Entropic Lattice Boltzmann Method for Simulation of Thermal Flows

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Abstract

A new thermal entropic lattice Boltzmann model on the standard two-dimensional nine-velocity lattice is introduced for simulation of weakly-compressible flows. The new model covers a wider range of flows than the standard isothermal model on the same lattice, and is computationally efficient and stable.

Key words: Entropic lattice Boltzmann method, thermal flows.

1 Introduction

Lack of energy conservation in the isothermal lattice Boltzmann models (ILBM) [1–5] leads to spurious bulk viscosity and limits their use in many applications such as slow convective flows and microflows. Early attempts to include the energy conservation suffered from severe numerical instabilities. Nonlinearly stable thermal models were proposed [5], but they remaind so far less efficient because the advection term cannot be fitted on a lattice. So-called passive scalar models [6] are often used to simulate thermal flows. In these models, dynamics of the temperature field is done on a separate lattice. Apart from doubling the lattice, also the collision requires gradient terms to be evaluated

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at each lattice cite which deprives the scheme from the locality pertinent to the lattice Boltzmann method.

In this paper we revisit derivation of the thermal lattice Boltzmann model on the standard nine-velocity lattice ($D2Q9$). With an extension of the previous derivation of the isothermal entropic lattice Boltzmann model from continuous kinetic theory [5], we derive a novel thermal model on the same lattice. This model is valid for small temperature deviations and is pertinent to weakly-compressible flows. The lattice Bhatnagar-Gross-Krook scheme for the new thermal equilibrium is validated with the Couette flow between parallel walls at different temperatures, and the thermal convection flow in a cavity.

2 $D2Q9$ thermal entropic lattice BGK model

Discrete velocities are defined as the nodes of the third-order, two-dimensional Gauss-Hermit quadrature [3],

$$\mathbf{c}_i = \begin{cases} 0, & i = 0, \\ \{\cos((i-1)\pi/2), \sin((i-1)\pi/2)\}, & i = 1,2,3,4, \\ \sqrt{2}\{\cos[(i-5)\pi/2 + \pi/4], \sin[(i-5)\pi/2 + \pi/4]\}, & i = 5,6,7,8. \end{cases} \quad (1)$$

Generating function for the equilibrium (the H-function) has the form [5],

$$H = \sum_{i=0}^{8} f_i \ln\left(\frac{f_i}{W_i}\right), \quad (2)$$

where W_i are the weights of the nodes of the quadrature. The thermal local equilibrium is the minimum of H (2) under fixed mass, momentum, and energy,

$$\sum_{i=0}^{8} \left\{f_i, \mathbf{c}_i, c_i^2\right\} = \left\{\rho, \rho\mathbf{u}, D\rho T + \rho u^2\right\}, \quad (3)$$

where T is the temperature, and $D = 2$ is the dimension.

Starting from (2), and minimizing it under constraints (3), the equilibrium is found as: $f_i^{\text{eq}} = W_i \exp\left(\mu + \zeta_x c_{ix} + \zeta_y c_{iy} + \gamma c_i^2\right)$, where μ, ζ_x, ζ_y and γ are Lagrange multipliers. Their values can be found by perturbation in the momentum. At $\mathbf{u} = \mathbf{0}$, Lagrange multipliers can be evaluated exactly, and we obtain,

$$f_i^{eq}(\rho, \mathbf{0}, T) = \rho W_i(T) = \rho(1-T)^2 \left(\frac{T}{2(1-T)}\right)^{c_i^2}. \tag{4}$$

Note that the weights $W_i(T)$ in (4) are only seemingly independent of the weights of the Gauss-Hermit quadrature W_i. Indeed, for $T = T_0 = 1/3$ (reduced reference temperature of the Gaussian weight of the quadrature), we have $W_i(1/3) = W_i$. This implies that the present thermal model reduces to the standard isothermal equilibrium on the same lattice. Equation (4) also tells us that the variation of the reduced temperature is restricted to the interval $(0, 1)$. Variation of the temperature around the reference value T_0 is further restricted by the accuracy of the higher-order moments of the equilibrium populations (see below). For non-zero values of the momentum, equilibrium populations $f_i^{\text{eq}}(\rho, \boldsymbol{u}, T)$ are evaluated in terms of a series in u_α^n, and we here present the polynomial approximation of this series to the order u^3 in component notation:

$$\begin{aligned}
f_0^{eq} &= \rho\left\{(T-1)^2 + (T-1)u^2\right\} \qquad (5)\\
f_1^{eq} &= \frac{\rho}{2}\left\{(1-T)(T+u_x) + \frac{(1+T-4T^2)u^2}{4T} - \frac{(1-T){u_y}^2}{2T} - \frac{(3T-1)u_x^3}{4T} - \frac{(1+T)u_x u_y^2}{4T}\right\}\\
f_2^{eq} &= \frac{\rho}{2}\left\{(1-T)(T+u_y) + \frac{(1+T-4T^2)u^2}{4T} - \frac{(1-T){u_x}^2}{2T} - \frac{(3T-1)u_y^3}{4T} - \frac{(1+T)u_x^2 u_y}{4T}\right\}\\
f_3^{eq} &= \frac{\rho}{2}\left\{(1-T)(T-u_x) + \frac{(1+T-4T^2)u^2}{4T} - \frac{(1-T){u_y}^2}{2T} + \frac{(3T-1)u_x^3}{4T} + \frac{(1+T)u_x u_y^2}{4T}\right\}\\
f_4^{eq} &= \frac{\rho}{2}\left\{(1-T)(T-u_y) + \frac{(1+T-4T^2)u^2}{4T} - \frac{(1-T){u_x}^2}{2T} + \frac{(3T-1)u_y^3}{4T} + \frac{(1+T)u_x^2 u_y}{4T}\right\}\\
f_5^{eq} &= \frac{\rho}{4}\left\{T^2 + T(u_x+u_y) + u_x u_y + Tu^2 + \frac{3T-1}{4T}\left(u_x^3 + u_y^3\right) + u_x u_y(u_x+u_y)\frac{1+T}{4T}\right\}\\
f_6^{eq} &= \frac{\rho}{4}\left\{T^2 + T(u_y-u_x) - u_x u_y + Tu^2 + \frac{3T-1}{4T}\left(u_y^3 - u_x^3\right) - u_x u_y(u_y-u_x)\frac{1+T}{4T}\right\}\\
f_7^{eq} &= \frac{\rho}{4}\left\{T^2 + T(u_x-u_y) - u_x u_y + Tu^2 + \frac{3T-1}{4T}\left(u_x^3 - u_y^3\right) - u_x u_y(u_x-u_y)\frac{1+T}{4T}\right\}\\
f_8^{eq} &= \frac{\rho}{4}\left\{T^2 - T(u_x+u_y) + u_x u_y + Tu^2 - \frac{3T-1}{4T}\left(u_x^3 + u_y^3\right) - u_x u_y(u_x+u_y)\frac{1+T}{4T}\right\}
\end{aligned}$$

Note that at $T = 1/3$, and retaining the quadratic in u terms, (5) reduces to the standard isothermal equilibrium on the $D2Q9$ lattice [2].

With the equilibrium (5), we consider the simplest single relaxation time BGK equation,

$$\partial_t f_i + c_{i\alpha}\partial_\alpha f_i = -\tau^{-1}(f_i - f_i^{\rm eq}(\rho, \boldsymbol{u}, T)), \tag{6}$$

With the Chapman-Enskog method, and assuming small variation of the temperature around the reference temperature (a precise estimate will be given below), we derive the non-equilibrium pressure tensor and the heat flux of the present model:

$$P^{\rm neq}_{\alpha\beta} = -\tau\rho T\left[\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3}\delta_{\alpha\beta}\partial_\gamma u_\gamma\right], \tag{7}$$

$$q^{\rm neq}_\alpha = -2\tau\rho T\partial_\alpha T, \tag{8}$$

whereupon the transport coefficients are identified as $\mu = \tau\rho T$ (viscosity) and $\kappa = 2\tau\rho T$ (thermal conductivity). Note that, unlike the isothermal lattice Boltzmann models, the non-equilibrium (Newtonian) stress (7) is traceless, as pertinent to the classical case of Boltzmann's fluid considered herein. That is, by preserving the energy conservation in the derivation, we eliminated the spurious bulk viscosity of ILBM. The heat flux (8) obeys the Fourier law.

Let us comment on the domain of validity and accuracy of the present thermal model. The leading-order error is $\sim u\Delta T$, where ΔT is a characteristic deviation of the temperature from the reference value $T_0 = 1/3$ (error terms in the diagonal part of the third-order tensor $Q_{\alpha\beta\gamma} = \sum_{i=0}^{8} f_i^{\rm eq} c_{i\alpha}c_{i\alpha}c_{i\alpha}$). Thus, in order to maintain the same accuracy as in the isothermal lattice Boltzmann models, we need to choose the values for $u \sim 10^{-1} - 10^{-4}$ and $\Delta T/T_0 \sim 10^{-3} - 5.10^{-1}$ such that the product $u\Delta T$ is less than 10^{-3}. This accuracy is sufficient for simulations of weakly-compressible flows.

The lattice Boltzmann method is the second-order accurate implicit scheme for the kinetic equation (6), and is derived as follows: (i) Integrate (6) over the time δt, (ii) Apply trapezoidal rule in order to evaluate the collision term (second-order accuracy in δt), (iii) use the map, $f_i \to g_i = f_i + (\delta t/2\tau)(f - f^{\rm eq}(f))$, and note the property $f_i^{\rm eq} = g_i^{\rm eq}$. The result is the discrete-time scheme for (6):

$$g_i(\mathbf{x} + \mathbf{c}_i\delta t, t + \delta t) = g_i(\mathbf{x}, t) + \frac{2\delta t}{2\,\tau + \delta t}\left[g_i^{\rm eq}(\mathbf{x}, t) - g_i(\mathbf{x}, t)\right]. \tag{9}$$

Furthermore, fixing the grid points in such a way that if $\mathbf{x}$ is a grid point then also $\mathbf{x} \pm \mathbf{c}_i\delta t$ are the grid points, equation (9) becomes the lattice Bhatnagar-Gross-Krook scheme (LBGK). Note that the implicit second-order scheme for the populations f_i (9) can be interpreted as the explicit first-order scheme for the variables g_i obtained from a kinetic equation of the form (6) with a renormalized relaxation time $\tau' = \tau + (\delta t)/2$. We note in passing that a nonlinearly stable entropic version of the scheme (6) can be written for the populations f_i rather than for the functions g_i, where the factor $(2\delta t)/(2\tau+\delta t)$ in (9) is replaced with $(\alpha\delta t)/(2\tau + \delta t)$, and α is the solution to the entropy estimate, $H(f) = H(f + (\alpha/\tau)(f^{\rm eq} - f))$, with $\alpha \to 2\tau$ in the hydrodynamic limit (see, e. g. Eq. (9) in Ref. [5].)

We present the results of the validation studies performed. We simulate Couette flow between two parallel isothermal plates of which one is at rest and the other is moving with a constant velocity of U_0 (in grid units) parallel to the stationary wall. The temperature of the moving wall is maintained at $T_0+\Delta T$ while the other wall is at a constant temperature of T_0 (reference temperature). For these boundary conditions, the steady state solution for non-dimensional temperature reads as $T' = \frac{T(X)-T_0}{\Delta T} = X + \frac{\mu U_0^2}{2\kappa\rho\Delta T} X(1 - X)$, where X denotes non-dimensional width of the channel. Diffusive wall boundary condition [7] was used in the simulation. Comparison of the simulation with the analytical solution is given in Fig. 1.

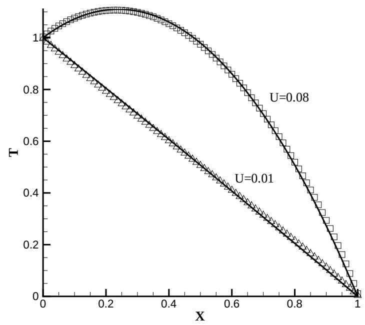

Fig. 1. Comparison of ELBM(symbol) with analytical solution(line) for thermal Couette flow problem.

Natural convection in a square cavity was also simulated using the present model. The fluid enclosed in a square cavity is suddenly heated on one side (left) and cooled on the opposite side (right) via isothermal walls; the other two walls are adiabatic. Gravitational force is perpendicular to the adiabatic walls. We present the results of simulations up to Rayleigh numbers $\mathrm{Ra} = 10^5$ in Fig. 2 where the temperature field in the cavity for various Ra is demonstrated. Results are found to be in a qualitative agreement with other studies. However, the use of the single relaxation time model (fixed Prandtl number) precludes a quantitative comparison which is out of the scope of this paper.

In conclusion, the main result of this paper is that the construction of the isothermal entropic lattice BGK models of Refs. [4,5] can be extended to the lattice Boltzmann models capable of simulating weakly-compressible thermal flows. The thermal BGK model retains all the features of the genuine lattice

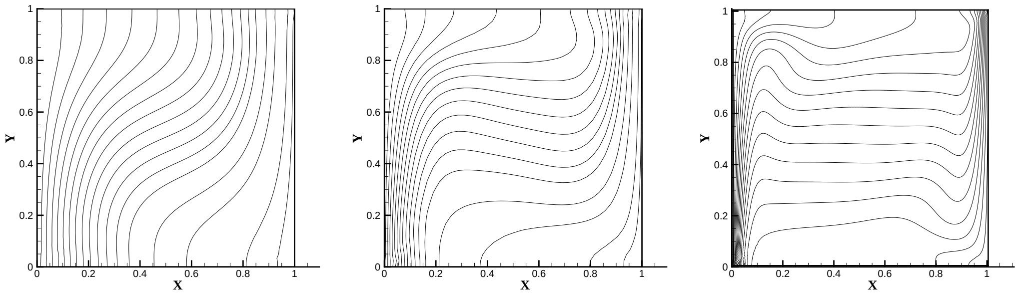

Fig. 2. Isotherms of the steady-state convection in the cavity at $Ra = 10^3$, $Ra = 10^4$, and $Ra = 10^5$ (from left to right).

Boltzmann, that is, locality of collisions, ease and efficiency of the numerical implementation, and stability. Unlike the isothermal model, the present thermal model has no spurious bulk viscosity, and thus is a valid model of Boltzmann's fluid. It is straightforward to switch from the standard isothermal LBGK code to the present thermal model by just changing the isothermal equilibrium to that given by equation (5). Extension of the present LBGK to a model with a tailored Prandtl number, as well as the stability enhancement via the entropy estimate, will be done in our subsequent publications. IVK was supported by the BFE-Project Nr. 100862. SSC and NIP were supported by ETH Projects 0-20280-05 and 0-20235-05.

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