T$ (where $\Delta T$ is a devi-

ation from the reference temperature) from the target
Maxwell-Boltzmann form,

$$P_{\alpha\beta}^{\text{MB}} = \rho T \delta_{\alpha\beta} + \frac{j_\alpha j_\beta}{\rho}. \quad (5)$$

Hence, as the first step towards establishing the lat-
tice Boltzmann method for thermal flow simulations, we
need to modify the construction of the equilibrium which
would remove this deviation from the pressure tensor.

B. Guided local equilibrium

In order to remove the aforementioned deviation in
the equilibrium pressure tensor, we use the method of
guided equilibrium introduced in [8] for a generic lattice
Boltzmann model. Following [8], we minimize the en-
tropy function (2) under an extended set of conditions
which includes the local conservations (4) and the condi-
tion which stipulates that the equilibrium pressure tensor
would remove this deviation from the pressure tensor.

In the consistent lattice Boltzmann method [3], the local
conservations include mass, momentum and energy,

$$\begin{align*}
\sum_{i=0}^{8} f_i^{\text{eq}} &= \rho, \\
\sum_{i=0}^{8} c_{i\alpha} f_i^{\text{eq}} &= j_\alpha, \\
\sum_{i=0}^{8} c_{i\alpha}^{2} f_i^{\text{eq}} &= 2\rho T + \frac{j_\alpha^2}{\rho}
\end{align*} \quad (4)$$

where $\rho$, $j_\alpha = \rho u_\alpha$, and $T$ are the density, momentum and
temperature fields, correspondingly. Note that the con-
sistent lattice Boltzmann construction includes energy
conservation among the constraints (4). Note that this
is at variance with the standard isothermal lattice Boltz-
mann method on the same lattice [11] where the entropy
function is minimized under the constraints of mass and
momentum only [10].

Derivation of the equilibrium populations as a mini-
mizer of the entropy function (2) under constraints (4)
can be found in Refs. [3, 9], and is not reproduced here.
We remind that at the reference temperature $T_0 = 1/3$, the consistent lattice Boltzmann model recov-
ers the Navier-Stokes-Fourier hydrodynamic equations and results in the nonequilibrium pressure tensor without
a spurious bulk viscosity of the standard lattice Boltz-
mann model. However, the consistent lattice Boltzmann
model itself is not yet capable of simulating accurately
thermal flows with significant temperature and density
variations. In particular, the equilibrium pressure ten-
sor of the consistent lattice Boltzmann model shows de-
viations of the order of $u^2 \Delta T$ (where $\Delta T$ is a devi-

ation from the reference temperature) from the target
Maxwell-Boltzmann form,

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which includes the local conservations (4) and the condi-
tion which stipulates that the equilibrium pressure tensor
$P_{\alpha\beta}^{\text{eq}}$ is in the MB form (5),

$$\begin{align*}
\sum_{i=0}^{8} c_{i\alpha} c_{i\beta} f_i^{\text{eq}} &= \rho T \delta_{\alpha\beta} + \frac{j_\alpha j_\beta}{\rho}.
\end{align*} \quad (6)$$

Hence, as the first step towards establishing the lat-
tice Boltzmann method for thermal flow simulations, we
need to modify the construction of the equilibrium which
would remove this deviation from the pressure tensor.
Minimization of the entropy function \( \mathcal{S} \) under the extended list of constraints, \([4]\) and \([5]\) leads to the equilibrium populations of the form

\[
    f_i^{\text{eq}} = w_i \exp \{ \mu + \zeta_\alpha c_{i\alpha} + \chi_{\alpha\beta} c_{i\alpha} c_{i\beta} + \gamma c_i^2 \},
\]

where summation convention in two repeated spatial indices is assumed, and where \( \mu, \zeta_\alpha, \chi_{\alpha\beta}, \gamma \) are Lagrange multipliers of the constraints. Their values are found upon substitution of (7) into (4) and (6). Equilibrium at zero velocity \((j_\alpha = 0)\) can be found exactly and coincides with the one reported in \([7, 9]\). Equilibria at non-zero velocity are then derived by perturbation around the zero-velocity state, and \(f_i^{\text{eq}}\) are represented in terms of a series in the momentum. For what will follow, expansion up to the fourth order in velocity is required. This solution procedure is quite standard, hence, we reproduce only the result in terms of the velocity \(u_\alpha = j_\alpha/\rho\).

\[
    \begin{align*}
    f_0^{\text{eq}} &= \rho(T + u_x^2 - 1)(T + u_y^2 - 1), \\
    f_1^{\text{eq}} &= \frac{\rho}{2}(T + u_x + u_y^2)(1 - T - u_y^2), \\
    f_2^{\text{eq}} &= \frac{\rho}{2}(1 - T - u_x^2)(T + u_y + u_y^2), \\
    f_3^{\text{eq}} &= \frac{\rho}{2}(T + u_x^2)(1 - T - u_y^2), \\
    f_4^{\text{eq}} &= \frac{\rho}{2}(1 - T - u_x^2)(T + u_y + u_y^2), \\
    f_5^{\text{eq}} &= \frac{\rho}{4}(T + u_x + u_y^2)(T + u_y + u_y^2), \\
    f_6^{\text{eq}} &= \frac{\rho}{4}(T - u_x + u_y^2)(T + u_y + u_y^2), \\
    f_7^{\text{eq}} &= \frac{\rho}{4}(T - u_x + u_y^2)(T - u_y + u_y^2), \\
    f_8^{\text{eq}} &= \frac{\rho}{4}(T + u_x + u_y^2)(T - u_y + u_y^2).
    \end{align*}
\]

Note that equilibrium populations at zero velocity remain positive for temperature values \(0 < T < 1\). The equilibrium pressure tensor satisfies the MB relation per construction,

\[
    P_{\alpha\beta}^{\text{eq}} = P_{\alpha\beta}^{\text{MB}}.
\]

The properties of the higher-order moments in the equilibrium \([8]\) are studied in the next section.

### C. Deviations in higher-order moments

Apart from the equilibrium pressure tensor, also the third- and fourth-order moments of the equilibrium must satisfy the Maxwell-Boltzmann relations in order to recover the Navier-Stokes and the temperature equation in the hydrodynamic limit,

\[
    \begin{align*}
    Q_{\alpha\beta\gamma}^{\text{MB}} &= T(j_\alpha \delta_{\beta\gamma} + j_\beta \delta_{\alpha\gamma} + j_\gamma \delta_{\alpha\beta}) + \frac{j_\alpha j_\beta j_\gamma}{\rho^2}, \\
    R_{\alpha\beta}^{\text{MB}} &= T \left( \frac{j_\beta^2}{\rho} + 4T \right) \delta_{\alpha\beta} + 6T \frac{j_\alpha j_\beta}{\rho} + \frac{j_\alpha j_\beta j_\gamma}{\rho^3}.
    \end{align*}
\]

Using the equilibrium populations \([8]\) to evaluate the functions

\[
    \begin{align*}
    Q_{\alpha\beta\gamma}^{\text{eq}} &= \sum_{i=0}^{8} c_{i\alpha} c_{i\beta} c_{i\gamma} f_i^{\text{eq}}, \\
    R_{\alpha\beta}^{\text{eq}} &= \sum_{i=0}^{8} c_{i\alpha} c_{i\beta} c_{i\gamma}^2 f_i^{\text{eq}},
    \end{align*}
\]

and introducing, for a generic moment \(M\), a deviation \(M'\) of its equilibrium value \(M^{\text{eq}}\) from the Maxwell-Boltzmann value \(M^{\text{MB}}\),

\[
    M^{\text{eq}} = M^{\text{MB}} + M',
\]

we find the following deviations of the third- and fourth-order moments:

\[
    \begin{align*}
    Q'_{xxx} &= j_x(1 - 3T) - \frac{j_x^3}{\rho^3}, \\
    Q'_{yyy} &= j_y(1 - 3T) - \frac{j_y^3}{\rho^3}, \\
    R'_{xx} &= (1 - 3T)\rho T + (1 - 6T)\frac{j_x^2}{\rho} - \frac{j_x^4}{\rho^3}, \\
    R'_{yy} &= (1 - 3T)\rho T + (1 - 6T)\frac{j_y^2}{\rho} - \frac{j_y^4}{\rho^3}, \\
    R'_{xy} &= 2(1 - 3T)\frac{j_x j_y}{\rho} - \frac{j_x j_y j_z^2}{\rho^3}.
    \end{align*}
\]

Note that the off-diagonal elements of the third-order moment \(Q_{\alpha\beta\gamma}^{\text{eq}}\) already satisfy the Maxwell-Boltzmann relations,

\[
    Q_{\alpha\beta\gamma}^{\text{eq}} = Q_{\alpha\beta\gamma}^{\text{MB}}, \quad Q_{\alpha\beta\gamma}^{\text{eq}} = Q_{\alpha\beta\gamma}^{\text{MB}}.
\]

Thus, the deviation of the contracted third-order moment \(q_{\alpha}^{\text{eq}} = \sum_{i=0}^{8} c_{i\alpha} c_{i\gamma}^2 f_i^{\text{eq}}\) (the energy flux) is due to the deviation of the diagonal elements,

\[
    q_{\alpha}' = Q_{\alpha\alpha\alpha}'.
\]

Deviations of the diagonal components of the third-order moments are well known for the low-symmetry D2Q9 lattice, and stem from the fact that the velocity set satisfies a relation, \(c_{\alpha\beta\gamma}^2 = c_{\alpha\alpha}\). This lattice constraint precludes construction of equilibrium different from \([8]\) in such a way that also the energy flux would be guided by the Maxwell-Boltzmann relation.

In the next section, we shall identify the impact of the deviations \([13]\) on the hydrodynamic equations. Once this will be done, we shall remove the anomalous terms in the hydrodynamic equations by introducing correction terms into the kinetic equation.
III. DEVIATIONS IN THE HYDRODYNAMIC EQUATIONS

A. Bear BGK model

In this section, the impact of deviations of the moments on the hydrodynamic equations will be identified using the single relaxation time Bhatnagar-Gross-Krook (BGK) model for the collision integral:

\[ \partial_t f_i + c_{ia} \partial_i f_i = -\frac{1}{\tau} (f_i - f_i^{eq}), \]  

(16)

where \( \tau \) is the relaxation time, and the equilibrium populations are given by Eq. (5). The hydrodynamic limit of the BGK kinetic equation (16) can be studied via the Chapman-Enskog expansion. Details of the Chapman-Enskog analysis are given in the Appendix A. Here we shall summarize the results of this analysis.

In order to recover the Navier-Stokes equation, we will need to introduce additional terms into Eq. (16) in order to annihilate the right hand side of the momentum equation (17) (see section IV).

B. Deviations in the momentum equation

To the first order of the Chapman-Enskog expansion, the momentum equation reads:

\[ \partial_t j_\alpha + \partial_j P_{\alpha\beta}^{MB} + \partial_j P_{\alpha\beta}^{neq} = -\partial_j P_{\alpha\gamma}', \]  

(17)

where \( P_{\alpha\beta}^{neq} \) is the nonequilibrium pressure tensor in the form required for the Navier-Stokes equation,

\[ P_{\alpha\beta}^{neq} = -\tau \rho T \left[ \partial_\alpha \left( \frac{j_\beta}{\rho} \right) + \partial_\beta \left( \frac{j_\alpha}{\rho} \right) - \delta_{\alpha\beta} \partial_\gamma \left( \frac{j_\gamma}{\rho} \right) \right], \]

(18)

while \( P_{\alpha\gamma}' \) is the deviation of the nonequilibrium pressure tensor from \( P_{\alpha\beta}^{neq} \):  

C. Deviations in the energy equation

Similarly, the energy density equation reads,

\[ \partial_t \left( \frac{j_\alpha}{\rho} + 2 \rho T \right) + \partial_\alpha q_{\alpha a}^{MB} + \partial_\alpha q_{\alpha a}^{neq} = -\partial_\alpha q_{\alpha}' - \partial_\alpha q_{\alpha}'', \]

(20)

where

\[ q_{\alpha}' = 3\tau \rho T \partial_\alpha T \]

\[ -\tau \left[ \frac{3j_\alpha j_\beta}{\rho^2} \partial_\alpha (\rho T) + 3j_\alpha T \partial_\beta \left( \frac{j_\beta}{\rho} \right) - \frac{3j_\alpha j_\beta}{2\rho} \partial_\beta T \right] \]

\[ -\tau \left[ (1 - 3T) \left( \partial_\beta \left( \frac{j_\alpha j_\beta}{\rho^2} \right) - \frac{j_\alpha}{2\rho} \partial_\beta j_\beta \right) \right] \]

\[ -\tau \left[ \frac{2j_\alpha j_\beta}{\rho^2} \partial_\alpha j_\beta + \frac{3j_\alpha j_\beta}{\rho^2} \partial_\beta \left( \frac{j_\alpha j_\beta}{\rho^2} \right) + \frac{j_\alpha}{2\rho} \partial_\beta \left( \frac{j_\beta}{\rho^2} \right) \right] \]

\[ + \tau \partial_\beta \epsilon_{\alpha\beta}'', \]

(22)

\[ \epsilon_{xx}'' = \frac{j_x j_x}{\rho^3} + \frac{j_x^2}{\rho^3}, \]

\[ \epsilon_{yy}'' = \frac{j_y j_y}{\rho^3} + \frac{j_y^2}{\rho^3}, \]

\[ \epsilon_{xy}'' = \frac{j_x j_y}{\rho^3}. \]

(23)

It should be noted that, in certain situations, many terms in (22) and (23) can be safely neglected. For example, deviations of the order \( j^4 \) affect the viscous heat dissipation and can be ignored in cases where viscous heating
is unimportant. However, we shall use the full expressions (22) and (23) for the deviation in the numerical implementation below.

The deviations in the hydrodynamic equations identified in this section are due to the lattice constraints of the D2Q9 lattice, and they cannot be removed by introducing a set of the equilibrium distribution functions different from (8). These deviations can be removed only by introducing correction terms into the kinetic equation which we address in the next section.

### IV. CORRECTION OF BGK EQUATION

To this end, we have computed the deviations due to the lattice constraints. In this section, an efficient way to remove these deviations by adding correction terms in the Boltzmann equation is introduced:

\[
\partial_t f_i + c_{i\alpha} \partial_\alpha f_i = -\frac{1}{r} (f_i - f_i^{eq}) + \Psi_i + \Phi_i. \tag{24}
\]

The purpose of the \(\Psi_i\) terms is to correct the momentum equation, while the purpose of the \(\Phi_i\) terms is to correct the energy equation.

#### A. Momentum equation correction terms \(\Psi_i\)

We require that the \(\Psi_i\) term affects only the momentum equation and delivers there a term which compensates \(-\partial_\gamma P''_{\alpha\gamma}\). Thus,

\[
\begin{align*}
\sum_{i=0}^{8} \Psi_i &= 0, \\
\sum_{i=0}^{8} c_{i\alpha} \Psi_i &= \partial_\gamma P''_{\alpha\gamma}, \\
\sum_{i=0}^{8} c_i^2 \Psi_i &= 0, \\
\sum_{i=0}^{8} c_{i\alpha} c_{i\beta} \Psi_i &= 0, \\
\sum_{i=0}^{8} c_{i\alpha} c_{i\beta} c_i^2 \Psi_i &= 0, \\
\sum_{i=0}^{8} c_{i\alpha} c_{i\beta} c_i^4 \Psi_i &= 0.
\end{align*} \tag{25}
\]

Among these equations only nine are independent, and the unique solution is:

\[
\begin{align*}
\Psi_0 &= 0, \\
\Psi_1 &= \partial_\gamma P''_{x\gamma}, \\
\Psi_2 &= \partial_\gamma P''_{y\gamma}, \\
\Psi_3 &= -\partial_\gamma P''_{x\gamma}, \\
\Psi_4 &= -\partial_\gamma P''_{y\gamma}, \\
\Psi_5 &= -\frac{1}{4} (\partial_\gamma P''_{x\gamma} + \partial_\gamma P''_{y\gamma}), \\
\Psi_6 &= \frac{1}{4} (\partial_\gamma P''_{x\gamma} - \partial_\gamma P''_{y\gamma}), \\
\Psi_7 &= \frac{1}{4} (\partial_\gamma P''_{x\gamma} + \partial_\gamma P''_{y\gamma}), \\
\Psi_8 &= \frac{1}{4} (-\partial_\gamma P''_{x\gamma} + \partial_\gamma P''_{y\gamma}).
\end{align*} \tag{26}
\]

#### B. Energy equation correction terms \(\Phi_i\)

Similarly, it is required that \(\Phi_i\) terms appear only in the energy equation,

\[
\begin{align*}
\sum_{i=0}^{8} \Phi_i &= 0, \\
\sum_{i=0}^{8} c_{i\alpha} \Phi_i &= 0, \\
\sum_{i=0}^{8} c_i^2 \Phi_i &= \partial_\alpha (q''_{\alpha} + q''_{\alpha}), \\
\sum_{i=0}^{8} c_{i\alpha} c_{i\beta} \Phi_i &= 0, \\
\sum_{i=0}^{8} c_{i\alpha} c_{i\beta} c_i^2 \Phi_i &= 0, \\
\sum_{i=0}^{8} c_{i\alpha} c_{i\beta} c_i^4 \Phi_i &= 0.
\end{align*} \tag{27}
\]
The solution of that system is:

\[
\begin{align*}
\Phi_0 &= -\frac{3}{2} \partial_a (q'_a + q''_a), \\
\Phi_1 &= \frac{1}{2} \partial_a (q'_a + q''_a), \\
\Phi_2 &= \frac{1}{2} \partial_a (q'_a + q''_a), \\
\Phi_3 &= \frac{1}{2} \partial_a (q'_a + q''_a), \\
\Phi_4 &= \frac{1}{2} \partial_a (q'_a + q''_a),
\end{align*}
\]

(28)

The fluid corresponds to the ideal gas equation of state, \(p = \rho T\), with specific heats \(c_v = 1.0\) and \(c_p = 2.0\), in lattice units, and with the adiabatic exponent \(\gamma = c_p/c_v = 2.0\). The viscosity coefficient \(\mu\) and thermal conductivity \(\kappa\) can be identified as

\[
\mu = \tau \rho T, \quad \kappa = \frac{2}{\Pr} \tau \rho T.
\]
The Prandtl number is a tunable parameter and can take arbitrary values. A wide range of gases and fluids whose physics is described by equations \[6\] can be simulated. We now proceed with a time-space discretization of the kinetic equation \[24\].

V. LATTICE BOLTZMANN DISCRETIZATION

Derivation of the lattice Boltzmann scheme for the kinetic equation \[24\] proceeds essentially along the lines of

\[
f_i(x + c_i \delta t, t + \delta t) = f_i(x, t) + \int_{t}^{t+\delta t} \frac{1}{\tau} (f_i^\text{eq}(t') - f_i(t')) dt' + \int_{t}^{t+\delta t} \Phi_i(t') dt' + \int_{t}^{t+\delta t} \Psi_i(t') dt'.
\] (34)

The time integrals of the collision term as well as of the correction terms is evaluated using the second-order accurate trapezoidal rule. Second, in order to establish a semi-implicit scheme, the following transformation is applied \[6\]:

\[
g_i = f_i + \frac{\delta t}{2\tau} (f_i - f_i^\text{eq}) - \frac{\delta t}{2} [\Psi_i + \Phi_i].
\] (35)

This leads to a semi-explicit scheme,

\[
g_{i+\delta t} = g_i + \frac{2\delta t}{\delta t + 2\tau} [f_i^\text{eq} - g_i + \frac{2\tau\delta t}{2\tau + 2\tau} [\Psi_i(f) + \Phi_i(f)].
\] (36)

Note that the simple scheme \[36\] is semi-explicit due to the presence of the correction terms \(\Psi_i\) and \(\Phi_i\) (and not fully explicit, as in the standard case without any corrections). The scheme utilizes the transformed populations \(g\). The equilibrium \(f^\text{eq}\) can be computed using equations that relate the locally conserved moments of the populations \(f\) with those of the \(g\)-populations. In order to do this, we evaluate the moments of the transformation \[36\] :

\[
\rho(f) = \rho(g),
\] (37)

\[
j_x(f) = j_x(g) + \frac{\delta t}{2} \sum_{i=0}^{8} c_{i,x} \Psi_i(f),
\] (38)

\[
j_y(f) = j_y(g) + \frac{\delta t}{2} \sum_{i=0}^{8} c_{i,y} \Psi_i(f),
\] (39)

\[
T(f) = \frac{1}{2\rho} \left( \sum_{i=0}^{8} c_i^2 g_i - \frac{j^2(f)}{\rho} + \frac{\delta t}{2} \sum_{i=0}^{8} c_i^2 \Phi_i(f) \right).
\] (40)

The above set of equations can be simplified using Eqs. \[26\] and \[28\]:

\[
\rho(f) = \rho(g),
\] (41)

\[
j_x(f) = j_x(g) + \frac{\delta t}{2} (\partial_x P_\alpha''(f)),
\] (42)

\[
j_y(f) = j_y(g) + \frac{\delta t}{2} (\partial_y P_\alpha''(f)),
\] (43)

\[
T(f) = \frac{1}{2\rho} \left( \sum_{i=0}^{8} c_i^2 g_i - \frac{j^2(f)}{\rho} + \frac{\delta t}{2} \partial_\alpha (q'_\alpha(f) + q''_\alpha(f)) \right).
\] (44)

Finally, discretization in space is done as in the standard lattice Boltzmann method: if \(x\) is a grid node then also \(x \pm c_i \delta t\) is the grid node.

In the simulation, the following algorithm was implemented for the collision step:

Step 1. Calculate \(\rho, j_\alpha, T\) using \([41-44]\), \((\partial_\gamma P_\alpha''(f))^t\), \((\partial_\alpha (q'_\alpha + q''_\alpha))^t\) and \(g_t\) values;

Step 2. Calculate \((\partial_\gamma P_\alpha''(f))^t, (\partial_\alpha (q'_\alpha + q''_\alpha))^t\) using values of \(\rho, j_\alpha, T\) from Step 1;

Step 3. Calculate again \(\rho, j_\alpha, T\) using \([41-44]\), \(g_t\) and the values calculated in Step 2;

Step 4. Use \(\rho, j_\alpha, T\) from Step 3 for the calculation of the equilibrium values \([38]\);

Step 5. Use \((\partial_\gamma P_\alpha''(f))^t, (\partial_\alpha (q'_\alpha + q''_\alpha))^t\) from Step 2 in the discrete equation \[36\] along with the equilibrium values calculated in Step 4.

The terms \(\partial_\gamma P_\alpha''\) and \(\partial_\alpha (q'_\alpha + q''_\alpha)\) are evaluated using a second-order accurate finite-difference scheme.

A few comments on the computational efficiency of our model are in order. First, the present thermal model is
only about 2.7 times slower as compared to the standard isothermal LB method on the same D2Q9 lattice due to evaluations of the deviation terms \([19]\) and \([22]\). Note that, depending on the desired accuracy and the optimization level, faster and simpler algorithms can be readily designed. For example, for the natural convection problem considered below in section VI, deviations of the order \(j^3\), \(j^2\Delta T\), and \(j^4\) can be safely neglected in the energy equation, which removes the computational overhead with respect to the standard isothermal D2Q9 code without sacrificing the accuracy of the results in the thermal case. It should be stressed that optimization of the code was not pursued in the present study so that the above estimates are only qualitative.

Second, as compared to the thermal model on two lattices \([6]\) in terms of memory use, the present model requires storage of twelve values per node, that is, nine for the populations \(g_i\), two for the terms \((\partial_n P_{\alpha\gamma}^\prime)_{\ast}\), and one for the term \((\partial_n (q_{\alpha}^\prime + q_{\alpha}^\prime))_{\ast}\). In the case of the two distribution function thermal models \([6]\), the storage of at least eighteen values per node is required, without taking into account the additional computational effort needed in order to recover viscous dissipation terms.

These estimates show that the present one-lattice thermal model is viable. We shall now proceed with a numerical validation of the present scheme.

VI. NUMERICAL EXAMPLES

In this section, the thermal model developed above is validated numerically. Equilibrium populations are expanded till the fourth order in the velocity and the corrections described in previous sections are applied. The same model is used in all simulations, even though viscous heat dissipation could have been ignored in the Rayleigh-Bénard setup.

A. Necessity of guided equilibrium

In our first example, we compare the three different models: the original consistent LB model \([7,9]\), the model using the guided equilibrium \([8]\) without any correction terms, and the full model after the correction terms are applied. In order to demonstrate the necessity of the guided equilibrium, we simulate the two-dimensional Couette flow between two parallel moving plates at different temperatures. Isothermal walls are separated by a distance \(H\) and move parallel to the \(x\)-axis. The diffusive wall boundary conditions \([12]\) is implemented for the isothermal walls, and periodic boundary condition is applied for the rest. Analysis similar to the one presented in \([13]\) results in the following relation at the steady state:

\[
P - N^{eq} = \text{const},
\]

where \(P = P^{eq} = P_{xx} + P_{yy}\) is the trace of the pressure tensor and \(N = P_{xx} - P_{yy}\) is the normal stress difference. On one hand, using the guided equilibrium \([8]\) in \([16]\) results in the constant pressure in the whole domain:

\[
\rho T = \text{const}.
\]

This is consistent with the correct Maxwell-Boltzmann relation for the pressure tensor. On the other hand, as we have already mentioned in section II, the equilibrium normal stress difference \(N^{eq}\) of the consistent LB model \([7,9]\) exhibits a deviation of the order \(\sim j^2\Delta T\), where \(\Delta T\) is a variation around the reference temperature \(T_0 = 1/3\). In this case, equation \([45]\) yields a different result, namely, the pressure \(p = \rho T\) varies along the \(y\)-axis according to the variation of the momentum,

\[
\rho T - (1 - 3T) \frac{j^2}{4T} = \text{const}.
\]

In Fig. 2 simulation results for the pressure in the Couette flow with all the three models are presented and compared with the analytical solution \([40]\). While the variation of the pressure \(p = \rho T\) away from the constant value is numerically small for the original model \([7,9]\), it is still visible, and it verifies the analytical solution \([47]\) rather than \([40]\). On the other hand, the LB model with the guided equilibrium verifies the constancy of the pressure with machine precision. Same holds also for the LB model with the guided equilibrium when all the correction terms are applied, as expected. This demonstrates necessity of the guided equilibrium in our construction.
B. Viscous heat dissipation

We simulate the thermal Couette flow as in the preceding section but for a small temperature differences. In this case, the viscous heat dissipation is important and affects the temperature profile. As is well known, the Navier-Stokes and Fourier equations (32) predict that the temperature profile depends on the Prandtl number, Pr, and on the Eckert number, Ec, where

\[ Ec = \frac{u^2}{c_p \Delta T}, \quad (48) \]

with \( u \) the difference of the velocities of the plates, and \( \Delta T \) the difference of temperatures of the plates. This simulation enables to verify that the correction terms do recover the right Prandtl number. In the simulation, we used \( Ec = 3 \) and \( \Delta T = 2 \times 10^{-3} T_0 \), where \( T_0 = 1/3 \) is the reference temperature. Three different cases were considered:

Case 1. LB with the guided equilibrium (8) and the corrections \( \Psi_i \) and \( \Phi_i \), which deliver \( Pr = 1 \) (that is, without the transformation (30));

Case 2. As in Case 1 plus the transformation (30) to match \( Pr = 0.71 \) (air).

Case 2. As in Case 1 plus the transformation (30) to match \( Pr = 4 \).

Simulation results for the temperature profile are presented in Fig. 3 and are in excellent agreement with the analytical solution. For the current setup, with the present implementation of boundary condition, simulation results remain in agreement with the analytical solution for Prandtl numbers ranging from 0.01 to 20.

C. Rayleigh-Bénard convection

The Rayleigh-Bénard convection flow is a classical benchmark on the thermal models. The fluid is enclosed between two parallel stationary walls, the hot (bottom) and the cold (top), and experiences the gravity force. Density variations caused by the temperature variations drive the flow, while the viscosity will counteract to equilibrate it.

In our LB model, gravity is implemented using the correction (31). We operate the model in the weakly compressible regime, however, without using the Boussinesq approximation. For that we set a temperature difference of the order of 3% of the reference temperature \( T_0 = 1/3 \).

At the top and the bottom walls we apply the diffusive wall boundary condition (12), whereas periodic boundary condition is applied on the vertical walls. For the nodes that belong to the isothermal walls, gravitational force was not applied.

\[ \frac{\beta g \Delta T H^3}{\nu^2}, \quad (49) \]

where \( g \) is the gravity acceleration, \( \Delta T \) is the wall temperature difference, \( H \) is the distance between the walls and \( \nu \) is the kinematic viscosity of the fluid. For the ideal gas equation of state, the thermal expansion coefficient \( \beta \) is defined as:

\[ \beta = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial T} \right)_p = \frac{1}{T}. \quad (50) \]

For the computation of the Rayleigh number, we used the thermal expansion coefficient evaluated at the reference temperature \( T_0 = 1/3 \), that is, \( \beta = 3 \). The heat transfer is described by the Nusselt number, Nu, defined as the ratio between convective heat transport to the heat transport due to temperature conduction:

\[ Nu = 1 + \langle u_y T \rangle_H \frac{H}{\kappa \Delta T}. \quad (51) \]

Here \( \langle u_y T \rangle_H \) denotes the average over the convection layer and \( \kappa \) is the thermal conductivity of the model (33). For the current simulations, a computation domain with the aspect ratio 2 : 1 was considered.

For this setup, the critical Rayleigh number was found to be \( Ra_{cr} = 1700 \pm 10 \), which is consistent with the reference data for the Boussinesq approximation [14, 15]. Any flow field was dissipated for values less than \( Ra_{cr} \). On the contrary, for values larger than \( Ra_{cr} \), the flow develops two or more cells (vortices) depending on the initial conditions.

FIG. 3: Temperature profile in the thermal Couette flow. Plotted is the reduced temperature, \( T_{norm} = (T - T_{cold})/(T_{hot} - T_{cold}) \), versus the reduced \( y \)-coordinate (as in Fig. 2). Eckert number Ec = 3. Line: Analytical solution for \( Pr = 4 \), \( Pr = 1 \), and \( Pr = 0.71 \). Reynolds number Re = 200. Symbol: Simulation results for the three cases (see text). Diamonds: Case 1; Squares: Case 2 (air); Circles: Case 3.
FIG. 4: Contour plot with 19 equidistant iso-temperature lines for Ra = $10^4$ (top) and Ra = $5 \times 10^4$ (bottom).

FIG. 5: Stream function contours for Ra = $10^4$ (top) and Ra = $5 \times 10^4$ (bottom). Difference between contour lines is 0.025 in units of $\rho_{\text{max}}U_{\text{max}}H$.

For different Rayleigh numbers, simulations for the 51, 101 and 201 grid nodes in the y-direction were performed. Extrapolating the obtained values of Nusselt number, an estimate of the final converged solution can be done ($N_{\text{ue}}$). In Fig. 4 the isotherms of Ra = $10^4$ and Ra = $5 \times 10^4$ are plotted for the case of 101 grid nodes in the y-direction. In Fig. 5 the contours of the stream function of the compressible flow field for Ra = $10^4$ and Ra = $5 \times 10^4$ are plotted. The extrapolated converged values of Nusselt number at various Rayleigh numbers are plotted in Fig. 6 and compared with the standard reference data [14, 15] in Table I. The present model is found to be in good agreement with [14], and it also agrees well with the thermal LB models on double lattices where the temperature dynamics is treated as a passive scalar [6, 16]. It should be noted that for Ra up to $10^4$ a uniform grid with 51 nodes in the y-direction was sufficient, while for larger values of Ra, larger grids provide more accurate results. In Fig. 7 a grid convergence study is performed. Natural convection of Ra = $3 \times 10^4$ in the same setup is considered. Fig. 7 reveals the second-order accuracy of the numerical scheme.
TABLE I: Simulation results of the present model compared to the simulation results of Ref. [14]. Left column: Rayleigh number; Central column: Nusselt number; Right column: Difference in percent from the values of Ref. [14].

| Rayleigh number | Nusselt number (NuR) | Difference from Ref. [14] |
|-----------------|----------------------|--------------------------|
| 2500            | 1.474                | 0.07 %                   |
| 5000            | 2.104                | 0.57 %                   |
| 10000           | 2.644                | 0.64 %                   |
| 30000           | 3.605                | 1.56 %                   |
| 50000           | 4.133                | 2.64 %                   |

FIG. 8: (Color online) Snapshot of the temperature field at Ra = 10^8, Pr = 0.71, using a uniform grid of 51 nodes for the y-direction. Contours of reduced temperature, T_{norm} = (T - T_{cold})/(T_{hot} - T_{cold}) are plotted.

Finally, it should be mentioned that on a grid with only 51 nodes in the y-direction, the code was run stably for Ra as high as at least 10^8 which proves a good numerical stability of the algorithm. In Fig. 8, a snapshot of the temperature field is presented at Ra = 10^8. However, a study of the natural convection at high Rayleigh numbers is out of the scope of this paper.

VII. SUMMARY

A reader who wishes to implement this model should execute the following steps:

- Use guided equilibrium populations [8];
- Calculate the correction terms Ψ_i and Φ_i with a second-order finite-difference scheme.
- Use the discretized equation [36].

VIII. CONCLUSION

In this paper, we have developed a new lattice Boltzmann model for simulation of thermal flows with the standard and most commonly used D2Q9 lattice. The important starting point of the derivation is the consistent LB method [1]. Unlike the previous approaches, the consistent LB model on standard lattices already includes energy as a locally conserved quantity, the nonequilibrium stress tensor is free of a spurious bulk viscosity, and a part of the moment relations satisfies the required Maxwell-Boltzmann relations. Hence, by using the consistent LB model, it becomes unnecessary to introduce a separate lattice for the energy field.

We have considerably refined the consistent LB model in two steps. First, following the concept of guided equilibrium [8], we recovered Galilean invariance of the pressure tensor at non-vanishing variations of the temperature. Second, we have identified the remaining deviations in the Navier-Stokes-Fourier equations, and have removed them by adding compensating terms into the kinetic equation. This step allowed us also to make the Prandtl number a tunable parameter, and to add external forces. It should be noted that additional terms also appear in the method based on two lattices [4] but there is no relation between the both. On the other hand, a numerical implementation of the kinetic equation with additional terms here has practically not much different from the method first developed in [4]. Finally, it is straightforward to extend the present model to three dimensions based on the D3Q27 consistent LB model [1].

We shall conclude this paper with a general comment on the construction of thermal lattice Boltzmann models. As we already mentioned in the introduction, there are two basic directions for such a development, one which uses larger and more isotropic sets of velocities, and the other which uses a small number of velocities and introduces non-local (dependent on the gradients of the fields) corrections to compensate for the deficit of lattice symmetry. This situation resembles the classical dilemma of extending the hydrodynamics into beyond the Navier-Stokes level: One way is the higher-order hydrodynamics (Burnett or super-Burnett) which means higher-order derivatives and more non-locality in the equations for the standard hydrodynamic fields. The other is to take more moments while staying local (Grad’s moment method). Both approaches have positive and negative aspects. In our case, the attractive features of large velocity sets...
(locality, isotropy, possibility of the exact treatment of propagation) should be waged against the necessity of handling many more fields (populations). On the other hand, the obvious attractive side of the small lattices approach has to be opposed by the fact that one has to evaluate more terms dependent on the gradients of the fields. While this proves to be possible, still, one needs to be careful about numerical errors brought in by such procedures. We believe that both these approaches, at present, show there advantages and disadvantages, so the decision about which to prefer should be the focus of future studies.

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### APPENDIX A: DERIVATION OF HYDRODYNAMIC EQUATIONS

We apply the Chapman-Enskog expansion in order to derive hydrodynamic equations corresponding to the BGK equation (10) with the equilibrium (8). Populations $f_i$ and the time derivative operator are expanded into powers of the relaxation parameter $\tau$

$$f_i = f_i^{eq} + \sum_{n=1}^{\infty} f_i^{(n)} \tau^n,$$

$$\partial_t = \sum_{n=0}^{\infty} \tau^n \partial_{t}^{(n)}.$$  

(A1)

(A2)

The non-equilibrium pressure tensor and energy flux to first order in $\tau$ are defined as:

$$P^{(1)}_{\alpha\beta} = \tau \sum_{i=0}^{8} c_i \epsilon_i \partial_{t}^{(1)} f_i,$$  

$$q^{(1)}_{\alpha} = \tau \sum_{i=0}^{8} c_i \epsilon_i \partial_{t}^{(1)} f_i.$$  

(A3)

On the zeroth order, equations for density, momentum, pressure tensor and energy flux are:

$$\partial_t^{(0)} \rho = -\alpha \partial_t j_\alpha,$$  

$$\partial_t^{(0)} j_\alpha = -\partial_t P^{MB}_{\alpha\beta},$$  

$$\partial_t^{(0)} \left[ \frac{j_\alpha^2}{\rho} + 2\rho T \right] = -\partial_t q^{MB}_{\alpha} - \partial_t q^{(1)}_{\alpha}.$$  

$$\partial_t^{(0)} P^{eq}_{\alpha\beta} = -\partial_t Q^{eq}_{\alpha\beta} - \frac{1}{\tau} P^{(1)}_{\alpha\beta},$$  

$$\partial_t^{(0)} q^{eq}_{\alpha} = -\partial_t R^{eq}_{\alpha} - \frac{1}{\tau} q^{(1)}_{\alpha},$$  

(A4)

(A5)

(A6)

(A7)

(A8)

where $Q^{eq}_{\alpha\beta\gamma}$ and $R^{eq}_{\alpha\beta\gamma}$ are the third- and the fourth-order moments evaluated at the local equilibrium (8). (explicit form of these function was given in section 11). From (A6), we derive the zeroth-order equation for the temperature,

$$\partial_t^{(0)} T = -T \partial_t \left( \frac{j_\alpha}{\rho} \right) - \frac{j_\alpha}{\rho} \partial_t \rho - \frac{1}{2\rho} \partial_t q^{(1)}_{\alpha}.$$  

(A9)

On the first order in $\tau$ we need equations for the locally conserved fields only,

$$\partial_t^{(1)} \rho = 0,$$  

$$\partial_t^{(1)} j_\alpha = -\frac{1}{\tau} \partial_t P^{(1)}_{\alpha\beta},$$  

$$\partial_t^{(1)} \left[ \frac{j_\alpha^2}{\rho} + 2\rho T \right] = \frac{1}{\tau} \partial_t q^{(1)}_{\alpha}.$$  

(A10)

(A11)

(A12)

Function $P^{(1)}_{\alpha\beta}$ is represented as a sum of two terms, $P^{neq}_{\alpha\beta}$, which results in the correct Navier-Stokes term in the momentum equation, and $P^{''}_{\alpha\beta}$, representing the deviation:

$$P^{(1)}_{\alpha\beta} = P^{neq}_{\alpha\beta} + P^{''}_{\alpha\beta},$$  

$$P^{neq}_{\alpha\beta} = -\tau \left[ \partial_t Q^{eq}_{\alpha\beta\gamma} + \partial_t^{(0)} P^{eq}_{\alpha\beta} \right],$$  

$$P^{''}_{\alpha\beta} = -\tau \left[ \partial_t Q^{MB}_{\alpha\beta\gamma} + \partial_t^{(0)} P^{MB}_{\alpha\beta} \right].$$  

(A13)

(A14)

(A15)

In order to derive $P^{(1)}_{\alpha\beta}$ from (A3), we note that the left hand side can be computed by chain rule,

$$\partial_t^{(0)} q^{eq}_{\alpha} = \frac{\partial P^{eq}_{\alpha\beta}}{\partial \rho} \partial_t^{(0)} \rho + \frac{\partial P^{eq}_{\alpha\beta}}{\partial j_\gamma} \partial_t^{(0)} j_\gamma + \frac{\partial P^{eq}_{\alpha\beta}}{\partial T} \partial_t^{(0)} T.$$  

(A16)

Using (A4), (A5), (A6) and (A10) in (A16), we obtain

$$P^{neq}_{\alpha\beta} = -\tau \rho T \left[ \partial_t \left( \frac{j_\alpha}{\rho} \right) + \partial_\beta \left( \frac{j_\alpha}{\rho} \right) - \partial_\gamma \left( \frac{j_\gamma}{\rho} \right) \delta_{\alpha\beta} \right],$$  

$$P^{''}_{\alpha\beta} = \tau \left[ \frac{1}{2 \rho} \frac{\partial P^{eq}_{\alpha\beta}}{\partial T} \partial_t q^{eq}_{\gamma} - \tau \partial_t Q^{eq}_{\alpha\beta\gamma} \right].$$  

(A17)

(A18)

Substituting (A17) and (A18) into (A11), and combining the latter with (A9), and also combining (A11) with (A10), we derive the equations for the density and velocity $u_\alpha = j_\alpha/\rho$ to first order,

$$\partial_t \rho = -\partial_\alpha (\rho u_\alpha),$$  

$$\partial_t u_\alpha = -u_\beta \partial_\beta u_\alpha - \frac{1}{\rho} \partial_\alpha (\rho T) - \frac{1}{\rho} \partial_\beta \Pi_{\alpha\beta} - \frac{1}{\rho} \partial_\gamma P^{''}_{\alpha\gamma},$$  

(A19)

(A20)

where

$$\Pi_{\alpha\beta} = -\tau \rho T \left[ \partial_\beta u_\alpha + \partial_\alpha u_\beta - \partial_\gamma u_\gamma \delta_{\alpha\beta} \right],$$  

(A21)

is the nonequilibrium pressure tensor of a Newtonian fluid, and $P^{''}_{\alpha\gamma}$ (A18) is the deviation. Expanding Eq. (A18), we arrive at the explicit form of the deviation, Eq. (19).

Derivation of the equation for the energy (or, equivalently, for the temperature) is done in a similar way upon computing the first-order correction $q^{(1)}_{\alpha}$ from equation (A8). The resulting equation for the temperature reads:
\[ \partial_t T = -u_\alpha \partial_\alpha T - T \partial_\alpha u_\alpha - \frac{1}{2\rho} \partial_\kappa q'_\kappa - \frac{1}{2\rho} \partial_\gamma q''_\gamma. \]  

(A22)

The last two terms in this equation represent the deviation. Note that, unlike in the case of the momentum equation (A20), the deviation also includes a zero-order term \( q'_\kappa \). This happens because, with the choice of the guided equilibrium (8), we have set the equilibrium pressure tensor in the required Maxwell-Boltzmann form but not the equilibrium energy flux (why the latter is impossible on the \( D2Q9 \) was explained in section II). Finally, the first-order deviation (last term in (A22)) has the form given by Eqs. (22) and (23).

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