

A Hydrodynamically Correct Thermal Lattice Boltzmann Model

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A three-dimensional lattice-Boltzmann model which yields correct hydrodynamics at the Navier–Stokes level of the Chapman–Enskog expansion requires a minimum of 26 velocities. We present results for a model with one additional velocity, determined by maximizing the equilibrium entropy. For compressible Rayleigh–Bénard convection the model is more accurate but considerably less stable, than a previous, approximate 21-speed model.

KEY WORDS: Lattice-Boltzmann equation; Rayleigh–Bénard convection; numerical stability.

1. INTRODUCTION

The lattice gas automaton (LGA) method^(1,2) models fluid-dynamic behavior by creating a fictitious molecular dynamical world of particles moving on a regular lattice. These particles travel between neighboring lattice sites, arriving synchronously at the lattice sites at integral multiples of the simulation time step, where they engage in collisions that conserve particle number, momentum, and (for thermal models) energy. The LGA models are Boolean systems that allow only zero or one particle at each site for each of the permitted particle velocities. Macroscopic quantities, such as mass density and fluid velocity, are obtained by spatial or temporal averaging to eliminate the large amount of statistical noise in the LGA calculations.

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The lattice Boltzmann equation (LBE)⁽³⁻⁵⁾ model eliminates this statistical noise by directly simulating the ensemble-averaged behavior of an LGA system. The LGA's Boolean variables are replaced by floating point variables $f_\alpha(\mathbf{r})$ representing the expected number of particles traveling in the α th direction at position \mathbf{r} of the lattice. The linearized LBE collision operator redistributes the incoming particle mass amongst the outgoing particle velocities in such a way as to relax toward a local equilibrium distribution determined from the local conserved densities.

Initially, LBE models included only mass and momentum as conserved quantities. They involved transcriptions of particle collision rules for the effect of the collision operator on the velocity distribution. These models, for example for the Kelvin-Helmholtz instability, were encouragingly found to be somewhat more stable than the standard numerical schemes for solving the Navier-Stokes equations. To include thermal effects as well but approximately, the similarity between the Navier-Stokes velocity and temperature equations can be exploited to formulate LBE models that treat temperature as an additional velocity component. Such an example is the simulation of Rayleigh-Bénard convection using a single-speed LBE model of the Boussinesq equations.⁽⁶⁾ To evaluate thermal effects more accurately multispeed LBE models must be employed to include energy conservation explicitly. In order to simplify the calculation the number of velocities considered was reduced in earlier work, but they then did not exactly model the full Navier-Stokes equations.^(7,8) This article addresses the problem of how to build an exact model (neglecting Burnett-level corrections) and the model's resulting numerical stability.

2. THERMAL LBE MODEL

Construction of an LBE model requires specification of the structure of the lattice and the set of permitted particle velocities $\{\mathbf{c}_\alpha\}$, the collision operator $\Omega_{\alpha\beta}$, and the local equilibrium mass distribution $f_\alpha^{(0)}$. The following conventions are used in describing an LBE model. The time required for particles to travel from source to destination sites between successive collisions τ is taken as the unit of time. For models using the Lax-Wendroff streaming operator (see below), this time will differ from the simulation time step δt . The nearest neighbor spacing of the lattice becomes the unit of length, and the model's particles are taken to have unit mass, $m = 1$. We take the Boltzmann factor k to be unity, which establishes a temperature scale through the relation $\varepsilon = (3/2)k/mT$, where ε is the internal energy per unit mass. Greek indices are used to iterate over the directions of particle motion, Latin subscripts to denote the Cartesian components of vectors and tensors.

The most general restriction on the form of $f_{\alpha}^{(0)}$ required to obtain Navier–Stokes behavior demands that its lowest 26 velocity moments match those of the Maxwell–Boltzmann distribution.⁽⁹⁾ It so happens that the velocity set consisting of speed $\sqrt{2}$, $\sqrt{3}$, and speed 2 particles on a cubic lattice contains 26 elements, and the symmetries of this set match those of the 26 Maxwell–Boltzmann moments. Moreover, all of these moments may be independently specified and thus this velocity set constitutes a minimal LBE model yielding correct Navier–Stokes hydrodynamic behavior with the equilibrium mass distribution $f_{\alpha}^{(0)}$ uniquely determined. Unfortunately, this model is found to be numerically unstable unless its transport coefficients are made quite large.

To improve stability, the velocity set can be decreased or increased. If the velocity set is decreased then the model will necessarily violate some of the velocity-moment constraints, and thus will deviate from Navier–Stokes behavior. With care, these deviations can be made to be of sufficiently high order in the fluid velocity \mathbf{u} that the resulting model may still be useful for simulating low-Mach-number flows. Such a thermal LBE model, with comparatively modest numerical stability, using a three-dimensional cubic lattice with 21 particle velocities has been described previously.⁽¹⁰⁾

In this paper the velocity set is increased from the 26-velocity minimal set by one additional speed, specifically, a zero-velocity (i.e., stopped) particle population in the hope of increasing the numerical stability of the scheme while retaining the correct Navier–Stokes solution. The extra degree of freedom provided by the stopped particle population is used to maximize the entropy at zero fluid velocity. The equilibrium entropy S in the 27-velocity model is then

$$S = -f_0^{(0)} \ln f_0^{(0)} - 12f_{\sqrt{2}}^{(0)} \ln f_{\sqrt{2}}^{(0)} - 8f_{\sqrt{3}}^{(0)} \ln f_{\sqrt{3}}^{(0)} - 6f_2^{(0)} \ln f_2^{(0)} \quad (1)$$

where the subscripts identify the particle speeds. At zero fluid velocity the 26 moment constraints reduce to

$$\begin{aligned} f_0^{(0)} + 12f_{\sqrt{2}}^{(0)} + 8f_{\sqrt{3}}^{(0)} + 6f_2^{(0)} &= \rho \\ 24f_{\sqrt{2}}^{(0)} + 24f_{\sqrt{3}}^{(0)} + 24f_2^{(0)} &= 2\rho\varepsilon \\ 48f_{\sqrt{2}}^{(0)} + 72f_{\sqrt{3}}^{(0)} + 96f_2^{(0)} &= (20/3)\rho\varepsilon^2 \end{aligned} \quad (2)$$

where ε is the internal energy per unit mass and ρ is the mass density. Maximizing S under these constraints yields

$$f_0^{(0)} \approx 0.693\varepsilon^2 - 1.248\varepsilon + 0.903 \quad (3)$$

which uniquely determines the equilibrium distribution at zero fluid velocity. This value of $f_0^{(0)}$ is also used at nonzero fluid velocity as an approximate solution to the more general problem of maximizing entropy in a moving fluid.

The collision operator is best described in terms of velocity moments of the mass distribution. The postcollisional mass distribution f'_α is generated from the precollisional distribution f_α through the collision operator

$$f'_\alpha(\mathbf{r}, t) = f_\alpha(\mathbf{r}, t) + \sum_\beta \omega_{\alpha\beta} f_\beta^{(\text{neq})}(\mathbf{r}, t) \quad (4)$$

where $f_\alpha^{(\text{neq})} = f_\alpha - f_\alpha^{(0)}$. The collision operator is fully defined by specifying its effect on a complete set of velocity moments; the present model has 27 particle velocities and thus 27 independent moments are required for a complete specification. The five lowest velocity moments are just the conserved densities. The conserved densities are contained entirely in the equilibrium distribution, and thus the action of the collision operator on these moments is irrelevant. Higher moments are associated with viscous and thermal transport properties; in particular, the action of the collision operator on the nonequilibrium part of the trace-free second moments determines the viscosity of the model. Similarly, relaxation of the traceful nonequilibrium third moments controls the thermal conductivity. These viscous and thermal transport moments are taken to be eigenvectors of the collision operator, i.e.,

$$\sum_\alpha (c_{\alpha a} c_{\alpha b} - c_\alpha^2 \delta_{ab}/3) f'_\alpha^{(\text{neq})} = (\lambda_s + 1) \sum_\alpha (c_{\alpha a} c_{\alpha b} - c_\alpha^2 \delta_{ab}/3) f_\alpha^{(\text{neq})} \quad (5)$$

$$\sum_\alpha (\mathbf{c}_\alpha - \mathbf{u})^2 (c_{\alpha a} - \mathcal{Q}_a) f'_\alpha^{(\text{neq})} = (\lambda_e + 1) \sum_\alpha (\mathbf{c}_\alpha - \mathbf{u})^2 (c_{\alpha a} - \mathcal{Q}_a) f_\alpha^{(\text{neq})} \quad (6)$$

where λ_s and λ_e are eigenvalues of Ω . The kinematic viscosity ν and the thermal diffusivity χ are determined by

$$\nu = \frac{2}{\lambda_s} \delta t \varepsilon \left(\frac{1}{\lambda_s} + \frac{1}{2} \right), \quad \chi = -\frac{2}{3} \delta t \varepsilon \left(\frac{1}{\lambda_e} + \frac{1}{2} \right) \quad (7)$$

The bulk viscosity is zero, as must be the case for any ideal energy-conserving gas (since $\sum_\alpha c_\alpha^2 f_\alpha^{(\text{neq})}$ must be zero).

The provision of separate eigenvalues for the relaxation of the viscous and thermal transport moments allows this model to simulate fluids with arbitrary Prandtl number $\text{Pr} = \nu/\chi$. The thermal lattice BGK (LBGK)⁽¹¹⁾ or single-relaxation-time (SRT)⁽¹²⁾ models, in which the nonequilibrium distribution is relaxed uniformly to equilibrium using a single eigenvalue,

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are restricted to $Pr = 1$. Previous thermal lattice Boltzmann models with two relaxation times contained an error in the energy equation when the Prandtl number was not equal to one, namely the term representing dissipation and transport of energy by the viscous forces was multiplied by the thermal conductivity rather than by the viscosity. This defect is removed in the present model by relaxing the third moments in the frame of the moving fluid, rather than in the frame of the lattice. Cross terms in the third powers of $(c_\alpha - u)$ appearing in Eq. (6) couple second moments of the nonequilibrium distribution, $\sum_\alpha c_{\alpha a} c_{\alpha b} f_\alpha^{(neq)}$, into the energy equation. This coupling corrects the transport coefficient multiplying the viscous term.

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Higher even moments of the nonequilibrium distribution are relaxed using the viscous eigenvalue λ_v and higher odd moments are relaxed using λ_e . This scheme was found to produce somewhat better stability than relaxing higher moments straight to equilibrium.

The collision operator is not directly implemented as a matrix product as suggested by Eq. (4); rather, the various velocity moments discussed above are first projected out of $f_\alpha^{(neq)}$. In this velocity-moment basis the collision operator becomes diagonal and its action on $f_\alpha^{(neq)}$ may then be easily computed. The output of the collision operator is then transformed back to the particle-population basis of Eq. (4), and then added to $f_\alpha^{(0)}$.

3. STABILITY CONSIDERATIONS

Standard mathematical methods to stabilize the model have been tried since the conventional LBE scheme operates exactly at the Courant-Friedrichs stability criterion. In LBE models, time evolves in two steps: the collision process, in which the distributions at a site are relaxed toward equilibrium, and the advection process, in which the distributions are moved to their new lattice sites. The simplest advection scheme is to translate distributions by an integer displacement according to the speed of the distribution. However, since the accuracy of the collision process is only $O(\delta t^2)$, one may instead use an advection process that maintains $O(\delta t^2)$ accuracy yet improves total stability. For example, the Lax-Wendroff scheme⁽¹⁷⁾ discretizes the advection equation as

$$f_\alpha(\mathbf{r}, t + \delta t) = f'_\alpha(\mathbf{r}, t) - \frac{C}{2} (f'_\alpha(\mathbf{r} + \tau \mathbf{c}_{\alpha y}) - f'_\alpha(\mathbf{r} - \tau \mathbf{c}_{\alpha x}, t)) + \frac{C^2}{2} (f'_\alpha(\mathbf{r} + \tau \mathbf{c}_{\alpha y}) + f'_\alpha(\mathbf{r} - \tau \mathbf{c}_{\alpha y}) - 2f'_\alpha(\mathbf{r}, t)) \quad (8)$$

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where $C = \delta t/\tau$ is the Courant number. Note that a redistribution among neighboring sites is called for that involves distributions displaced upwind,

displaced downwind, and left in place. The appearance of δt in the expressions for the transport coefficients guarantees that the collision process will be appropriately adjusted to suit the reduced simulation time step. In general, one finds that the use of Lax–Wendroff scheme significantly improves stability with some loss of accuracy.⁽¹⁰⁾ Using a predictor-corrector formulation for the combined advection and collision processes yielded no significant improvement in the model's stability or accuracy.

4. SIMULATION RESULTS

The 27-velocity thermal LBE model has been used to simulate compressible Rayleigh–Bénard convection.⁽¹⁸⁾ The results are compared against those obtained from a 21-speed LBE model and an explicit MacCormack finite-difference (FD) solver.⁽¹⁹⁾ These simulations have been done primarily in two dimensions to reduce the CPU time required and to allow the use of larger grids having finer spatial resolution. However, full three-dimensional simulations were performed to verify the numerical stability of the model with respect to wave vectors lying off the x - y plane.

Lattice Boltzmann models often employ simplified boundary conditions (e.g., no-slip boundary conditions implemented by means of backreflecting boundary sites). While simple to implement, these schemes generate incorrect boundary layers^(13, 14) which have been addressed by more elaborate boundary rules.^(15, 16) Thermal LBE models introduce additional difficulty through the need to provide isothermal boundaries. This requirement may be satisfied by using techniques employed in standard finite-difference methods, namely extrapolation of fluid-dynamic quantities from the interior of the fluid onto the boundary of the computational domain. We used quadratic extrapolation for conserved quantities and linear extrapolation for nonequilibrium modes; see (ref. 10) for a detailed description.

Table I. Peak Fluid Velocity of Convective Flows Simulated by the LBE Model for Three Different Temperature Ratios and Two Different Grid Sizes^a

| T_H/T_C | $d=100$ | 200 |
|-----------|-------------------|---------|
| 1.2 | 0.04237 (0.04243) | 0.04231 |
| 1.4 | 0.07670 (0.07741) | 0.07662 |
| 1.5 | 0.09126 (0.09244) | 0.09115 |

^aThe values in parentheses are those produced by the MacCormack finite-difference code. Fluid velocities are normalized by the local speed of sound.

Table II. Normalized RMS Deviation for Density, Temperature, and Velocity Between LBE ($d=100$) and MacCormack Simulation Results for Different Temperature Ratios

| T_H/T_C | Density | Temperature | Velocity |
|-----------|---------|-------------|----------|
| 1.2 | 0.00105 | 0.00115 | 0.00120 |
| 1.4 | 0.00543 | 0.00555 | 0.00683 |
| 1.5 | 0.00860 | 0.00809 | 0.01103 |

The simulation models flow in a two-dimensional rectangular region of width L and height d bounded by rigid walls at the top and bottom and with periodic boundary conditions employed at the sides of the system. No-slip, isothermal boundary conditions are enforced at the top and bottom walls, which are maintained at temperatures T_C and T_H , respectively, with $T_C < T_H$. A gravitational force exerts a downward acceleration g on the fluid. An (x, z) coordinate system is adopted with x increasing to the right and z increasing downward. The locations of the top and bottom walls are taken to be $z = z_0$ and $z = z_0 + d$, respectively, where $z_0 = dT_C/(T_H - T_C)$. The fluid is set up with initial temperature, density, and pressure

$$T_0(z) = T_C z/z_0, \quad \rho_0(z) = \rho_C (z/z_0)^n, \quad p_0(z) = p_C (z/z_0)^{n+1} \quad (9)$$

where ρ_C and p_C are the density and pressure at the top wall and n is the polytropic index (i.e., $p \propto T^n$). The fluid velocity is initially zero plus a small perturbation which may be random or of the form $u_z = u_{z0} \sin(2\pi x/L) \sin[\pi(z - z_0)/d]$. The latter form leads to faster startup of the convective rolls, but selects a particular horizontal wave number for development of the convective instability.

The flow is characterized by six dimensionless parameters: the fluid's ratio of specific heats $\gamma = C_p/C_v$ and Prandtl number, the aspect ratio

Table III. Normalized RMS Deviation for Density, Temperature, and Velocity Between LBE ($d=200$) and MacCormack Simulation Results for Different Temperature Ratios

| T_H/T_C | Density | Temperature | Velocity |
|-----------|---------|-------------|----------|
| 1.2 | 0.00152 | 0.00151 | 0.00152 |
| 1.4 | 0.00679 | 0.00662 | 0.00889 |
| 1.5 | 0.01001 | 0.00912 | 0.01316 |

Table IV. Peak Normalized Fluid Velocity as a Function of Rayleigh Number and Lax-Wendroff Time Step for $d=50$ and $T_H/T_C=1.5^a$

| Ra | $\delta t = 0.95$ | 0.90 | 0.80 | MacCormack |
|--------|-------------------|--------|--------|------------|
| 8,000 | 0.0930 | 0.0939 | 0.0946 | 0.0924 |
| 16,000 | Unstable | 0.1529 | 0.1539 | 0.1518 |

^a Runs listed as unstable diverged due to numerical instability. The last column gives peak normalized fluid velocity obtained from the MacCormack solver on a 150×100 grid.

$A = L/d$, the temperature ratio T_H/T_C , the polytropic index n , and the Rayleigh number

$$Ra = \frac{gd^4}{T_C \nu_C \chi_C} \left(\frac{T_H - T_C}{d} - \frac{g}{C_p} \right) \quad (10)$$

where ν_C and χ_C are the values of the transport coefficients measured at density ρ_C . The transport coefficients are taken to be independent of T and to scale inversely with ρ . The simulations described here fix $\gamma = 5/3$ (since the LBE gas is ideal and monatomic), $Pr = 2/3$, $A = 1.5$, and $n = 0$. The last constraint implies the relation $g = k(T_H - T_C)/md$, so that gravity balances the temperature difference and the initial data (uniform density, linear temperature gradient) form an unstable equilibrium solution.

After an initial transient, the system settles into a state of steady convective flow. For $Ra = 8000$, the peak fluid velocities achieved in runs with three different temperature ratios are shown in Table I. These velocities have been normalized by the local speed of sound (which varies with T). The root mean square deviations between the LBE and the MacCormack FD results are given in Tables II and III. The RMS density deviation is

Table V. RMS Error in Normalized Fluid Velocity Between the LBE Lax-Wendroff Runs (75×50 grid) and the MacCormack Simulations (150×100 Grid) for $T_H/T_C = 1.5^a$

| Ra | $\delta t = 0.95$ | 0.90 | 0.80 |
|--------|-------------------|--------|--------|
| 8,000 | 0.0073 | 0.0139 | 0.0200 |
| 16,000 | Unstable | 0.0119 | 0.0209 |

^a Runs listed as unstable diverged due to numerical instability.

calculated as $\langle (\rho_{\text{LBE}} - \rho_{\text{FD}})^2 \rangle^{1/2} / \langle (\rho_{\text{FD}} - \rho_0)^2 \rangle^{1/2}$, where the angle brackets indicate averaging over all interior lattice sites; the temperature and velocity deviations are calculated similarly. For both grid sizes the RMS error varies with the peak fluid velocity as u^a , where $a \approx 2.5$ for the density and temperature deviations and $a \approx 3$ for the velocity deviations. In contrast, for the 21-speed LBE model, all three deviations varied as u^1 due to the errors introduced by employing a reduced velocity set. In the 27-velocity set not only is the absolute error reduced by an order of magnitude, but it seems to be dominated by higher order terms in the Chapman-Enskog expansion beyond the validity of Navier-Stokes hydrodynamics as indicated by the observation that the cubic velocity deviation persists and gets even larger for the finer grid size. Thus, in comparing absolute error in the 21- and 27-velocity models, the RMS density and temperature deviations are smaller by a factor of 17 and the RMS velocity deviations by a factor of 7 in the low-speed case ($T_H/T_C = 1.2$). The 27-speed model was found to be numerically unstable even at moderate Rayleigh number (e.g., $Ra \approx 10,000$ for $d = 50$) with a stability range smaller than that of the 21-speed model. The stability can be improved using the Lax-Wendroff scheme, but at the expense of accuracy (see Tables IV and V).

5. CONCLUSIONS

This paper describes a three-dimensional multispeed thermal LBE model which produces fully correct hydrodynamic behavior at the Navier-Stokes level of the Chapman-Enskog expansion. Good agreement (less than about 1% error) is found when comparing this model with a conventional explicit finite-difference Navier-Stokes solver in modeling compressible Rayleigh-Bénard convective flows. However, the numerical stability leaves much to be desired. We ascribe the earlier, quite good stability of the momentum-only calculation to the use of a very physical particle-like collision operator, while in the present model, which includes energy, that particle-like aspect is lost in the requirement of satisfying moment conditions. Since standard numerical methods to stabilize the solution showed only moderate success, it seems that the only option for stabilization is to still further increase the number of velocities, since we know that in the limit of having a very large set of velocities leads to the Maxwell-Boltzmann distribution that has stability. The problem is that one does not know off hand by what criterion to determine the additional velocities and besides that increasing the number of velocities beyond the already rather large number of 27 velocities defeats the whole purpose of the enterprise to have a simple model, with only a few degrees of freedom, of hydrodynamic behavior. The large number of particle velocities required

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for the LBE model also results in greatly increased computer memory requirements relative to a conventional solver, roughly a factor of 5 (27 velocities vs. 5 conserved densities for the conventional solver). The LBE method also ran somewhat slower ^{than} the finite-difference method, with running times less than a factor of 2 greater than the MacCormack scheme on comparable size grids.

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Considering that the LBE model took comparable computer time to the explicit finite-difference MacCormack calculation, that the boundary conditions are treated analogously, that memory requirements are significantly greater, and that numerical stability is significantly poorer, we find no potential advantage in using an LBE model over a conventional Navier–Stokes solver for thermal systems.

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