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Simulating Thermohydrodynamics with Lattice BGK Models

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In this paper, we propose new lattice BGK models for one-, two- and three-dimensional thermohydrodynamics. A proper internal energy is introduced and the energy equation is obtained. The derivation of the thermohydrodynamic equations is systematic and numerical simulations are carried out to verify the theoretical values of the sound speed, the shear viscosity and the conductivity. One-dimensional shock-tube problem and two-dimensional Rayleigh-Bénard convection are simulated. Good performance and satisfactory results are obtained. These models can be applied to many interesting cases, in particular, the transonic regimes where the compressibility can not be neglected.

KEY WORDS: Kinetic theory; thermohydrodynamics; computational technique; lattice gas; BGK model.

1. INTRODUCTION

Recently, there has been an increasing interest in modeling complicated physical phenomena by simple methods. One example is the lattice gas method which was initially introduced by Frisch *et al.*, (1986) to solve the two-dimensional Navier-Stokes equation. Different variants of the first FHP model have been proposed and used for many applications (see more details by Doolen (1991)). The first three-dimensional lattice gas model was introduced by d'Humières *et al.*, (1986). A variety of physical phenomena have been studied. Examples include the Burgers dynamics [Boghosian and Levermore (1987)], flows in porous media [Rothman (1990)], MHD [Chen and Matthaeus (1989)] and phase separation [Zaleski (1989)]. The ingredients of all lattice gas models are the following:

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on each node of a well-chosen lattice, a set of variables $\{n_i\}$, $(i \in 1,..., b)$ describes the state of occupation of the particles with given velocities $\mathbf{c}_i$'s. The time evolution of the system consists of a collision step and a propagation step. During the collision step, particles are redistributed locally according to conservation laws while in the propagation step the particles move from node to node according to their velocities. The use of such simplified models for complicated phenomena impose some constraints to be satisfied [Frisch *et al.*, (1987); Qian (1990); and Rivet (1988)]. The symmetry of the underlying lattice, the conservation laws and the existence of scale-separation are some of such constraints. The recent intensive theoretical and numerical investigations have led to a better understanding of the advantages of lattice gas models and their drawbacks. More details of both the advantages and disadvantages of the lattice gas models can be found in Qian *et al.* (1990). The main strengths can be summarized as: (1) absolute numerical stability; (2) easy treatment of boundary conditions; (3) simple programming and high parallelism. These strengths are accompanied with some shortcomings. One fundamental weakness is that the lattice gas dynamics is intrinsically noisy, thus requiring the use of spatial or temporal averaging to obtain hydrodynamic information. Orszag and Yakhot (1986) discussed some consequences of the statistical noise, and Dahlburg *et al.*, (1987) showed the numerical weakness in low Mach number and low density simulations. Coupled with the intrinsic nonlinearity, this statistical noise leads to the divergence of transport coefficients in one-dimensional case [d'Humières *et al.*, (1989)] (by RNG method) and in two-dimensional case [Kadanoff *et al.*, (1989)] (by mode-mode coupling theory). A second weakness is that the lattice gas dynamics is not Galilean invariant because of the presence of a factor $g(\rho)$ in the nonlinear advection term and the pressure depends on velocity [Frisch *et al.*, (1987); Qian (1990); and Rivet (1988)].

Several modifications have been proposed however to overcome some of these drawbacks. The lattice Boltzmann equation (LBE) [McNamara and Zanetti (1988)] is the simplest one for two-dimensional models of the FHP family (FHP-I, -II, -III and -IV). A simplification is due to Higuera *et al.*, (1988), in which they introduced the enhanced collision matrix regardless of detailed collisions. As a result, three-dimensional application is straightforward. Qian (1990) and Qian *et al.*, (1991) proposed to consider directly the Maxwellian gas instead of Fermions or Bosons. They obtained some models which are Galilean invariant with a velocity-independent pressure. All these different versions of LBE however have numerical instability problems when the viscosity is very close to zero. In order to achieve better numerical stability, a lattice version of BGK model [Bhatnagar *et al.*, (1954)] was recently proposed in Qian *et al.*, (1992), and

Chen *et al.*, (1992). A nonlinear deviation from the Navier-Stokes equation was also studied in Chapman and Cowling (1970). The organization of the paper is the following: We shall give the description of the kinetics and the thermohydrodynamical equations in the Section 2. Section 3 will be devoted to the choice of the equilibrium state for different models, and numerical simulations will be reported in the Section 4. The last section will consist of a discussion and conclusion.

2. KINETICS AND MACROSCOPICAL EQUATIONS

Let us first define the kinetic variables and thermohydrodynamic quantities. $N_i(\mathbf{x}, t)$ is the particle density related to the given velocity $\mathbf{c}_i$. The finite set of discrete velocities $\{\mathbf{c}_i\}$ determines completely the underlying lattice structure. All the thermohydrodynamic quantities are defined by the moments of N_i,

$$\rho = \sum_i N_i \tag{2.1}$$

$$\rho \mathbf{u} = \sum_i \mathbf{c}_i N_i \tag{2.2}$$

$$\rho \left(e + \frac{u^2}{2} \right) = \sum_i \frac{c_i^2}{2} N_i \tag{2.3}$$

where ρ, $\mathbf{u}$ and e are density, velocity and internal energy. Other quantities include the momentum flux tensor $P_{\alpha\beta}(\Pi_{\alpha\beta})$ and the heat flux $q_\alpha(Q_\alpha)$,

$$P_{\alpha\beta} = \sum_i (c_{i\alpha} - u_\alpha)(c_{i\beta} - u_\beta) N_i \tag{2.4}$$

$$\Pi_{\alpha\beta} = \sum_i c_{i\alpha} c_{i\beta} N_i \; (= P_{\alpha\beta} + \rho u_\alpha u_\beta) \tag{2.5}$$

$$q_\alpha = \sum_i \frac{1}{2} (c_{i\alpha} - u_\alpha)(c_{i\beta} - u_\beta)^2 N_i \tag{2.6}$$

$$Q_\alpha = \sum_i \frac{1}{2} c_{i\alpha} c_{i\beta}^2 N_i \left(= q_\alpha + \rho u_\alpha \left(e + \frac{u^2}{2} \right) + u_\beta P_{\alpha\beta} \right) \tag{2.7}$$

Following Qian *et al.*, (1992), we use the same kinetic equation as the starting point,

$$N_i(\mathbf{x} + \mathbf{c}_i \tau, t + \tau) = N_i(\mathbf{x}, t) + \omega [N_i^e(\mathbf{x}, t) - N_i(\mathbf{x}, t)] \tag{2.8}$$

where ω is the collision frequency (or the relaxation parameter) and τ is time step unit ($\tau = 1$). Assuming that a scale-separation exists, we apply the

classic Chapman-Enskog expansion [Qian and Orszag (1993)] to Eq. (2.8), and thus the first-order approximation leads to the following Euler equations [Harris (1971)],

$$\partial_t \rho + \partial_\alpha(\rho u_\alpha) = 0 \tag{2.9}$$

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p \tag{2.10}$$

$$\partial_t(\rho e) + \partial_\beta(\rho e u_\beta) = -p\partial_\beta u_\beta \tag{2.11}$$

where p is the pressure which is related to the density by the equation of state,

$$p = \frac{2}{D}\rho e \tag{2.12}$$

D is the space dimension. We can obtain easily an expression for the sound speed a_s,

$$a_s = \sqrt{\gamma e}, \qquad \gamma = \frac{D+2}{D} \tag{2.13}$$

where γ is the ratio of specific heat.

The Navier-Stokes equations are the second-order approximation for which the space gradient effect is accounted [Frisch *et al.*, (1987); Qian (1990); Rivet (1988); Chen *et al.*, (1992); Qian and Orszag (1993); and Harris (1971)]. The continuity equation is the same as Eq. (2.9) while the momentum and energy equations include diffusive terms,

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) = -\partial_\alpha p + \partial_\beta[\nu\partial_\beta(\rho u_\alpha) + \zeta\partial_\alpha(\rho u_\beta)] \tag{2.14}$$

$$\partial_t(\rho e) + \partial_\beta(\rho e u_\beta) = -p\partial_\beta u_\beta + \partial_\alpha(\kappa\rho\partial_\alpha e) + \partial_\alpha[u_\beta(\nu\partial_\beta(\rho u_\alpha) + \zeta\partial_\alpha(\rho u_\beta))] \tag{2.15}$$

$$\nu = \frac{\sigma}{2}\left(\frac{2}{\omega} - \tau\right)e, \qquad \zeta = \left(\sigma - \frac{2+D}{D^2}\right)\left(\frac{2}{\omega} - \tau\right)e,$$
$$\kappa = \frac{D+2}{2D}\left(\frac{2}{\omega} - \tau\right)e \tag{2.16}$$

where σ is a parameter which will be described in the next section.

3. CHOICE OF THE EQUILIBRIUM STATE N_i^e FOR DIFFERENT MODELS

The thermohydrodynamic equations presented in the last section are obtained by a proper choice of the local equilibrium state in Eq. (2.8)

which is a key point [Qian *et al.*, (1992); Chen *et al.*, (1992); and Chapman and Cowling (1970)]. Now we shall discuss more details regarding the choice and give some concrete models. The models are still based on the lattice structures described in detail in Bhatnagar *et al.*, (1954). Here we recall some basic elements. The finite set of velocities $\mathbf{c}_i$ consists of different sub-lattices depending on the number of nonzero components of velocities and velocity moduli. We denote p as the sub-lattice index and $\mathbf{c}$ as velocity unit (The index p should not be confused with the pressure p). The rest particles mean $p=0$ while $p=1$ describes the particles on the sub-lattice along the principal axis. Now we make the choice for N_i^e as the truncated Maxwellian distribution as follows:

$$N_i^e = A_p\rho + B_p c_{i\alpha}\rho u_\alpha + \frac{t_p}{2c_s^4}(c_{i\alpha}c_{i\beta} - c_s^2\delta_{\alpha\beta})\rho u_\alpha u_\beta + D_p c_{i\alpha}u_\alpha \rho u^2 \quad (3.1)$$

where c_s is a constant which will be given next. The requirements of isotropy of a 4th-order tensor of velocity [Frisch *et al.*, (1987); Qian (1990); and Rivet (1988)] and that of Galilean invariance impose some constraints on the weights t_p, which are model-dependent. We simply give some values in Table I for the *DdQb* models in d space dimensions and with b particles from [Qian (1990); Qian *et al.* (1992); and Chapman and Cowling (1970)] (These models will be explained later in this section).

The point is to determine the different constants A_p, B_p and D_p in Eq. (2.16). The physical conservation laws of mass, momentum and energy lead to the following constraints,

$$\sum_p b_p A_p = 1 \quad (3.2)$$

$$\sum_p \frac{c_p^2}{2} b_p A_p = e \quad (3.3)$$

$$\sum_p c_p^2 b_p B_p = D \quad (3.4)$$

$$\sum_p \frac{c_p^2}{2} b_p D_p = 0 \quad (3.5)$$

Table I. Values for *DdQb* Models

Model	t_0	t_1	t_2	t_3	t_4	c_s^2
D1Q5	1/2	1/6	0	0	1/12	1
D2Q13	4/9	1/9	1/36	0	0	1/3
D3Q21	2/9	1/9	0	1/72	0	1/3
D3Q25	1/3	1/18	1/36	0	0	1/3

where b_p is the number of particles residing on the sub-lattice p (with $c_p^2 = c_{i\alpha} c_{i\alpha}$). Three additional constraints come from the consideration of the energy dependence of transport coefficients and the isotropy of the viscous term. These additional constraints can be written as,

$$\sum_p c_p^4 b_p A_p = 2(D+2)\,\sigma e^2 \tag{3.6}$$

$$\sum_p c_p^4 b_p B_p = D(D+2)\,\sigma e \tag{3.7}$$

$$\sum_p \frac{c_p^4}{p} b_p B_p = 3D\sigma e \tag{3.8}$$

where σ is a nondimensional parameter. The system is still undetermined since we have more unknowns than the number of constraints. Therefore, we have certain degrees of freedom to choose the parameters and concrete models in one, two and three dimensions are presented next.

(1) One-dimensional $D1Q5$ Model.

This purely one-dimensional model has no spurious invariants d'Humières *et al.*, (1989) and can be used to test new ideas. A suitable choice of A_p, B_p and D_p are the following,

$$A_0 = 1 - \frac{5e}{2c^2} + \frac{3e^2}{c^4}, \qquad A_1 = \frac{4e}{3c^2} - \frac{2e^2}{c^4}, \qquad A_4 = -\frac{e}{12c^2} + \frac{e^2}{2c^4} \tag{3.9}$$

$$B_1 = \frac{4c^2 - 3\sigma e}{6c^4}, \qquad B_4 = \frac{3\sigma e - c^2}{24c^4} \tag{3.10}$$

$$D_1 = -\frac{1}{6c^4}, \qquad D_4 = \frac{1}{24c^4} \tag{3.11}$$

we choose $\sigma = 2$ for this model.

(2) Two-dimensional $D2Q13$ Model.

The two-dimensional $D2Q9$ model [Qian (1990) and Qian *et al.*, (1992)] is modified by adding 4 more velocities along the x and y directions with velocity modulus $2c$. So we have 13 different velocities of particles on each node of lattice.

We take the following values for A_p, B_p and D_p,

$$\begin{aligned} A_0 &= 1 - \frac{5e}{2c^2} + \frac{9e^2}{4c^4}, \qquad A_1 = \frac{2e}{3c^2} - \frac{5e^2}{6c^4}, \\ A_2 &= \frac{e^2}{8c^4}, \qquad A_4 = -\frac{e}{24c^2} + \frac{7e^2}{48c^4} \end{aligned} \tag{3.12}$$

$$B_1 = \frac{2c^2 - 3\sigma e}{3c^4}, \qquad B_2 = \frac{\sigma e}{4c^4}, \qquad B_4 = \frac{3\sigma e - c^2}{24c^4} \tag{3.13}$$

$$D_1 = -\frac{1}{18c^4}, \qquad D_2 = -\frac{1}{12c^4}, \qquad D_4 = \frac{1}{18c^4} \tag{3.14}$$

σ is set to 1 for this model.

(3) Three-dimensional $D3Q21$ Model.

We add 6 faster particles with speed modulus equal to $2c$ along the x, y and z axis to the $D3Q15$ model [Qian (1990) and Qian *et al.*, (1992)].

The following values for A_p, B_p and D_p are suitably chosen,

$$A_0 = 1 - \frac{5e}{2c^2} + \frac{11e^2}{4c^4}, \qquad A_1 = \frac{4e}{9c^2} - \frac{23e^2}{36c^4},$$
$$A_3 = \frac{e^2}{16c^4}, \qquad A_4 = -\frac{e}{36c^2} + \frac{7e^2}{72c^4} \tag{3.15}$$

$$B_1 = \frac{2c^2 - 3\sigma e}{3c^4}, \qquad B_3 = \frac{\sigma e}{8c^4}, \qquad B_4 = \frac{3\sigma e - c^2}{24c^4} \tag{3.16}$$

$$D_1 = -\frac{1}{36c^4}, \qquad D_3 = -\frac{5}{36c^4}, \qquad D_4 = \frac{1}{18c^4} \tag{3.17}$$

σ is also set to 1 for this model.

(4) Three-dimensional $D3Q25$ Model.

This is the $D3Q19$ model with 6 faster particles with speed modulus equal to $2c$ along the x, y, and z axis [Qian (1990) and Qian *et al.*, (1992)].

We use the following values for A_p, B_p and D_p,

$$A_0 = 1 - \frac{5e}{2c^2} + \frac{3e^2}{c^4}, \qquad A_1 = \frac{4e}{9c^2} - \frac{7e^2}{9c^4},$$
$$A_2 = \frac{e^2}{12c^4}, \qquad A_4 = -\frac{e}{36c^2} + \frac{e^2}{9c^4} \tag{3.18}$$

$$B_1 = \frac{4c^2 - 9\sigma e}{6c^4}, \qquad B_2 = \frac{\sigma e}{4c^4}, \qquad B_4 = \frac{3\sigma e - c^2}{24c^4} \tag{3.19}$$

$$D_1 = 0, \qquad D_2 = -\frac{1}{16c^4}, \qquad D_4 = \frac{1}{16c^4} \tag{3.20}$$

and $\sigma = 1$ is used for this model.

4. NUMERICAL SIMULATIONS

Several numerical simulations are carried out for verifying the theoretical results. Good agreements are obtained for the sound speed a_s which depends on the internal energy e, for the viscosity ν and for the conductivity κ. With the $D2Q13$ model either the relaxation or the forced Poiseuille flows are used to measure the viscosity while the conductivity is obtained by keeping a constant heat flux and comparing with the Fourier law. Figure 1 for the sound speed a_s, Fig. 2 for ν and Fig. 3 for κ. Solid lines are theoretical results while the points (squares or crosses) are numerical measurements. Good agreements are thus achieved. The second test is the shock-tube problem. This is a classic benchmark problem for testing different numerical schemes. Here we use the $D1Q5$ model to mimic the flow. The initial conditions are uniform energy with zero velocity everywhere. A step function of density is used in the middle of the tube. Figure 4 shows the density and energy profiles for different times. A right-running shock and a left-running rarefaction wave are clearly generated. Detailed comparison with high-order method is to be done. A third numerical simulation concerns the Rayleigh-Bénard convection in two dimensions on a lattice of 64×32 at Rayleigh number $\mathrm{Ra} = 8666$ by using

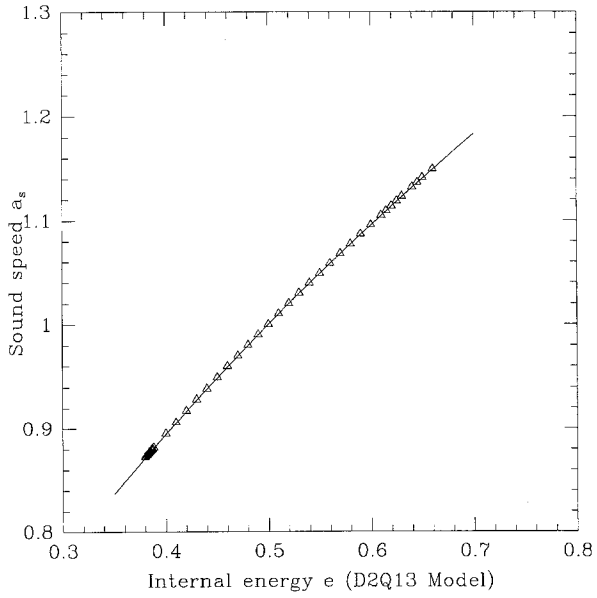

Fig. 1. The sound speed a_s in function of the internal energy e; solid line is the formula $a_s = (\gamma e)^{1/2}$ and points are numerical results.

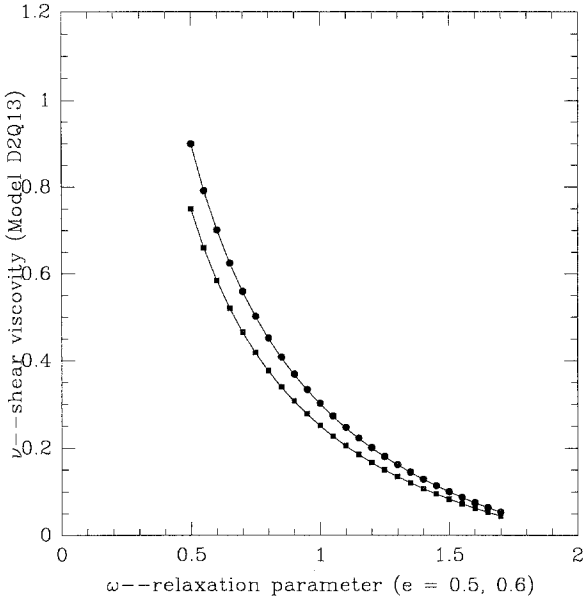

Fig. 2. Shear viscosity ν in function of the parameter ω for different e; solid line is the formula $\nu = e/2(2/\omega - 1)$ and points are numerical results. Squares for $e = 0.5$ and circles for $e = 0.6$.

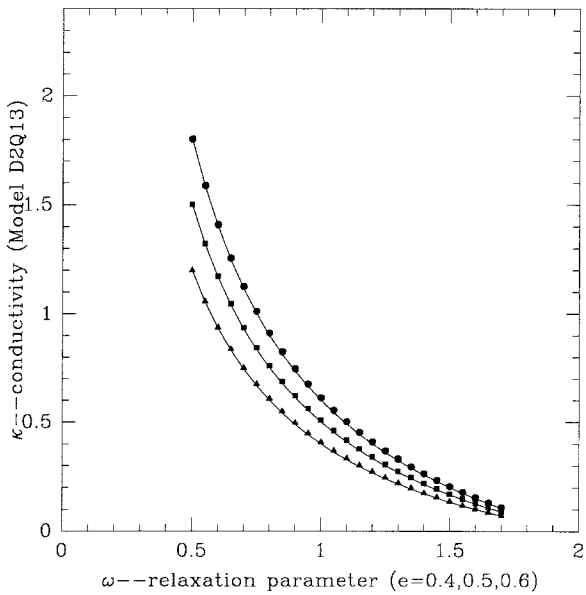

Fig. 3. Heat conductivity κ in function of the parameter ω for different e; solid line is the formula $\kappa = e(2/\omega - 1)$ and points are numerical results. Triangles for $e = 0.4$, squares for $e = 0.5$ and circles for $e = 0.6$.

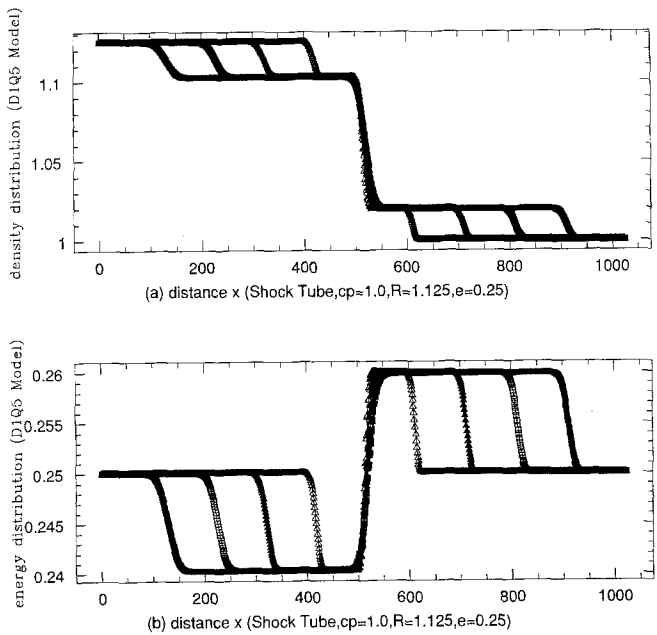

Fig. 4. Upper: density profile for times = 80, 160, 240, and 320 with open triangle, solid triangle, open square and solid square; Bottom: the same but for the internal energy e. $R = 1.125$, $\omega = 1.0$, and $e = 0.25$.

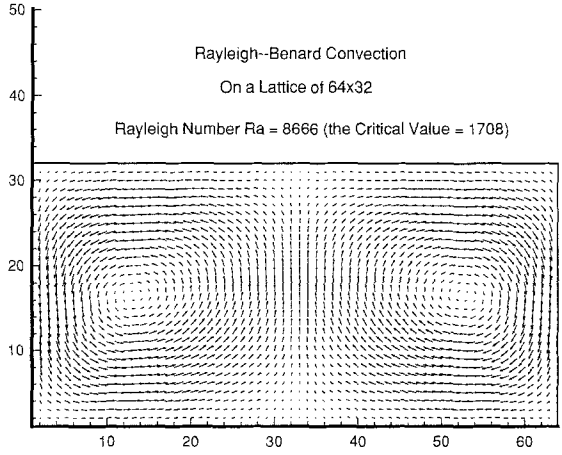

Fig. 5. Rayleigh-Benard Convection Simulation, velocity field with Rayleigh number $Ra = 8666$ (Note: the critical $Ra = 1708$ for this case). The two counter-rotating rolls are well reproduced.

$D2Q13$ model. Higher Rayleigh numbers can be achieved with large systems. The gravity is incorporated into the simulation by the method described in Qian (1990). More detailed results with experimental comparison Tilgner *et al.*, will be presented elsewhere.

5. CONCLUSION

In this paper we have proposed new lattice BGK models for thermohydrodynamics which have yet to be studied either by lattice gas or by lattice Boltzmann equation. Different models for one, two and three dimensions are investigated and numerical simulations confirm well the theoretical results concerning the second speed, the shear viscosity and the conductivity. Two other simulations for shock-tube in one dimension and Rayleigh-Bénard convection in two dimensions are carried out. The comparison with real experiments remains to be done in the near future. As a flexible and efficient numerical method, the lattice BGK method can be used in fundamental studies since it provides a connection between microdynamics and macrodynamics, examples include the dynamical phase transition, pattern formation [Qian and Orszag, to be published] and turbulence study, it can be applied as well to many industry-interested problems, like flows in porous media. One shortcoming of the actual lattice BGK method is that we can not change the Prandtl number. It is a fixed constant. This can be understood in the following way since we have only one relaxation parameter ω, therefore the dynamical and thermal relaxations take the same order. This shortcoming may be overcome by using multi-relaxation parameters ω_i instead of a single one. In the lattice Boltzmann equation, this may not be a problem by using the enhanced collision matrix [Higuera *et al.*, (1989)]. An important problem which is worth paying more attention to is a rigorous analysis of the stability. Personal experience shows that the $D2Q9$ model is more stable than the triangular FHP model of the lattice BGK version [Qian]. Another slightly different approach is the moment method which is studied recently by McNamara and Alder (preprint).

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