Lattice-Boltzmann Simulation Code Development for Micro-Fluidic Systems

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Complex fluid dynamics problems in the micron to hundred micron size range are currently not amenable to conventional simulation methods, but this capability is critically important to support the design and testing of micro-chemical components and systems. A promising new method for simulating fluid flow at this scale is the lattice Boltzmann algorithm, which has recently been developed from lattice gas automata. One major advantage of the lattice Boltzmann method over other fluid dynamics simulation techniques is the ability to incorporate interaction terms directly into the equations of motion. This makes possible the simulation of multiphase-multicomponent systems in a straightforward way, without the introduction of complicated front tracking routines. However, most of the current lattice Boltzmann algorithms are unable to model the effects of thermal transport and only describe systems that can be considered isothermal. The few algorithms that have been developed for thermal flow are only applicable to a very limited range of problems[1, 2]. Many micro-fluid systems, particularly those involving thermal flow or chemical reactions, require thermal as well as flow analysis. This paper will describe initial efforts to incorporate a general model of thermal behavior into a lattice Boltzmann algorithm for single phase fluid flow.

Lattice Boltzmann simulations represent a discretized version of the Boltzmann equation in which space is divided up into a regular lattice and the velocities are represented by a finite number of vectors instead of a continuous distribution. Instead of solving for the continuous one particle distribution function $f(\mathbf{r}, \mathbf{v})$, the lattice Boltzmann algorithm is based on a discretized distribution $f_i(\mathbf{r})$ where i represents one of the discrete velocities and replaces the variable $\mathbf{v}$ in the continuous distribution. The discrete velocities are denoted by the displacement vectors to neighboring lattice sites $\mathbf{e}_i$ where $i = 1, ..., b$ where b is the total number of displacement directions. The magnitude of the displacements is $|\mathbf{e}_i| = c$. A zero displacement vector $\mathbf{e}_0$ is also included in the set to represent particles with zero velocity. Two sets of distributions, f_i and F_i, are assigned to each site. The distribution f_i represents the transport of mass and momentum and satisfies the two relations

$$\rho = \sum_{i=0}^{b} f_i \tag{1}$$

$$\rho \mathbf{u} = \sum_{i=1}^{b} \mathbf{e}_i f_i \tag{2}$$

where ρ is the density and $\mathbf{u}$ is the macroscopic velocity of the fluid. The distribution F_i models the movement of energy around the system and satisfies the relation

$$\epsilon \rho = \sum_{i=0}^{b} F_i \tag{3}$$

where ϵ is the specific energy per particle. Using a second distribution to model the energy is similar to the passive scalar approach proposed by Shan[2].

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The distributions are defined for each of the lattice sites in the system and are updated at each time step by first performing a collision to obtain a new set of distributions. Each of the new distributions f_i and F_i are then displaced along the vector $\mathbf{e}_i$ to get a new set of distributions at each site. The collisions and displacement of the distributions are summarized by the equations of motion

$$f_i(\mathbf{r}+\mathbf{e}_i, t+1) - f_i(\mathbf{r}, t) = -\frac{1}{\tau_\rho}(f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t)) \quad (4)$$

$$F_i(\mathbf{r}+\mathbf{e}_i, t+1) - F_i(\mathbf{r}, t) = -\frac{1}{\tau_\epsilon}(F_i(\mathbf{r}, t) - F_i^{eq}(\mathbf{r}, t)) \quad (5)$$

where the $\mathbf{r}$ are lattice sites and t is the discrete time. The collisions are assumed to take the familiar BGK form[3] and are characterized for the two distributions by the relaxation times τ_ρ and τ_ϵ. Because there is no explicit coupling between the equations of motion for the f_i and F_i, the total internal energy of the system is a conserved quantity, which implies that there is no viscous heating in the system. For many problems of practical importance, the contribution from viscous heating is small.

The equilibrium distributions f_i^{eq} and F_i^{eq} are given by the expressions

$$f_i^{eq} = \frac{\rho(1-d_0)}{b} + \frac{\rho D}{bc^2}\mathbf{e}_i\cdot\mathbf{u} + \frac{\rho D(D+2)}{2bc^4}\mathbf{u}\cdot\mathbf{e}_i\mathbf{e}_i\cdot\mathbf{u} - \frac{\rho D}{2bc^2}\mathbf{u}\cdot\mathbf{u} \quad (6)$$

$$f_0^{eq} = \rho d_0 - \frac{\rho}{c^2}\mathbf{u}\cdot\mathbf{u} \quad (7)$$

$$F_i^{eq} = \epsilon f_i^{eq} \quad (8)$$

$$F_0^{eq} = \epsilon f_0^{eq} \quad (9)$$

where D is the dimension of the system and d_0 is a parameter that is determined by the local thermodynamic conditions. The f_i^{eq} are identical to those developed for simulating a multiphase-multicomponent system[4], except that in this case d_0 is not a constant. The parameter d_0 controls the partition between fast and slow moving particles. Particles moving less than some value u_0 could be assigned to the zero velocity distribution f_0, while particles moving faster than u_0 are assigned to the f_i. This implies that d_0 is related to the temperature T; if T increases then d_0 should decrease. If the specific energy ϵ and the density ρ are known at a given lattice site, then in principle the temperature and pressure can be calculated. By constructing a model connecting d_0 to the temperature, it is possible to incorporate the effects of thermal flow into a lattice Boltzmann algorithm consisting of the following steps

i) Calculate ρ, $\mathbf{u}$, and ϵ at each site.

ii) Based on the value of ρ and ϵ calculate the temperature T at each site. Use the value of T to evaluate d_0.

iii) Evaluate f_i^{eq} and F_i^{eq} at each site and complete the collision step.

iv) Translate the f_i and F_i.

The key feature of this algorithm is that d_0 is allowed to vary as a function of the local temperature at each site. This provides an implicit coupling between the two distributions f_i and F_i. The hydrodynamic equations corresponding to this model can be obtained by applying the usual Chapman-Enskog expansion[5] to the equations of motion. This yields

$$\frac{\partial}{\partial t}\rho + \nabla\cdot\rho\mathbf{u} = 0 \quad (10)$$

$$\begin{aligned}
\frac{\partial}{\partial t}\rho\mathbf{u} + \nabla\cdot\rho\mathbf{u}\mathbf{u} &= -\nabla\rho(1-d_0)\frac{c^2}{D} - \nabla(\zeta\nabla\cdot(\rho\mathbf{u})) + (\nabla\mu)(\nabla\cdot(\rho\mathbf{u})) \\
&+ (\nabla\mu)\cdot(\nabla(\rho\mathbf{u})) + \nabla\cdot(\mu\nabla(\rho\mathbf{u})) + \nabla(\xi\rho\mathbf{u}\cdot\nabla\epsilon) \\
&+ 2\mu\nabla(\nabla\cdot\rho\mathbf{u}) \qquad (11) \\
\frac{\partial}{\partial t}\epsilon\rho + \nabla\cdot\epsilon\rho\mathbf{u} &= \nabla\cdot(\kappa\nabla\epsilon) \qquad (12)
\end{aligned}$$

where the functions μ, ζ, ξ, and κ can be obtained as closed form functions of the parameters defining the original lattice Boltzmann model and the local thermodynamic variables. The quantity $\rho(1-d_0)c^2/D$ can be identified with the pressure and the transport coefficients μ and κ are the kinematic viscosity and thermal diffusivity. The remaining coefficients ξ and ζ are artifacts left over from the approximations made in developing the lattice Boltzmann model. Their significance requires further study.

This algorithm was tested using a Van der Waals equation of state for the fluid, which required finding expressions for the both the temperature T and pressure P as function of the local internal energy and density. The boundary conditions used for the distributions f_i and F_i are similar to those proposed by Chen *et al.*[6]. For the boundary conditions on the f_i, a linear extrapolation is made of each component to an outside boundary layer of lattice points. The linear extrapolation was generalized for application to the energy distributions F_i. For the simulations described below, both constant temperature boundary conditions and adiabatic boundary conditions were used. All results are reported using arbitrary units and are only meant to illustrate some of the basic features of the model.

As a test of the qualitative behavior of the model, two-dimensional simulations of a linear temperature gradient, flow through a constriction, and Rayleigh-Bénard convection between two plates at different temperatures were performed. The simulations of Rayleigh-Bénard convection also required the introduction of a gravity field, which was incorporated into the model as described by Martys and Chen[7]. Periodic boundary conditions were used in the horizontal direction.

To simulate the linear temperature profile, the gravitational acceleration was set equal to zero and the system was allowed to equilibrate. A plot of the temperature and density is shown in Figure 1.

Figure 1 Plot of temperature and density as a function of position.

The temperature can be seen rising from the bottom plate to the top while the density decreases. The temperature and density profiles are not strictly linear because the transport coefficient κ depends on the density and temperature and the large changes in both these quantities cause some deviations from linearity. However, the results indicate that the basic physics for simulating natural convection is contained in the model.

Figure 2 Contour plot of temperature distribution for flow through a constriction.

The temperature distribution for a flow through a constriction is shown in Figure 2. Adiabatic boundary conditions are applied at the walls so that no energy is lost to the boundaries. The flow is from the left of the figure and the darker regions represent higher temperatures. The fluid heats up in the region in front of the constriction and and then cools back down as it flows through the constriction and expands into the region downstream. This is the expected behavior for a nonideal fluid, although for many real-life applications, other effects such as viscous heating may be significant for this kind of system.

Figure 3 Plot of vector field for half of the Rayleigh-Bénard simulation.

The simulations of Rayleigh-Bénard convection were performed by turning on the gravitational acceleration and adding some arbitrary velocities to the initial condition to help initiate the Raleigh-Bénard instability. After 10,000 timesteps, the simulation appeared to reach a steady-state with four convective cells forming in the system. The velocity field representing two of the cells (half the system)

are shown in Figure 3. The upward circulation is at the two sides of the figure and the downwards circulation is at the center. Examination of the temperature distribution (not shown) reveals a plume of cool liquid pressing down into the center of the region shown in Figure 3 between the two cells while a plume of warm liquid is rising at either side. Plots of the density are similar to the temperature, showing a downward moving plume of dense liquid at the center of the system and upward moving plumes of lower density at either side. The simulations clearly show that the model is capable of reproducing the expected behavior of coupled momentum and heat transfer systems, at least in simple cases.

The results presented here indicate that modeling the internal energy using a second distribution is a viable way to incorporate thermal effects into the lattice Boltzmann algorithm. It should also be possible to couple this approach to the nonlocal lattice Boltzmann algorithms used to model multiphase-multicomponent isothermal systems and use these combined models to analyze the effects of thermal transport on the dynamics of phase changes and chemical reactions in multiphase environments. This will allow detailed simulation of many microscale systems, including microscale heat pumps and microscale chemical reactors.

NOMENCLATURE

b: total number of lattice displacement vectors

c: magnitude of lattice displacement vectors

D: dimension of system

d: partition coefficient between fast and slow velocities

$\mathbf{e}$: lattice displacement vector

f: distribution describing local momentum and density

F: distribution describing local energy density

P: pressure

$\mathbf{r}$: position vector

t: time

T: temperature

$\mathbf{u}$: macroscopic velocity vector

$\mathbf{v}$: microscopic velocity vector

ϵ: local energy density

μ: local kinematic viscosity

κ: local energy transport coefficient

ρ: local density

τ: local relaxation time

ξ: transport coefficient

ζ: transport coefficient

Superscripts

eq: equilibrium distribution

Subscripts

i: displacement vector direction

0: zero displacement vector

ϵ: energy equation

ρ: density-momentum equation

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