

## Lattice Boltzmann thermohydrodynamics

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(Received 23 July 1992)

We introduce a lattice Boltzmann computational scheme capable of modeling thermohydrodynamic flows of monatomic gases. The parallel nature of this approach provides a numerically efficient alternative to traditional methods of computational fluid dynamics. The scheme uses a small number of discrete velocity states and a linear, single-time relaxation collision operator. Numerical simulations in two dimensions agree well with exact solutions for adiabatic sound propagation and Couette flow with heat transfer.

PACS number(s): 47.10.+g, 02.70.-c

The lattice Boltzmann (LB) method is a discrete, in space and time, microscopic, kinetic-equation description for the evolution of the velocity distribution function of a fluid [1–3]. Like lattice-gas (LG) automata [4], LB methods are well suited for simulating a variety of physical systems in a parallel computing environment. As a result, the LB approach has found recent successes in a host of fluid dynamical problems, including flows in porous media [5], magnetohydrodynamics [6], immiscible fluids [5], and turbulence [7,8]. Its efficiency competes with, and in some cases exceeds, that of traditional numerical methods, while its physical interpretation is transparent.

Noticeably absent, though, from the list of successful applications of LG and LB methods is a model that can simulate the full set of thermohydrodynamic equations. Previous attempts at developing such a model have *exclusively* involved LG automata [9,10] whose Fermi-Dirac equilibrium distributions do not have sufficient flexibility to guarantee the correct form of the energy equation (3). LB methods are considerably more flexible, but have not, until now, been applied to this problem.

The thermohydrodynamic equations of classical kinetic theory result from a Chapman-Enskog expansion of the *continuum* Boltzmann equation, with the assumption of a Maxwellian equilibrium distribution. Since an exact Maxwellian distribution with a continuous distribution of velocities, both in angle and magnitude, cannot be implemented in a system that is discrete in both space and time, we seek an alternative distribution that will nevertheless give rise to the same macroscopic physics. In this Rapid Communication we address this issue and introduce a LB scheme that can simulate the following continuity, momentum, and energy equations for viscous, compressible, and heat-conducting flows:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_\alpha} (nu_\alpha) = 0, \quad (1)$$

$$n \frac{\partial u_\alpha}{\partial t} + nu_\beta \frac{\partial u_\alpha}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\alpha} \left[ \lambda \frac{\partial u_\gamma}{\partial x_\gamma} \right] + \frac{\partial}{\partial x_\beta} \left[ \mu \left( \frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial x_\beta} \right) \right], \quad (2)$$

and

$$n \frac{\partial \epsilon}{\partial t} + nu_\alpha \frac{\partial \epsilon}{\partial x_\alpha} = -p \frac{\partial u_\gamma}{\partial x_\gamma} + \frac{\partial}{\partial x_\beta} \left[ \kappa \frac{\partial T}{\partial x_\beta} \right] + \mu \left[ \frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right] \frac{\partial u_\beta}{\partial x_\alpha} + \lambda \left[ \frac{\partial u_\gamma}{\partial x_\gamma} \right]^2, \quad (3)$$

where  $n$  is the fluid mass density,  $\epsilon$  is the internal energy per unit mass and is proportional to the temperature  $T$ ,  $u$  is the local velocity,  $p$  is the pressure, and  $\lambda$ ,  $\mu$ , and  $\kappa$  are the second viscosity, shear viscosity, and thermal conductivity, respectively.

The starting point of the LB method is the kinetic equation for the velocity distribution function,  $f_{\sigma i}(\mathbf{x}, t)$ :

$$f_{\sigma i}(\mathbf{x} + \mathbf{e}_{\sigma i}, t + 1) - f_{\sigma i}(\mathbf{x}, t) = \Omega_{\sigma i}, \quad (4)$$

where the non-negative, real number  $f_{\sigma i}(\mathbf{x}, t)$  is the mass of fluid at lattice node  $\mathbf{x}$  and time  $t$ , moving in direction  $i$  with speed  $|\mathbf{e}_{\sigma i}| = \sigma$ ,  $\sigma = 1, 2, \dots, N$ , where  $N$  is the number of speeds. The  $\sigma = 0$  speed corresponds to the component of the fluid that is at rest. The term  $\Omega_{\sigma i}$  represents the rate of change of  $f_{\sigma i}$  due to collisions. For computational efficiency, it is desirable to find the minimal set of  $\sigma$  and  $i$ , for which a coarse graining of the kinetic equation (4) leads to the macroscopic dynamics of interest.

The microscopic dynamics associated with Eq. (4) can be viewed as a two-step process: free streaming and collision. During the free-streaming step,  $f_{\sigma i}(\mathbf{x} + \mathbf{e}_{\sigma i})$  is replaced by  $f_{\sigma i}(\mathbf{x})$ . Thus each site exchanges mass with its neighbors, i.e., sites connected by lattice vectors  $\mathbf{e}_{\sigma i}$ . In the collision step the distribution functions at each site then relax toward a state of local equilibrium. For simplicity, we consider the linearized, single-time-relaxation model of Bhatnagar, Gross, and Krook [11], which has recently been applied to LB models [6,12–14]:

$$\Omega_{\sigma i} = -\frac{1}{\tau} (f_{\sigma i} - f_{\sigma i}^{\text{eq}}). \quad (5)$$

The collision operator  $\Omega_{\sigma i}$  conserves the local mass, momentum, and kinetic energy:  $\sum_{\sigma, i} \Omega_{\sigma i} = 0$ ,

$\sum_{\sigma,i} \Omega_{\sigma i} \mathbf{e}_{\sigma i} = 0$ , and  $\sum_{\sigma,i} \Omega_{\sigma i} \mathbf{e}_{\sigma i}^2 / 2 = 0$ , and the parameter  $\tau$  controls the rate at which the system relaxes to the local equilibrium,  $f_{\sigma i}^{\text{eq}}$ .

The LB method, unlike LG's, has considerable flexibility in the choice of the local equilibrium distribution. A general equilibrium distribution is given by a truncated power series in the local velocity  $\mathbf{u}$ , valid for  $|\mathbf{u}| \ll 1$ ,

$$f_{\sigma i}^{\text{eq}} = A_{\sigma} + B_{\sigma} \mathbf{e}_{\sigma i} \cdot \mathbf{u} + C_{\sigma} (\mathbf{e}_{\sigma i} \cdot \mathbf{u})^2 + D_{\sigma} u^2 + E_{\sigma} (\mathbf{e}_{\sigma i} \cdot \mathbf{u})^3 + F_{\sigma} (\mathbf{e}_{\sigma i} \cdot \mathbf{u}) u^2, \quad (6)$$

where the velocity is defined by  $n\mathbf{u} = \sum_{\sigma,i} f_{\sigma i} \mathbf{e}_{\sigma i}$ . The coefficients  $A, B, \dots, F$  are functions of the local density  $n = \sum_{\sigma,i} f_{\sigma i}$  and internal energy  $n\varepsilon = \sum_{\sigma,i} f_{\sigma i} (\mathbf{e}_{\sigma i} - \mathbf{u})^2 / 2$ , and their functional forms depend on the geometry of the underlying lattice.

The long-wavelength, low-frequency behavior of the system is obtained by a Taylor-series expansion of Eq. (4) to second order in the lattice spacing and time step:

$$\frac{\partial f_{\sigma i}}{\partial t} + \mathbf{e}_{\sigma i} \cdot \nabla f_{\sigma i} + \frac{1}{2} \mathbf{e}_{\sigma i} \mathbf{e}_{\sigma i} : \nabla \nabla f_{\sigma i} + \mathbf{e}_{\sigma i} \cdot \nabla \frac{\partial f_{\sigma i}}{\partial t} + \frac{1}{2} \frac{\partial}{\partial t} \frac{\partial}{\partial t} f_{\sigma i} = \Omega_{\sigma i}. \quad (7)$$

In order to derive the macroscopic hydrodynamic equations, we adopt the following Chapman-Enskog multi-scale expansions. We expand the time derivative as

$$\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \dots, \quad (8)$$

where  $\epsilon$  is a small parameter, and the lower-order terms in  $\epsilon$  vary more rapidly. Because we are interested in small departures from local equilibrium, we expand the distribution function as

$$f_{\sigma i} = f_{\sigma i}^{\text{eq}} + \epsilon f_{\sigma i}^{(1)} + \epsilon^2 f_{\sigma i}^{(2)} + \dots, \quad (9)$$

and the collision operator as

$$\frac{\Omega_{\sigma i}}{\epsilon} = -\frac{1}{\tau \epsilon} (\epsilon f_{\sigma i}^{(1)} + \epsilon^2 f_{\sigma i}^{(2)} + \dots). \quad (10)$$

Substituting the above expansions into the kinetic equation, we find

$$\frac{\partial}{\partial t_1} f_{\sigma i}^{\text{eq}} + \mathbf{e}_{\sigma i} \cdot \nabla f_{\sigma i}^{\text{eq}} = -\frac{1}{\tau} f_{\sigma i}^{(1)} \quad (11)$$

to order  $\epsilon$ , and

$$\frac{\partial}{\partial t_1} f_{\sigma i}^{(1)} + \frac{\partial}{\partial t_2} f_{\sigma i}^{\text{eq}} + \mathbf{e}_{\sigma i} \cdot \nabla f_{\sigma i}^{(1)} + \frac{1}{2} \mathbf{e}_{\sigma i} \mathbf{e}_{\sigma i} : \nabla \nabla f_{\sigma i}^{\text{eq}} + \mathbf{e}_{\sigma i} \cdot \nabla \frac{\partial}{\partial t_1} f_{\sigma i}^{\text{eq}} + \frac{1}{2} \frac{\partial^2}{\partial t_1^2} f_{\sigma i}^{\text{eq}} = -\frac{1}{\tau} f_{\sigma i}^{(2)} \quad (12)$$

to order  $\epsilon^2$ . With Eq. (11) and some algebra, we can rewrite Eq. (12) as

$$\frac{\partial}{\partial t_2} f_{\sigma i}^{\text{eq}} + \left[ 1 - \frac{1}{2\tau} \right] \left[ \frac{\partial}{\partial t_1} f_{\sigma i}^{(1)} + \mathbf{e}_{\sigma i} \cdot \nabla f_{\sigma i}^{(1)} \right] = -\frac{1}{\tau} f_{\sigma i}^{(2)}. \quad (13)$$

Summing moments of Eqs. (11) and (13), we obtain to

order  $\epsilon^2$ , the continuity equation

$$\frac{\partial n}{\partial t} + \nabla \cdot n\mathbf{u} = 0, \quad (14)$$

the momentum equation

$$\frac{\partial n\mathbf{u}}{\partial t} + \nabla \cdot \mathbf{\Pi} = 0, \quad (15)$$

and the energy equation

$$\frac{\partial n\varepsilon}{\partial t} + \nabla \cdot (n\varepsilon\mathbf{u}) + \nabla \cdot \mathbf{q} + \mathbf{P} : \nabla \mathbf{u} = 0. \quad (16)$$

The momentum flux tensor

$$\mathbf{\Pi} = \sum_{\sigma,i} \left[ f_{\sigma i}^{\text{eq}} + \left[ 1 - \frac{1}{2\tau} \right] f_{\sigma i}^{(1)} \right] \mathbf{e}_{\sigma i} \mathbf{e}_{\sigma i};$$

the heat flux,

$$\mathbf{q}_{\alpha} = \frac{1}{2} \sum_{\sigma,i} \left[ f_{\sigma i}^{\text{eq}} + \left[ 1 - \frac{1}{2\tau} \right] f_{\sigma i}^{(1)} \right] (\mathbf{e}_{\sigma i} - \mathbf{u})^2 (\mathbf{e}_{\sigma i} - \mathbf{u})_{\alpha},$$

and  $\mathbf{P}$  is the pressure tensor,

$$\mathbf{P}_{\alpha\beta} = \frac{1}{2} \sum_{\sigma,i} \left[ f_{\sigma i}^{\text{eq}} + \left[ 1 - \frac{1}{2\tau} \right] f_{\sigma i}^{(1)} \right] (\mathbf{e}_{\sigma i} - \mathbf{u})_{\alpha} (\mathbf{e}_{\sigma i} - \mathbf{u})_{\beta}.$$

To recover the Euler equations, we neglect the order  $\epsilon^2$  terms and impose four further constraints on the equilibrium distribution function. The first of these constraints requires that the momentum flux tensor  $\mathbf{\Pi}_{\alpha\beta}^{\text{eq}}$  be isotropic. The velocity-independent portion of the tensor is then identified as the pressure, and this immediately results in the equation of state for an ideal gas,  $p = n\varepsilon$ . The remaining two constraints require that the convective terms be a Galilean invariant, and that the heat flux vanish to first order in  $\epsilon$ ,  $\mathbf{q}^{\text{eq}} = 0$ . Thus we obtain the equations for compressible, inviscid, and nonconducting flow of a monatomic gas.

Retaining terms to order  $\epsilon^2$  and imposing two additional constraints, we recover the Navier-Stokes level equations. These constraints are that the momentum flux tensor  $\mathbf{\Pi}^{(1)}$  be isotropic and that the heat flux  $\mathbf{q}^{(1)}$  be proportional to the gradient of the temperature,  $\mathbf{q}^{(1)} \sim \nabla T$ . Note that the order  $\epsilon^2$  terms describe diffusive processes and, as assumed in Eq. (8), evolve on a slower time scale than the convective terms associated with the order  $\epsilon$  Euler equations.

To demonstrate the utility of the above LB method, we apply it to a two-dimensional triangular lattice. The model has one rest particle state,  $\sigma = 0$ , for which  $\mathbf{e}_{\sigma i} = 0$ ; and two nonzero speeds for which  $\mathbf{e}_{\sigma i} = \sigma (\cos(2\pi i/6), \sin(2\pi i/6))$  for  $i = 0, 1, \dots, 6$  and  $\sigma = 1, 2$ . The extension to three dimensions is straightforward and will be discussed elsewhere [15].

For this lattice geometry and the constraints discussed above, we can solve for the coefficients of the distribution function. One possible solution is the following:

$$A_0 = -\frac{5}{2} n\varepsilon + n + 2n\varepsilon^2, \quad A_1 = \frac{4}{9} n\varepsilon - \frac{4}{9} n\varepsilon^2, \\ A_2 = \frac{1}{9} n\varepsilon^2 - \frac{1}{36} n\varepsilon,$$

$$\begin{aligned}
 B_1 &= \frac{4}{9}n - \frac{4}{9}n\epsilon, & B_2 &= \frac{1}{9}n\epsilon - \frac{1}{36}n, \\
 C_1 &= \frac{8}{9}n - \frac{4}{3}n\epsilon, & C_2 &= -\frac{1}{72}n + \frac{1}{12}n\epsilon, \\
 D_0 &= -\frac{5}{4}n + 2n\epsilon, & D_1 &= -\frac{2}{9}n + \frac{2}{9}n\epsilon, & D_2 &= \frac{1}{72}n - \frac{1}{18}n\epsilon, \\
 E_1 &= -\frac{4}{27}n, & E_2 &= \frac{1}{108}n, & F_1 &= 0, & F_2 &= 0.
 \end{aligned}$$

Identifying the coefficients in Eqs. (1)–(3) with the corresponding terms from the Chapman-Enskog expansion, we determine the values for the transport coefficients. The shear viscosity and the thermal conductivity are given by  $\mu = n\epsilon(\tau - \frac{1}{2})$  and  $\kappa = 2n\epsilon(\tau - \frac{1}{2})$ , respectively, and yield a Prandtl number  $\text{Pr} = \frac{1}{2}$ . As in the case of a monatomic gas, the bulk viscosity vanishes because  $\lambda = -\mu$ .

We carried out four numerical tests to determine the accuracy of this method for simulating Eqs. (1)–(3). Each test focused on one aspect of thermohydrodynamic transport.

We determined the viscosity  $\mu$  by simulating an isothermal Poiseuille flow. Numerical results demonstrate that our model accurately reproduces a parabolic momentum profile (not shown here). The viscosity is related to the momentum at the channel center by  $\mu = W^2 f / 8u_{\text{cen}}$ , where  $f$  is the magnitude of the forcing,  $u_{\text{cen}}$  is the velocity at the center, and  $W$  is the channel width [16]. In Fig. 1, we show the dependence of viscosity on the relaxation time  $\tau$  and two internal energies  $\epsilon$ . The resulting viscosities from measurements agree with the Chapman-Enskog theory to within around 1% over the entire range of parameters simulated.

We determined the thermal conductivity  $\kappa$  by measuring the heat transfer across a temperature gradient, using Fourier's law  $\mathbf{q} = -\kappa\nabla T$ . By fixing the temperatures at the channel walls, we obtain a linear temperature profile and thus a constant gradient. Again, numerical results agree with the theoretical predictions quite well. Since the thermal conductivity has the same functional form as the viscosity, we also display the results in Fig. 1.

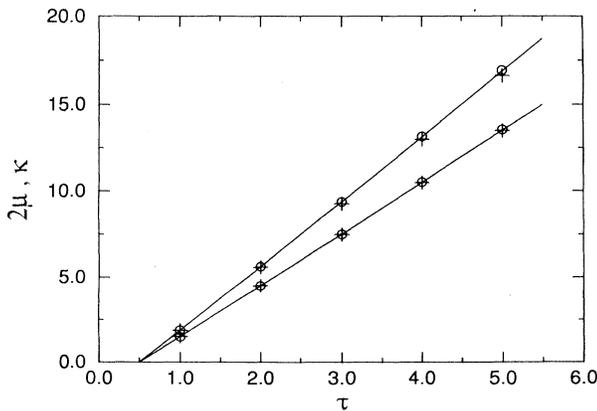


FIG. 1. Shear viscosity (+) and thermal conductivity (o), as functions of relaxation parameter  $\tau$ . Upper curve corresponds to internal energy  $\epsilon = 0.625$ ; lower curve,  $\epsilon = 0.5$ . The solid lines are the theoretical predictions.

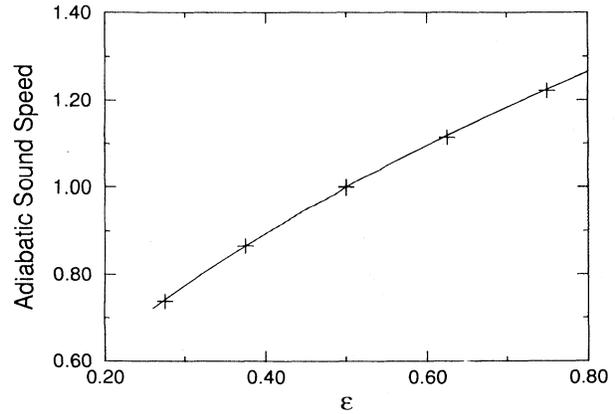


FIG. 2. Numerical simulations of adiabatic sound speed (+) as a function of internal energy  $\epsilon$ . The solid line is the function  $\sqrt{2\epsilon}$ .

For the two-dimensional LB scheme, linearized perturbation theory gives a simple relation between the adiabatic sound speed  $c_s$  and internal energy  $c_s = \sqrt{2\epsilon}$ . In Fig. 2, we present the sound speed as a function of internal energy for both numerical measurements and theory—the agreement is evident.

We simulated a Couette shear flow with a temperature gradient between the boundaries [17]. For small temperature gradients the pressure is essentially constant across the channel, and the temperature profile has an analytic solution given by  $\epsilon^* = (\epsilon - \epsilon_0) / (\epsilon_1 - \epsilon_0) = \frac{1}{2}(1 + y^*) + (\text{Br}/8)(1 - y^{*2})$ , where  $y^*$  is the normalized distance from the center of the channel;  $\epsilon_1$  and  $\epsilon_0$  are the internal energies of the upper and lower walls, respectively. The Brinkman number  $\text{Br}$  is the product of the Prandtl and Eckert numbers. The agreement between theory and simulation, as shown in Fig. 3, demonstrates the validity of the method in simulating flows in which energy dissipation is an important factor.

In conclusion, we have developed a lattice Boltzmann scheme for the simulation of viscous, compressible, heat-

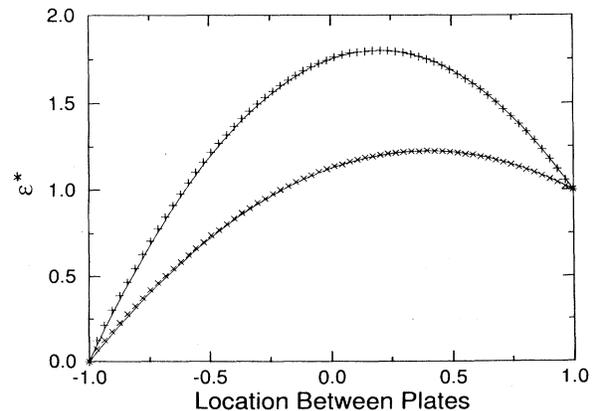


FIG. 3. Normalized internal energy  $\epsilon^*$  for Couette flow with heat transfer for Brinkman numbers  $\text{Br} = 5$  (+) and  $\text{Br} = 10$  (x). The upper wall is moving with speed  $U_1 = 0.1$ , and the lower wall is stationary. The solid lines represent analytical results.

conducting flows of an ideal monatomic gas. The kinetics of this model can be easily implemented on a parallel architecture machine. We have demonstrated theoretically and numerically that the macroscopic behavior of this model corresponds to that of Eqs. (1)–(3). Several issues remain. First, the current model uses the single-time-relaxation approximation, and this restricts simulations to flows with Prandtl number  $Pr = \frac{1}{2}$ . In order to simulate flows with other Prandtl numbers, we should use a full matrix collision operator, which leads to a multi-time-scale relaxation [15]. Second, the equation of state in the present model is that of ideal monatomic gas. To simulate nonideal gases we may incorporate some inter-

nal degrees of freedom. An analysis of the numerical stability of the current model and its benchmarking against other computational fluid dynamical schemes are under investigation.

We thank G. D. Doolen, D. W. Grunau, B. Hasslacher, S. A. Janowsky, J. L. Lebowitz, L. Luo, R. Mainieri, and W. Matthaeus for encouragement and helpful discussions. This work is supported by the U.S. Department of Energy at Los Alamos National Laboratory. Numerical simulations were performed on the CM-200 at the Advanced Computing Laboratory at Los Alamos National Laboratory.

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