

# THE FUTURE OF LATTICE-GAS AND LATTICE BOLTZMANN METHODS

LI-SHI LUO

*ICASE*

*MS 403, NASA Langley Research Center*

*6 North Dryden Street, Building 1298*

*Hampton, Virginia 23681-0001*

## 1. Brief History

Although the lattice-gas automata (LGA) or lattice-gas cellular automata (LGCA) and the lattice Boltzmann equation (LBE) have a rather short history extending only over a decade or so, they have attracted much attention among physicists in various disciplines. The reason is that the methods of LGA and LBE have demonstrated their great potentials to study various complex systems such as the hydrodynamics of multi-phase and multi-component fluids (Luo, 1998), magneto-hydrodynamics (Chen & Matthaeus, 1987; Chen *et al.*, 1988; Chen *et al.*, 1991), chemical reactive flows (Chen *et al.*, 1995; Boon *et al.*, 1996), where the application of other methods would be difficult or impractical.

Before the methods of lattice-gas automata and lattice Boltzmann equation, there were similar models. In 1964 Broadwell proposed using the Boltzmann equation with only a few discrete velocities to study aerodynamics (Broadwell, 1964). In 1973 Hardy, de Pazzis, and Pomeau (HPP) proposed the first single speed lattice-gas cellular automaton model on a 2D square-lattice space to study statistical mechanical properties of two-dimensional fluids, such as the divergence of 2D transport coefficients (Hardy *et al.*, 1973). It should be stressed that both the Broadwell model and the HPP model were more proposed as theoretical models than as computational tools.

In 1986, Frisch, Hasslacher, and Pomeau (Frisch *et al.*, 1986), and Wolfram (Wolfram, 1986) proposed the first 2D lattice-gas automaton model for the specific purpose of computational fluid dynamics. The 3D lattice-gas automaton model was soon introduced (d'Humières *et al.*, 1986). In

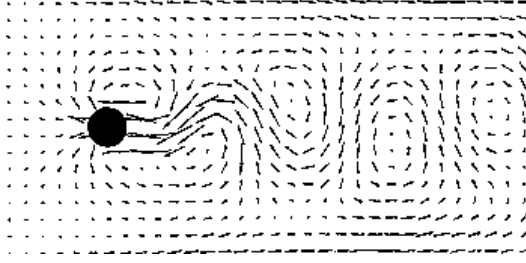
1988, the first proposal to use the lattice Boltzmann equation to simulate fluid dynamics was made (McNamara & Zanetti, 1988). The evidence that simple models such as the lattice-gas automaton and its floating-number counterpart, the lattice Boltzmann equation, can faithfully simulate hydrodynamics opens a new avenue in computational physics. Some of the key ideas of the LGA and LBE methods may indeed be revolutionary.

Although only in their infancy, the methods of the lattice-gas automata and lattice Boltzmann equation have demonstrated their capabilities in many areas of computational fluid dynamics, such as turbulent external flow over structures with complicated geometries (Strumolo & Viswanathan, 1997), multi-phase and multi-component fluids through porous media (Chen & Doolen, 1998), chemical reactive flows (Boon *et al.*, 1996), and other complex systems (Doolen, 1990; Rothman & Zaleski, 1997; Chen *et al.*, 1998). The advantages of the LGA and LBE methods are:

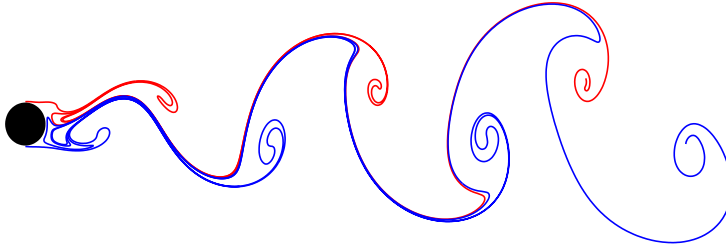
1. Broad applicability to various complex systems;
2. Ability to handle complicated boundary geometries;
3. Preservation of the conservation laws exactly (LGA);
4. Unconditional stability (LGA);
5. Memory efficiency (LGA);
6. Inherent parallelism — linear scalability on computers with massively parallel processors (MPP) (Amati *et al.*, 1997a);
7. Capability to include model interactions among particles;
8. Very simple to program.

However, one must be very careful in stating what precisely are the advantages of the LGA and LBE methods over conventional methods of solving the Navier-Stokes equations, *i.e.*, one must carefully identify the areas where the LGA and LBE methods are more suitable because of the physical nature of the problems. I shall briefly address this issue in this article.

Before we discuss any technical details, it would be appropriate for us to gain a sense of history first, to review how much the LGA and LBE methods have evolved since their inception. Here we show simulations of the 2D flow past a cylinder, a classic example in fluid dynamics, using the lattice gas method (Wolfram, 1988) and the lattice Boltzmann method (He & Doolen, 1997a). Fig. 1 from (Wolfram, 1988) shows that LGA can indeed mimic hydrodynamics: it reproduces von Kármán vortex street behind a cylinder, although the simulation was qualitative in nature. About one decade later, He and Doolen demonstrated that the LBE method can faithfully simulate hydrodynamics. Figs. 2 shows the von Kármán vortex street behind a cylinder with a Reynolds number of 100. Various quantities, such as drag coefficient and lift coefficient, are accurately measured and compared with existing numerical and experimental results (He & Doolen, 1997a). Furthermore, the computational speed of the LBE method is comparable to that of conven-



*Figure 1.* LGA simulation of flow past a cylinder in 2D space. Shown in the Figure are velocity vectors. The Reynolds number of the system is approximately 100. [From (Wolfram, 1988). Copyright 1988 by the Board of Trustees of the University of Illinois. Used with the by permission of University of Illinois Press.]



*Figure 2.* LBE simulation of flow past a cylinder in 2D space. Shown in the Figure are streak lines. (Courtesy of He and Doolen.)

tional methods of solving Navier-Stokes equations. The 2D flow past impulsively started cylinder with much higher Reynolds number ( $Re = 9500$ ) has also been simulated by using the LBE method and accurate results have been obtained (He & Doolen, 1997b). There are other examples of direct numerical simulation by using the lattice Boltzmann method (Hou *et al.*, 1995; Luo, 1997; Mei & Shyy, 1997), including turbulent flows (Benzi *et al.*, 1996; Amati *et al.*, 1997b). It is fair to say that nowadays the LGA and LBE methods have attained a state of maturity and can be very competitive in many areas.

This article is organized as follows. Sec. 2 provides an introduction of the lattice-gas and lattice Boltzmann methods. The philosophy behind the LGA and LBE methods is discussed. The details of the LGA and LBE hydrodynamics are also given. Sec. 3 addresses the issues concerning the future development of the methods, including hardware, modeling, and applications. Sec. 4 concludes this the article.

## 2. Introduction to LGA and LBE

### 2.1. PHILOSOPHY OF LGA AND LBE METHODS

It is a well known fact that a fluid is really a discrete system with a large number ( $\sim 10^{23}$ ) of particles (molecules). A system of many particles can be described by either molecular dynamics (MD) or a hierarchy of kinetic equations (the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy), and these two descriptions are equivalent. With the molecular chaos assumption due to Boltzmann, the BBGKY hierarchy can be closed with a single equation: the Boltzmann equation for the single particle distribution function. On the other hand, a fluid can also be treated as a continuum described by a set of partial differential equations for fluid density, velocity, and temperature: the Navier-Stokes equations.

It is usually convenient to use the Navier-Stokes equations to some fluid problems. Unfortunately these equations can be very difficult or even impossible to solve under some circumstances including inhomogeneous multi-phase or multi-component flow, and granular flow. In the case of multi-component or multi-phase flow, interfaces between different fluid components (*e.g.* oil and water) or phases (*e.g.* vapor and water) are what cause trouble. Computationally, one might be able to track a few, but hardly very many interfaces in a system. Realistic simulations of fluid systems with density or composition inhomogeneities by direct solution of the Navier-Stokes equations is therefore impractical. We can also look at the problem from a different perspective: interfaces between different components or phases of a fluid system are thermodynamic effects which result from interactions among molecules. To solve the Navier-Stokes equations, one needs to know the equation of state, which is usually unknown at an interface. It is therefore difficult to incorporate thermodynamics into the Navier-Stokes equations in a consistent or *a priori* fashion. Hence we encounter some fundamental difficulties. In the case of granular flow, the situation is even worse: it is not even clear that there exists a set partial differential equations analogous to the Navier-Stokes equations which correctly model such systems. Instead, granular flow is usually modeled by equations completely lacking the fundamental validity of the Navier-Stokes equations.

Although the Navier-Stokes equations are inadequate in some circumstances, either molecular dynamics nor the Boltzmann equation are practical alternatives because solutions of molecular dynamics or the Boltzmann equation pose formidable tasks which demand much more computational effort than the Navier-Stokes equations. Thus, we face the following predicament: although the Navier-Stokes equations are inadequate, molecular dynamics or the Boltzmann equation are much too difficult to solve and are even unnecessarily complicated if only hydrodynamic moments are

required. It is within this context that the lattice-gas automata (simplified molecular dynamics) and the lattice Boltzmann equation (simplified Boltzmann equation) become alternatives. It has been realized that hydrodynamics is insensitive to the details of the underlying microscopic or mesoscopic dynamics — the Navier-Stokes equations are merely statements of conservation laws, which reflect the same conservation laws in microscopic dynamics, and constitutive relations, which reflect the irreversible nature of the macroscopic dynamics. Different inter-molecular interactions would only result in different numerical values of the transport coefficients. Since the details of the microscopic dynamics are not important if only the hydrodynamic behavior of system is of interest, one may ask the following question: What constitutes a minimal microscopic or mesoscopic dynamic system which can provide desirable physics at the macroscopic level (hydrodynamics, thermodynamics, *etc.*). It turns out that the essential elements in such a microscopic or mesoscopic dynamic system are the conservation laws and associated symmetries. In what follows, we will demonstrate how the models of the lattice gas automata and the lattice Boltzmann equations are realized.

## 2.2. LATTICE GAS AUTOMATA

In a series of articles published in 1980's (Wolfram, 1994), Wolfram showed that cellular automata, despite their simple construction, have sufficient complexity to accomplish universal computing: that is, beginning with a particular initial state, the evolution of some automaton could implement any chosen finite algorithm. Based upon kinetic theory and the previous experience of HPP model (Hardy *et al.*, 1973) that a 2D square lattice does not possess the sufficient symmetry for hydrodynamics, Frisch *et al.* (Frisch *et al.*, 1986) and Wolfram (Wolfram, 1986) independently discovered that a simple cellular automaton on a two-dimensional triangular lattice can simulate the Navier-Stokes equations.

The LGA model Frisch *et al.* and Wolfram proposed evolves on a 2D triangular lattice space. The particles have momenta which allow them to move from one site on the lattice to another in discrete time steps. On a particular lattice site, there is either no particle or one particle with a particular momentum pointing to a nearest neighbor site. Therefore, there are at most six particles at one site simultaneously, hence this model is called the 6-bit model or FHP model. The evolution of the LGA model consists of two steps: collision and advection. The collision process is partially described in Fig. 3. For example, two particles colliding with opposite momenta will rotate their momenta  $60^\circ$  clockwise or counter-clockwise with equal probability. In Fig. 3, we do not list those configurations which can

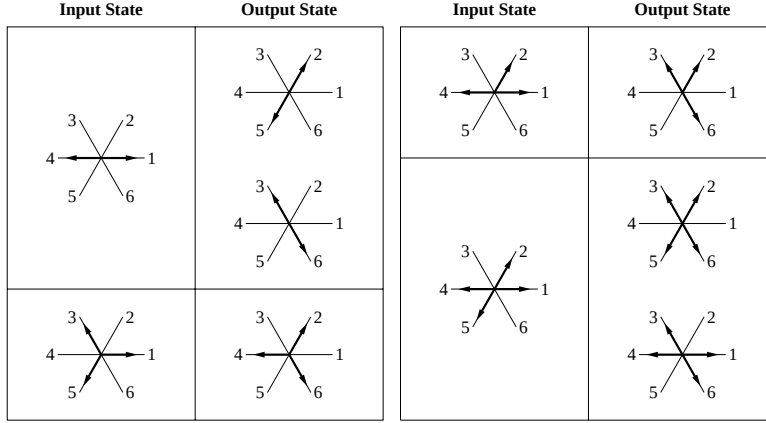


Figure 3. Collisions of FHP LGA model.

be easily obtained by rotational transformation, and which are invariant under the collision process. It should be noticed that the particle number, the momentum, and the energy are conserved in the collision process locally and exactly. (Because the FHP model has only one speed, the energy is no longer an independent variable: it is equivalent to the particle number. However, for multi-speed models, the energy is an independent variable.)

The evolution equation of the LGA can be written as:

$$n_{\alpha}(\mathbf{x} + \mathbf{e}_{\alpha}\delta_t, t + \delta_t) = n_{\alpha}(\mathbf{x}, t) + C_{\alpha}, \quad (1)$$

where  $n_{\alpha}$  is the Boolean particle number with the velocity  $\mathbf{e}_{\alpha}$ ,  $C_{\alpha}$  is the collision operator,  $\mathbf{x}$  is a vector in the lattice space with lattice constant  $\delta_x$ ,  $t$  denotes discrete time with step size  $\delta_t$ . We usually set both  $\delta_x$  and  $\delta_t$  to unity. The subscript  $\alpha$  is an index for velocity; as illustrated in Fig. 3, for the FHP model,  $\alpha$  runs from 1 to 6. After colliding, particles advect to the next site according to their velocities. Fig. 4 illustrates the evolution of the system in one time step from  $t$  to  $t + \delta_t$ . In this Figure, solid and hollow arrows represent particles with corresponding velocity at time  $t$  and  $t + \delta_t$ , respectively. The system evolves by iteration of the collision and advection processes.

According to the collision rules prescribed in Fig. 3, the collision operator,  $C_{\alpha}$ , can be written as follows:

$$C_{\alpha}(\{n_{\alpha}(\mathbf{x}, t)\}) = \sum_{\mathbf{s}, \mathbf{s}'} (s'_{\alpha} - s_{\alpha}) \xi_{ss'} \prod_{\sigma} n_{\sigma}^{s_{\sigma}} (1 - n_{\sigma})^{(1-s_{\sigma})}, \quad (2)$$

where  $\mathbf{s} \equiv \{s_1, s_2, \dots, s_6\}$  and  $\mathbf{s}' \equiv \{s'_1, s'_2, \dots, s'_6\}$  are possible incoming and outgoing configurations at a given site  $\mathbf{x}$  and time  $t$ , respectively;

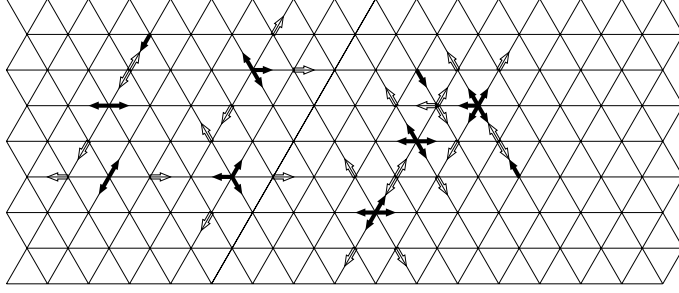


Figure 4. Evolution of FHP LGA model. Solid and hollow arrows represent particles with corresponding velocity at time  $t$  and  $t + 1$ , respectively. That is, the hollow arrows are the final configurations of the initial configurations of solid arrows after one cycle of collision and advection.

$\xi_{ss'}$  is a Boolean random number in space and time which determines the transition between state  $\mathbf{s}$  and  $\mathbf{s}'$  satisfying the following normalization condition:

$$\sum_{\mathbf{s}'} \xi_{ss'} = 1, \quad \forall \mathbf{s}. \quad (3)$$

The Boolean random number  $\xi_{ss'}$  must also have rotational symmetry, *i.e.*, for any states  $\mathbf{s}$  and  $\mathbf{s}'$ ,  $\xi_{ss'}$  is invariant if states  $\mathbf{s}$  and  $\mathbf{s}'$  are both subjected to simultaneous proper or improper rotations. It is obvious that for Boolean number  $n_\sigma$  and  $s_\sigma$ , the following equation holds:

$$n_\sigma^{s_\sigma} (1 - n_\sigma)^{(1-s_\sigma)} = \delta_{n_\sigma s_\sigma}, \quad (4)$$

where  $\delta_{n_\sigma s_\sigma}$  is the Kronecker delta symbol with two indices. Therefore, Eq. (2) can be written as

$$C_\alpha(\{n_\alpha(\mathbf{x}, t)\}) = \sum_{\mathbf{s}, \mathbf{s}'} (s'_\alpha - s_\alpha) \xi_{ss'} \delta_{\mathbf{n} \mathbf{s}}, \quad (5)$$

where  $\delta_{\mathbf{n} \mathbf{s}} \equiv \delta_{n_1 s_1} \delta_{n_2 s_2} \cdots \delta_{n_b s_b}$ . Eq. (2), or (5), is rather abstract, and the following is a specific example of the collision operator for the two-body collision:

$$\begin{aligned} C_\alpha^{(2)} = & \xi_R^{(2)} n_{\alpha+1} n_{\alpha+4} \bar{n}_\alpha \bar{n}_{\alpha+2} \bar{n}_{\alpha+3} \bar{n}_{\alpha+5} + \\ & \xi_L^{(2)} n_{\alpha+2} n_{\alpha+5} \bar{n}_\alpha \bar{n}_{\alpha+1} \bar{n}_{\alpha+3} \bar{n}_{\alpha+4} - \\ & (\xi_R^{(2)} + \xi_L^{(2)}) n_\alpha n_{\alpha+3} \bar{n}_{\alpha+1} \bar{n}_{\alpha+2} \bar{n}_{\alpha+4} \bar{n}_{\alpha+5}, \end{aligned} \quad (6)$$

where  $\bar{n}_\alpha \equiv 1 - n_\alpha$  is the complement of  $n_\alpha$ ,  $\xi_R^{(2)}$  and  $\xi_L^{(2)}$  are Boolean random numbers which determine the outcome of head-on two-body collisions. The Boolean random numbers reflect the randomness of the outcomes of

| INPUT STATE | OUTPUT STATE |
|-------------|--------------|
|             | 010010       |
| 001001      | 100100       |
| 010101      | 101010       |
| 001011      | 100110       |
|             | 110110       |
| 011011      | 101101       |

TABLE 1. Collision table for 6-Bit FHP model.

the two-body collision. Obviously, for the collision operator to satisfy the complete lattice symmetry group statistically (on average), they must satisfy

$$\langle \xi_R^{(2)} \rangle = \langle \xi_L^{(2)} \rangle, \quad (7)$$

where  $\langle \cdot \rangle$  denotes the ensemble average. The conservation laws of the particle number, momentum, and energy of the LGA micro-dynamics can be written as follows:

$$\sum_{\alpha} (s'_{\alpha} - s_{\alpha}) = 0, \quad (8a)$$

$$\sum_{\alpha} (s'_{\alpha} - s_{\alpha}) \mathbf{e}_{\alpha} = 0, \quad (8b)$$

$$\sum_{\alpha} (s'_{\alpha} - s_{\alpha}) \frac{1}{2} (\mathbf{e}_{\alpha} - \mathbf{u})^2 = 0. \quad (8c)$$

In practice, the collision can be implemented with various algorithms. One can either use logical operation [as indicated by Eq. (6)], or by table-lookup. The collision rules shown in Fig. 3 can also be represented by the collision table, as shown by Table 1. In Table 1, each bit in a binary number represents a particle number  $n_{\alpha}$ ,  $\alpha = 1, 2, \dots, 6$ , from right to left. The limitation of table lookup is the size of the table, which is  $2^b$ , where  $b$  is the number of bits of the model. Both logic operation and table lookup can be extremely fast on digital computers, and especially so on dedicated computers (Toffoli & Margolus, 1987; Adler *et al.*, 1995).



## 2.3. HYDRODYNAMICS OF LATTICE GAS AUTOMATA

The ensemble average of Eq. (1) leads to a lattice Boltzmann equation:

$$f_\alpha(\mathbf{x} + \mathbf{e}_\alpha \delta_t, t + \delta_t) = f_\alpha(\mathbf{x}, t) + \Omega_\alpha, \quad (9)$$

where  $f_\alpha \equiv m \langle n_\alpha \rangle$  and  $\Omega_\alpha \equiv \langle C_\alpha \rangle$ , where  $m$  is the particle mass. In addition, it is assumed that the correlations among colliding particles are negligible, *i.e.*,

$$\langle n_\alpha n_\beta \cdots n_\gamma \rangle = \langle n_\alpha \rangle \langle n_\beta \rangle \cdots \langle n_\gamma \rangle. \quad (10)$$

Above approximation is equivalent to the celebrated molecular chaos assumption of Boltzmann (*Stosszahlansatz*). With the molecular chaos approximation, the lattice Boltzmann collision operator is given by

$$\Omega_\alpha(\{f_\alpha(\mathbf{x}, t)\}) = \sum_{\mathbf{s}, \mathbf{s}'} (s'_\alpha - s_\alpha) A_{ss'} \prod_{\sigma} f_{\sigma}^{s_\sigma} (1 - f_{\sigma})^{(1-s_\sigma)}, \quad (11)$$

where  $A_{ss'} \equiv \langle \xi_{ss'} \rangle$  is the transition probability from state  $\mathbf{s}$  and  $\mathbf{s}'$ . The hydrodynamic moments are given by:

$$\rho = \sum_{\alpha} f_{\alpha}, \quad \rho \mathbf{u} = \sum_{\alpha} \mathbf{e}_{\alpha} f_{\alpha}, \quad \rho \varepsilon = \sum_{\alpha} \frac{1}{2} (\mathbf{e}_{\alpha} - \mathbf{u})^2 f_{\alpha}, \quad (12)$$

where  $\mathbf{u}$ , and  $\varepsilon$  are the mass density, the velocity, and the internal energy density, respectively.

Eq. (9) can be expanded in a Taylor series of  $\delta_t$  up to the second order:

$$(\partial_t + \mathbf{e}_{\alpha} \cdot \nabla) f_{\alpha} + (\partial_t + \mathbf{e}_{\alpha} \cdot \nabla)^2 f_{\alpha} = \Omega_{\alpha}. \quad (13)$$

The equilibrium distribution,  $f_{\alpha}^{(0)}$ , which is the solution of  $\Omega_{\alpha}(\{f_{\alpha}\}) = 0$ , must be a Fermi-Dirac distribution because the system is a binary one (Wolfram, 1986), that is,

$$f_{\alpha}^{(0)} = \frac{1}{1 + \exp(a + b \mathbf{u} \cdot \mathbf{e}_{\alpha})}, \quad (14)$$

where coefficients  $a$  and  $b$  are functions of  $\rho$  and  $\mathbf{u}^2$  in general. Because the coefficients  $a$  and  $b$  in  $f_{\alpha}^{(0)}$  cannot be determined exactly (Wolfram, 1986),  $f_{\alpha}^{(0)}$  must be expanded in a Taylor series of  $\mathbf{u}$  — the small velocity (low Mach number) expansion. With the small velocity expansion of the equilibrium  $f_{\alpha}^{(0)}$  and through Chapman-Enskog analysis, one can obtain the following hydrodynamic equations from the FHP LGA model (Frisch *et al.*, 1986; Wolfram, 1986):

$$\partial_t \rho + \nabla \cdot \rho \mathbf{u} = 0, \quad (15a)$$

$$\partial_t \rho \mathbf{u} + \nabla (g \rho \mathbf{u} \mathbf{u}) = -\nabla P + \nu \nabla^2 \rho \mathbf{u}, \quad (15b)$$

where  $g$  is a function of  $\rho$ ,

$$P = c_s^2 \rho \left[ 1 - g \frac{\mathbf{u}^2}{c^2} \right], \quad c_s = c/\sqrt{2}, \quad (16a)$$

$$\nu = -\frac{1}{8}(2\lambda^{-1} + 1)c\delta_x, \quad (16b)$$

$c_s$  is the sound speed,  $c = \delta_x/\delta_t$ , and  $\lambda$  is an eigenvalue of the linearized collision operator (Rothman & Zaleski, 1997):

$$J_{\alpha\beta} \equiv \left. \frac{\partial \Omega_\alpha}{\partial f_\beta} \right|_{f_\beta = f_\beta^{(0)}}.$$

The defects of the LGA hydrodynamics are obvious from the above equations:

1. Simulations are intrinsically noisy because of the large fluctuation in  $n_\alpha$ ;
2. The factor  $g(\rho)$  is not unity, thus Galilean invariance is destroyed;
3. It is difficult to increase the Reynolds number  $\text{Re}$ ;
4. The equation of state depends on  $\mathbf{u}^2$  (unphysical);
5. There exist (unphysical) spurious conserved quantities due to the simple symmetry of the lattice-gas automata.

However, all these defects can be fixed by using more sophisticated LGA models (Chen *et al.*, 1997), or the other alternative — the lattice Boltzmann equation.

#### 2.4. LATTICE BOLTZMANN EQUATION

Historically, models of the lattice Boltzmann equation evolved from their Boolean counterparts: the lattice-gas automaton. Eq. (9) is the original lattice Boltzmann model to replace the corresponding LGA model for hydrodynamics (McNamara & Zanetti, 1988). Later it was realized that the collision operator can be linearized and be replaced with a simple relaxation model (Chen *et al.*, 1992; Qian *et al.*, 1992). Recently, it has been shown that the LBE is a special discretized form of the continuous Boltzmann equation (He & Luo, 1997a; He & Luo, 1997b).

For the sake of simplicity, and without loss of generality, the Boltzmann equation with the Bhatnagar-Gross-Krook (BGK) approximation is used in the following analysis. The Boltzmann BGK equation can be written in the form of an ordinary differential equation:

$$D_t f + \frac{1}{\lambda} f = \frac{1}{\lambda} f^{(0)}, \quad (17)$$

where  $D_t \equiv \partial_t + \boldsymbol{\xi} \cdot \nabla$  is the Lagrangian derivative along the microscopic velocity  $\boldsymbol{\xi}$ ,  $f \equiv f(\mathbf{x}, \boldsymbol{\xi}, t)$  is the single particle distribution function,  $\lambda$  is the relaxation time due to collision, and  $f^{(0)}$  is the Maxwell-Boltzmann distribution function:

$$f^{(0)} \equiv \frac{\rho}{(2\pi RT)^{D/2}} \exp \left[ -\frac{(\boldsymbol{\xi} - \mathbf{u})^2}{2\theta} \right], \quad (18)$$

in which  $D$  is the dimension of the space;  $\rho$ ,  $\mathbf{u}$  and  $\theta = k_B T/m$  are the macroscopic density of mass, the velocity, and the normalized temperature, respectively,  $T$ ,  $k_B$  and  $m$  are temperature, the Boltzmann constant, and particle mass. The macroscopic variables are the moments of the distribution function  $f$  with respect to velocity  $\boldsymbol{\xi}$ :

$$\rho = \int f d\boldsymbol{\xi}, \quad \rho \mathbf{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi}, \quad \rho \theta = \frac{1}{2} \int (\boldsymbol{\xi} - \mathbf{u})^2 f d\boldsymbol{\xi}. \quad (19)$$

Equation (17) can be formally integrated over a time interval  $\delta_t$ :

$$\begin{aligned} f(\mathbf{x} + \boldsymbol{\xi} \delta_t, \boldsymbol{\xi}, t + \delta_t) &= e^{-\delta_t/\lambda} f(\mathbf{x}, \boldsymbol{\xi}, t) \\ &+ \frac{1}{\lambda} e^{-\delta_t/\lambda} \int_0^{\delta_t} e^{t'/\lambda} f^{(0)}(\mathbf{x} + \boldsymbol{\xi} t', \boldsymbol{\xi}, t + t') dt'. \end{aligned} \quad (20)$$

Assuming that  $\delta_t$  is small enough and  $f^{(0)}$  is smooth enough locally, and neglecting the terms of the order  $\mathcal{O}(\delta_t^2)$  or smaller in the Taylor expansion of the right hand side of Eq. (20), we obtain

$$f(\mathbf{x} + \boldsymbol{\xi} \delta_t, \boldsymbol{\xi}, t + \delta_t) - f(\mathbf{x}, \boldsymbol{\xi}, t) = -\frac{1}{\tau} [f(\mathbf{x}, \boldsymbol{\xi}, t) - f^{(0)}(\mathbf{x}, \boldsymbol{\xi}, t)], \quad (21)$$

where  $\tau \equiv \lambda/\delta_t$  is the dimensionless relaxation time.

The equilibrium distribution function  $f^{(0)}$  can be expanded as a Taylor series in  $\mathbf{u}$ . By retaining the Taylor expansion up to  $\mathbf{u}^2$ , we obtain:

$$f^{(\text{eq})} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp \left( -\frac{\boldsymbol{\xi}^2}{2\theta} \right) \left[ 1 + \frac{(\boldsymbol{\xi} \cdot \mathbf{u})}{\theta} + \frac{(\boldsymbol{\xi} \cdot \mathbf{u})^2}{2\theta^2} - \frac{\mathbf{u}^2}{2\theta} \right]. \quad (22)$$

For the purpose of deriving the Navier-Stokes equations, the above second-order expansion is sufficient.

To derive the Navier-Stokes equations, the following moment integral must be evaluated exactly:

$$\int \boldsymbol{\xi}^m f^{(\text{eq})} d\boldsymbol{\xi}, \quad (23)$$

where  $0 \leq m \leq 3$  for isothermal models. The above integral contains the following integral which can be evaluated by Gaussian-type quadrature:

$$I = \int \exp(-\xi^2/2\theta) \psi(\xi) d\xi = \sum_{\alpha} W_{\alpha} \exp(-\xi_{\alpha}^2/2\theta) \psi(\xi_{\alpha}), \quad (24)$$

where  $\psi(\xi)$  is a polynomial in  $\xi$ , and  $W_{\alpha}$  and  $\xi_{\alpha}$  are the weights and the abscissas (or discrete velocities) of the quadrature, respectively. Accordingly, the hydrodynamic moments of Eqs. (19) can be computed by quadrature as well:

$$\rho = \sum_{\alpha} f_{\alpha}, \quad \rho \mathbf{u} = \sum_{\alpha} \xi_{\alpha} f_{\alpha}, \quad \rho \theta = \frac{1}{2} \sum_{\alpha} (\xi_{\alpha} - \mathbf{u})^2 f_{\alpha}, \quad (25)$$

where  $f_{\alpha} \equiv f_{\alpha}(\mathbf{x}, t) \equiv W_{\alpha} f(\mathbf{x}, \xi_{\alpha}, t)$ . We shall use the 9-bit isothermal LBE model on square lattice space as a concrete example to illustrate the derivation of LBE models: the evolution equation (21) on a discretized phase space and time with a proper equilibrium distribution function leads to the Navier-Stokes equations.

To derive the 9-bit LBE model, a Cartesian coordinate system is used, and accordingly, we set  $\psi(\xi) = \xi_x^m \xi_y^n$ . The integral of Eq. (24) becomes:

$$I = (\sqrt{2\theta})^{(m+n+2)} I_m I_n, \quad (26)$$

where

$$I_m = \int_{-\infty}^{+\infty} e^{-\zeta^2} \zeta^m d\zeta, \quad (27)$$

and  $\zeta = \xi_x/\sqrt{2\theta}$  or  $\xi_y/\sqrt{2\theta}$ . Naturally, the third-order Hermite formula is the optimal choice to evaluate  $I_m$  for the purpose of deriving the 9-bit LBE model, *i.e.*,  $I_m = \sum_{j=1}^3 \omega_j \zeta_j^m$ . The three abscissas ( $\zeta_j$ ) and the corresponding weights ( $\omega_j$ ) of the quadrature are:

$$\begin{aligned} \zeta_1 &= -\sqrt{3/2}, & \zeta_2 &= 0, & \zeta_3 &= \sqrt{3/2}, \\ \omega_1 &= \sqrt{\pi}/6, & \omega_2 &= 2\sqrt{\pi}/3, & \omega_3 &= \sqrt{\pi}/6. \end{aligned} \quad (28)$$

Then, the integral of Eq. (26) becomes:

$$I = 2\theta [\omega_2^2 \psi(\mathbf{0}) + \sum_{\alpha=1}^4 \omega_1 \omega_2 \psi(\xi_{\alpha}) + \sum_{\alpha=5}^8 \omega_1^2 \psi(\xi_{\alpha})], \quad (29)$$

where  $\xi_{\alpha}$  is the zero velocity vector for  $\alpha = 0$ , the vectors of  $\sqrt{3\theta}(\pm 1, 0)$  and  $\sqrt{3\theta}(0, \pm 1)$  for  $\alpha = 1-4$ , and the vectors of  $\sqrt{3\theta}(\pm 1, \pm 1)$  for  $\alpha = 5-8$ . Note that the above quadrature is exact for  $(m+n) \leq 5$ .

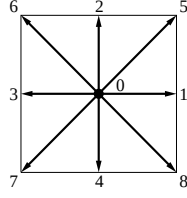


Figure 5. Discrete velocities of the 9-bit model on a square lattice.

Now momentum space is discretized with nine discrete velocities  $\{\xi_\alpha | \alpha = 0, 1, \dots, 8\}$ . To obtain the 9-bit model, configuration space is discretized accordingly, *i.e.*, it is discretized into a square lattice with lattice constant  $\delta_x = \sqrt{3\theta} \delta_t$ . It should be stressed that the temperature  $\theta$  has no physical significance here because we are only dealing with an isothermal model. We can therefore choose  $\delta_x$  to be a fundamental quantity instead, thus  $\sqrt{3\theta} = c \equiv \delta_x / \delta_t$ , or  $\theta = c_s^2 = c^2/3$ , where  $c_s$  is the sound speed of the model.

By comparing Eqs. (24) and (29), we can identify the weights defined in Eq. (24):

$$W_\alpha = 2\pi \theta \exp(\xi_\alpha^2 / 2\theta) w_\alpha, \quad (30)$$

where

$$w_\alpha = \begin{cases} 4/9, & \alpha = 0, \\ 1/9, & \alpha = 1, 2, 3, 4, \\ 1/36, & \alpha = 5, 6, 7, 8. \end{cases} \quad (31)$$

Then, the equilibrium distribution function of the 9-bit model is:

$$\begin{aligned} f_\alpha^{(\text{eq})} &= W_\alpha f^{(\text{eq})}(\mathbf{x}, \xi_\alpha, t) \\ &= w_\alpha \rho \left\{ 1 + \frac{3(\mathbf{e}_\alpha \cdot \mathbf{u})}{c^2} + \frac{9(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c^4} - \frac{3\mathbf{u}^2}{2c^2} \right\}, \end{aligned} \quad (32)$$

where

$$\mathbf{e}_\alpha = \begin{cases} (0, 0), & \alpha = 0, \\ (\cos \theta_\alpha, \sin \theta_\alpha) c, & \alpha = 1, 2, 3, 4, \\ (\cos \theta_\alpha, \sin \theta_\alpha) \sqrt{2} c, & \alpha = 5, 6, 7, 8, \end{cases} \quad (33)$$

and  $\theta_\alpha = (\alpha - 1)\pi/2$  for  $\alpha = 1-4$ , and  $(\alpha - 5)\pi/2 + \pi/4$  for  $\alpha = 5-8$ , as shown in Fig. 5. The Navier-Stokes equation derived from the above LBE model is:

$$\rho \partial_t \mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \rho \nu \nabla^2 \mathbf{u}, \quad (34)$$

where the equation of state is the ideal gas one,  $P = c_s^2 \rho$ , the sound speed  $c_s = c/\sqrt{3}$ , and the viscosity  $\nu = \frac{1}{6}(2\tau - 1)c \delta_x$  for the 9-bit model.

Similarly, we can also derive two-dimensional 6-bit, 7-bit, and three-dimensional 27-bit LBE models (He & Luo, 1997b).

In the above derivation, the discretization of phase space is accomplished by discretizing momentum space in such a way that a lattice structure in configuration space is simultaneously obtained. That is, the discretization of configuration space is determined by that of momentum space. Of course, the discretization of momentum space and configuration space can be done independently. This consideration has two immediate consequences: arbitrary mesh grids and significant enhancement of the Reynolds number in LBE hydrodynamic simulations.

To implement arbitrary mesh grids with the LBE method, one first discretizes the configuration space by generating a mesh adapted to the physics of the particular problem. Then at each grid point, one can discretize momentum space as before. Now, a local LBE is built on each mesh grid point. The evolution of this discretized Boltzmann equation (DBE) consists of the following three steps. The first two steps are the usual collision and advection process as in the previous LBE models. After collision and advection, interpolation follows. The interpolation process is what distinguishes the DBE from the LBE method. Because the mesh grids can be arbitrary, the distribution function  $f_\alpha$  at one mesh grid point, say  $\mathbf{X}$ , cannot go to another grid point in general through the advection process as it can in previous LBE models. Therefore, the interpolation step becomes necessary to construct  $f_\alpha(\mathbf{X}, t)$  on each and every mesh grid point from  $f_\alpha(\mathbf{X} + \mathbf{e}_\alpha \delta t, t)$  after the advection process. Of course, interpolation brings in additional numerical error, but it can be justified so long as the error induced by interpolation does not affect the DBE algorithm as a whole (He *et al.*, 1996). In addition, the separate discretization of momentum and configuration space allows us to increase the Reynolds number significantly in numerical simulations without enlarging mesh sizes or decreasing the viscosity by adjusting  $\tau$  (He *et al.*, 1996). In other words, the limitation posed by the lattice Reynolds number is completely overcome (He *et al.*, 1997) and the stability of the LBE method is greatly improved (He *et al.*, 1996; He *et al.*, 1997).

## 2.5. BOUNDARY CONDITIONS

In lattice-gas automata, non-slip boundary conditions can be realized by the bounce-back scheme: a particle colliding with the wall simply reverses its momentum. Also, slip boundary condition can be realized by the reflection scheme: a particle colliding with the wall reverses its momentum normal to the wall and maintains its tangential momentum unchanged. Both the bounce-back scheme and reflection scheme are easy to implement

and are very efficient computationally. Combination of the two can produce partial slip boundary condition. Both bounce-back or reflection schemes can be implemented in the lattice Boltzmann equation with some variations (Ginzbourg & d'Humières, 1996; Chen *et al.*, 1996; He *et al.*, 1997; Zou & He, 1997; Fang *et al.*, 1998). The ease of handling boundary conditions and complicated geometries is a very important feature of the lattice-gas and lattice Boltzmann methods.

### 3. The Future

In order to address the issues concerning the future development of the lattice-gas and lattice Boltzmann methods, a comparison between the conventional CFD methods and the LGA and LBE methods will be helpful.

1. The arithmetic operations in the conventional CFD solvers are floating number operations (FLOPs), while the LGA method and integer LBE method involve only logical (or integer) operations or table-lookups. Logical operations are certainly more natural and hence faster on digital computers.
2. Navier-Stokes solvers inevitably need to treat the nonlinear convective term,  $\mathbf{u} \cdot \nabla \mathbf{u}$ ; the LGA and LBE methods totally avoid the nonlinear convective term, because the convection becomes simple advection (uniform data shift) in the lattice-gas and lattice Boltzmann methods.
3. CFD solvers for the incompressible Navier-Stokes equations need to solve the Poisson equation for the pressure. This involves global data communication, in the LGA and LBE methods, data communication is always local.
4. Due to unstructured grids and domains, data communication in some conventional CFD solvers is nonuniform; the LGA and LBE methods usually employ the Cartesian grids and thus the data communication is always uniform.
5. The Courant-Fredrick-Levy (CFL) number is close to unity in most Navier-Stoke solvers with respect to the system size; in the LGA and LBE methods the CFL number is proportional to  $\delta_x^{-1}$ , where  $\delta_x$  is the grid size, *i.e.*, the grid CFL number is equal to 1 in the LGA and LBE methods. Consequently, the LGA and LBE methods are very inefficient for solving steady state problems, because their speed of convergence is dictated by acoustic propagation, which is very slow.
6. Boundary conditions, such as complicated geometries, sometimes are very hard to implement in conventional Navier-Stokes solvers; such boundary conditions can be trivially implemented in the LGA and LBE methods without affecting the computational speed;
7. Turbulence modeling is essential to the some conventional CFD meth-

ods, such modeling is implicit in the LGA and LBE methods. In addition, the LGA and LBE methods are intrinsically compressible;

8. The accuracy of the conventional Navier-Stokes solvers is well established. It has been shown that the accuracy of the LGA and LBE methods is of first order in time and second order in space. In contrast to the Navier-Stokes solvers, the LGA and LBE methods usually need comparable, or finer resolutions, depending on specific problems.

It is obvious that the problems the LGA and LBE methods encounter in their future development will be significantly different from what the conventional CFD methods will. In what follows, we briefly discuss the issues concerning hardware, modeling, and applications of the LGA and LBE methods.

### 3.1. HARDWARE

Because the LGA and LBE algorithms can be implemented with logical (binary) operations or table-lookups, these algorithms can be extremely fast on dedicated computers (Clouqueur & d'Humières, 1987; Toffoli & Margolus, 1987; Despain *et al.*, 1988). A recent study showed that a Cellular-Automata-Machine-8 (CAM-8) (Toffoli & Margolus, 1987) with 8 nodes achieved a speed of 7 million site updates per second for a 3D LGA algorithm (Adler *et al.*, 1995). An 8-node CAM-8 machine is similar to a low end workstation; it consists of 2 MB of SRAM, 64 MB of DRAM, and about two million gates CMOS logic, with a clock frequency of 25 MHz (Toffoli & Margolus, 1987; Adler *et al.*, 1995). However, the speed of the CAM-8 can be increased by four orders of magnitude ( $10^4$ ) with technology available today by putting logic directly into a DRAM memory chip and by exploiting the enormous memory bandwidth that can be made available on-chip (Margolus, 1998). This increased speed exceeds that of a Connection Machine 2, a SIMD supercomputer with 65,536 ( $= 2^{16}$ ) bit processors.

In recent years, we have seen a number of new ideas regarding models of computation in the future: the DNA model, the quantum model and the reversible model (Calude & Casti, 1998). In addition, there is an effort to use the quantum-dot as a computing device (Lent *et al.*, 1993; Tougaw & Lent, 1996; Lent & Tougaw, 1997). (There is a collections of papers on quantum engineering published by Nature (Nature, 1998).) The size of a quantum-dot can be a few ( $\text{\AA}$ ) to a few tens of ( $nm$ ). A quantum-dot has a few electronic bound states, and these states can be manipulated like a bit processor, which is a perfect model for cellular automata computing (Lent *et al.*, 1993; Tougaw & Lent, 1996; Lent & Tougaw, 1997). The progress made in these new areas will perhaps revolutionize the concept of computation, and thus enhance computing speeds by many orders of magnitude beyond



what we can now imagine.

### 3.2. MODELING

The LGA and LBE methods need solutions to the following modeling issues in the near future:

1. Thermo-hydrodynamics with large temperature gradient,  $\nabla T$ . Due to the limit of small number of discrete velocities, the existing LGA and LBE models are not very successful in problems of thermo-hydrodynamics with large temperature gradient. However, improvement can be achieved by increasing the number of discrete velocities (Pavlo *et al.*, 1998) or by other means (He *et al.*, 1997);
2. Compressibility, transonic and supersonic flows. Due to the low Mach number expansion of the equilibrium distribution function in the LBE method, the method is limited to incompressible or near incompressible flows. To overcome this limitation of the LBE method, one can decrease the sound speed in the existing models and reformulate the equilibrium. It should be pointed out that there exists other kinetic schemes which can effectively simulate compressible flows and shocks (Xu & Prendergast, 1993).
3. Plastic-elastic collisions, and consideration of internal degrees of freedom. In the existing LGA and LBE models the collisions are hard-sphere-like elastic ones because the particles are structureless. It is inevitable that particles with internal degrees of freedom and hence plastic-elastic collisions among them have to be taken into consideration if phase transition and compressibility are to be studied.
4. Correlations, long-range interactions, and dissipation. In the existing LGA and LBE models, the correlations among colliding particles are neglected due to the assumption of molecular chaos. The assumption may need some corrections if one is interested in something beyond the hydrodynamics of simple fluids. For instance, one must include non-local interactions in liquid-vapor phase transition. Also, dissipation mechanism is essential in systems such as granular flows.
5. Liquid-solid phase transition. Although the LGA and LBE methods are successful in modeling liquid-vapor phase transition, nothing has been done regarding the liquid-solid phase transition. The modeling of the liquid-solid phase transition is a difficult problem and one should expect some progress to be made in the near future when the full potential of kinetic theory is realized.
6. Turbulence modeling. Turbulence modeling is a mature subject and it has not been utilized in anyway in the LGA and LBE methods. Theory on the connection between the turbulence modeling and the LGA and

LBE methods will be of interest to many in the future.

7. Quantum systems. It has been shown that quantum lattice gas models can be effective algorithms to simulate quantum systems on quantum computer (Benzi & Succi, 1993; Succi, 1996; Meyer, 1997; Boghosian & Taylor, 1998). However, it is not clear yet whether the quantum lattice gas models can be used as effective algorithms on digital computers. This possibility needs to be further explored.

### 3.3. APPLICATIONS

The physical nature of the LGA and LBE methods makes them particularly well suited for certain problems but not others. One should expect significant progress made in the near future by using the LBE method in the area of interfacial dynamics related to the instability of either Rayleigh-Taylor or Richtmyer-Meshkov (Kotelnikov & Montgomery, 1997). The lattice Boltzmann method has been successfully applied to multicomponent fluids in complex three-dimensional geometries (Martys & Chen, 1996; Chen & Doolen, 1998) and interfacial gravity waves (Buick & Greated, 1998). In addition to interfacial dynamics, there are two types of problems on which the LGA and LBE methods may have a major impact: problems which are numerically stiff due to drastically different time scales in the system, and systems for which there exists no adequate macroscopic equation.

Stiff problems are ubiquitous in nature, and a few examples of them to which the LGA and LBE methods are well-suited are:

1. Flow-structure interaction (structural response time *vs.* hydrodynamic time). Aero-acoustics is a typical example of such a problem. This problem is not only stiff, but also involves moving boundaries. The LBE method is particularly suitable for solving this problem because: (a) CFL number of the LBE algorithm is very small and comparable to the structural response, yet the computation in each (small) time step is rather trivial so that the overall computation remains efficient and the structural response can be physically modeled; (b) The simplicity of implementing boundary conditions such as bounce-back boundary condition enables the LBE algorithms to deal with moving boundaries between structure-flow interfaces efficiently.
2. Combustion (chemical reaction time *vs.* hydrodynamic time). The LGA and LBE methods have been successful in dealing with reactive and hydrodynamic systems separately. It should not be too difficult to couple the two together since the models for reactive systems have already the underlying hydrodynamics in them.
3. Solidification (heat conduction time *vs.* hydrodynamic time). Solidification remains a challenging problem to model in general for any method.

Difficulties arise when the hydrodynamics is taken into consideration of the problem. In principle, kinetic theory is applicable to both fluid and solid phases, but much still remains to be done in this area.

The following are some problems of which there are no adequate or even commonly accepted *macroscopic* equations. Kinetic models such the lattice-gas automata or the lattice Boltzmann equation may be particularly useful to these problems:

1. Granular flows (no adequate macroscopic equation). Granular flows have attracted much interest recently. Currently, molecular dynamics remains the primary method to accurately simulate such systems. Although some preliminary theoretical results have been obtained by kinetic theory (Brey *et al.*, 1996), a realistic kinetic model has yet to be developed.
2. Rheology. The term “rheology” covers any fluid which is not described by the Navier-Stokes equations for Newtonian fluids. Examples include non-Newtonian, and polymeric flows. In many complex fluids, constitutive relations are difficult to obtain from first principles. Therefore, the LGA or LBE models which directly use model interactions among particles can be applicable and effective to study such systems.
3. Microscopic flows and heat-transfer. The Navier-Stokes equations break down in microscopic scales where kinetic effects are no longer negligible and may even be dominant, as in Micro-Electro-Mechanical-Systems (MEMS) (Ho & Tai, 1998). Because of kinetic nature of the LGA and LBE methods, they are particularly useful in studying microscopic or mesoscopic systems (Nie *et al.*, 1998).
4. Electronic transport in semiconductors. This is challenging problem in physics and important one in the semiconductor industry. Currently there are quantum molecular dynamic (microscopic) or hydrodynamic (macroscopic) simulations of the system, while mesoscopic theory is yet to be developed. Although there were previous successful attempts in this area by using the LGA method (Ancona, 1990; Komater *et al.*, 1992), a systematic pursuit of the application of the LGA and LBE methods to this particular area is still lacking.

#### 4. Conclusion

In this article, I have provided a brief review of some key aspects the lattice-gas automata and lattice Boltzmann methods, and some speculations on their future. There are two important lessons which should be learned from the lattice-gas automata and lattice Boltzmann equation. First of all, extremely simple microscopic dynamics may lead to extremely complicated macroscopic dynamics, the so-called emergent phenomena. Second, cellular

automata can accomplish very complex tasks of computation such as solving partial differential equations, and they are naturally suited to digital computers. I have also pointed out a few areas in which the new methods may be very effective and efficient. Hopefully more effort will be devoted to development of the methods for those interesting and important applications in the future.

Although this article mainly addresses the applications of the LGA and LBE methods to various problems, one should not be misled to the impression that these methods only amount to nothing more than practical numerical methods of not much theoretical value. To the contrary, the theoretical significance of these methods may well exceed their applied importance. We know that the Boltzmann equation, or kinetic theory in general, is a powerful theoretical means for us to understand transport phenomena associated with the systems near or far from equilibrium. However, the Boltzmann equation is difficult to solve analytically or numerically, thus its application is limited, especially in term of computing. In contrast, the lattice-gas automata and lattice Boltzmann equation are effective and efficient alternatives of the Boltzmann equation when it comes to computing. The derivation of the lattice Boltzmann equation shows that drastic approximations can be applied when hydrodynamic behavior of a system is of the interest. The fact that the entire velocity space can be replaced by a small number of discrete velocities while hydrodynamics of the system remains intact is an exemplary illustration of how a simple kinetic model can be constructed. It is well known that the Ising model is a paradigm of equilibrium statistical mechanics: it has almost everything one wishes to know about phase transition. Much like the Ising model, the lattice gas automata and lattice Boltzmann equation can serve as new paradigms of nonequilibrium statistical mechanics. Furthermore, the LGA and LBE methods can offer more than the Navier-Stokes equations can. Examples are multi-phase and multi-component fluids which are difficult to simulate by using the Navier-Stokes equations as discussed previously. Therefore, these methods are not only powerful computational tools to simulate, but also important theoretical means to understand various complex systems and novel paradigms of computation.

The author is grateful to Prof. N. Margolus for his insightful conversations on cellular automata computation and the information of several key references on the subject, and to Dr. S. Girimaji and Dr. R. Rubinstein for their editorial assistance and stimulating discussions on many subjects.

## References

- Adler, C., Boghosian, B.M., Flekkøy, E.G., Margolus, N. and Rothman, D.H. (1995) Simulating Three-Dimensional Hydrodynamics on a Cellular-Automata Machine,

- J. Stat. Phys.*, **81**, pp. 105–128.
- Amati, G., Succi, S. and Piva, R. (1997a) Massively Parallel Lattice-Boltzmann Simulation of Turbulent Channel Flow, *Int. J. Mod. Phys.*, **8**, pp. 869–877.
- Amati, G., Benzi, R. and Succi, S. (1997b) Extended Self-Similarity in Boundary-Layer Turbulence, *Phys. Rev. E*, **55**, pp. 985–998.
- Ancona, M.G. (1990) Lattice-Gas Approach to Semiconductor Device Simulation, *Solid-State Elec.*, **33**, pp. 1633–1642.
- Benzi, R. and Succi, S. (1993) Lattice Boltzmann-Equation for Quantum-Mechanics, *Physica D*, **69**, pp. 327–332.
- Benzi, R., Struglia, M.V. and Tripiccone, R. (1996) Extended Self-Similarity in Numerical Simulations of 3-Dimensional Anisotropic Turbulence, *Phys. Rev. E*, **53**, pp. R5565–R5568.
- Boghosian, B.M. and Taylor IV, W. (1998) Quantum Lattice-Gas Model for the Many-Particle Schrödinger Equation in  $d$ -Dimensions, *Phys. Rev. E*, **57**, pp. 54–66.
- Boon, J.-P., Dab, D., Kapral, R. and Lawniczak, A. (1996) Lattice Gas Automata for Reactive Systems, *Phys. Rep.*, **273**, pp. 55–147.
- Brey, J.J., Moreno, F. and Dufty, J.W. (1996) Model Kinetic Equation for Low-Density Granular Flow, *Phys. Rev. E*, **54**, pp. 445–456.
- Broadwell, J.E. (1964) Study of Rarefied Shear Flow by the Discrete Velocity Method, *J. Fluid Mech.*, **19**, pp. 401–414; (1964) Shock Structure in a Simple Discrete Velocity Gas, *Phys. Fluids*, **7**, pp. 1243–1247.
- Buick, J.M. and Greated, C.A. (1998) Lattice Boltzmann Modeling of Interfacial Gravity Waves, *Phys. Fluids*, **10**, pp. 1490–1511.
- Calude, C.S. and Casti, J.L. (1998) Parallel Thinking, *Nature*, **392**, pp. 549–551.
- Chen, H. and Matthaeus, W.H. (1987) New Cellular Automaton Model for Magnetohydrodynamics, *Phys. Rev. Lett.*, **58**, pp. 1845–1848.
- Chen, H., Matthaeus, W.H. and Klein, L.W. (1988) An Analytic Theory and Formulation of a Local Magnetohydrodynamic Lattice Gas-Model, *Phys. Fluids*, **31**, pp. 1439–1455.
- Chen, H., Chen, S. and Matthaeus, W.H. (1992) Recovery of the Navier-Stokes Equations Using a Lattice-Gas Boltzmann Method, *Phys. Rev. A*, **45**, pp. R5339–5342.
- Chen, H., Teixeira, C. and Molvig, K. (1997) Digital Physics Approach to Computational Fluid Dynamics, *Int. J. Mod. Phys.*, **8**, pp. 675–684.
- Chen, S., Chen, H., Martínez, D. and Matthaeus, W.H. (1991) Lattice Boltzmann Model for Simulation of Magnetohydrodynamics, *Phys. Rev. Lett.*, **67**, pp. 3776–3779.
- Chen, S., Dawson, S.P., Doolen, G.D., Janecky, D.R. and Lawniczak, A. (1995) Lattice Methods and Their Applications to Reacting Systems, *Comput. Chem. Eng.*, **19**, pp. 617–646.
- Chen, S., Martínez, D. and Mei, R. (1996) On Boundary Conditions in Lattice Boltzmann Methods, *Phys. Fluids*, **8**, pp. 2527–2536.
- Chen, S. and Doolen, G.D. (1998) Lattice Boltzmann Method for Fluid Flows, *Ann. Rev. Fluid Mech.*, **30**, pp. 329–364.
- Chen, S., Doolen, G., He, X., Nie, X. and Zhang, R. (1998) Recent Advances in Lattice Boltzmann Methods, to be submitted to *Proceedings of National Congress of Applied Mechanics*.
- Clouqueur, A. and d’Humières, D. (1987) RAP1, a Cellular Automaton Machine for Fluid Dynamics, *Complex Systems*, **1**, pp. 585–597.
- d’Humières, D., Lallemand, P. and Frisch, U. (1986) Lattice Gas Models for 3D Hydrodynamics, *Europhys. Lett.*, **2**, pp. 291–297.
- Despain, A., Max, C.E., Doolen, G. and Hasslacher, B. (1988) Prospects for a Lattice-Gas Computer, in (Doolen, 1990), pp. 211–218.
- Doolen, G.D., editor (1990) *Lattice Gas Methods for Partial Differential Equations*, Addison-Wesley, New York.
- Fang, H., Lin, Z. and Wang, Z. (1998) Lattice Boltzmann Simulation of Viscous Fluid Systems with Elastic Boundaries, *Phys. Rev. E*, **57**, pp. R25–R28.

- Frisch, U., Hasslacher, B. and Pomeau, Yv. (1986) Lattice-Gas Automata for the Navier-Stokes Equation, *Phys. Rev. Lett.*, **56**, pp. 1505–1508.
- Ginzbourg, I. and d'Humières, D. (1996) Local Second-Order Boundary Methods for Lattice Boltzmann Models, *J. Stat. Phys.*, **84**, pp. 927–971.
- Hardy, J., Pomeau, Yv. and de Pazzis, O. (1973) Time Evolution of a Two-Dimensional Classical Lattice System, *Phys. Rev. Lett.*, **31**, pp. 276–279; (1973) Time Evolution of a Two-Dimensional Model System. I. Invariant States and Time Correlation Functions, *J. Math. Phys.*, **14**, pp. 1746–1759.
- He, X., Luo, L.-S. and Dembo, M. (1996) Some Progress in Lattice Boltzmann Method. Part I. Nonuniform Mesh Grids, *J. Comput. Phys.*, **129**, pp. 357–363.
- He, X. and Luo, L.-S. (1997a) *A Priori* Derivation of the Lattice Boltzmann Equation, *Phys. Rev. E*, **55**, pp. R6333–R6336.
- He, X. and Luo, L.-S. (1997b) Theory of the Lattice Boltzmann Equation: From the Boltzmann Equation to the Lattice Boltzmann Equation, *Phys. Rev. E*, **56**, pp. 6811–6817.
- He, X. and Doolen, G. (1997a) Lattice Boltzmann Method on a Curvilinear Coordinate System: Vortex Shedding behind a Circular Cylinder, *Phys. Rev. E*, **56**, pp. 434–440.
- He, X. and Doolen, G. (1997b) Lattice Boltzmann Method on Curvilinear Coordinates System: Flow around a Circular Cylinder, *J. Comput. Phys.*, **134**, pp. 306–315.
- He, X., Luo, L.-S. and Dembo, M. (1997) Some Progress in the Lattice Boltzmann Method. Reynolds Number Enhancement in Simulations, *Physica A*, **239**, pp. 276–285.
- He, X., Chen, S. and Doolen, G. (1997) A Novel Thermal Model for the Lattice Boltzmann Method, submitted to *J. Comput. Phys.*
- He, X., Zou, Q., Luo, L.-S. and Dembo, M. (1997) Analytic Solutions of Simple Flows and Analysis of Nonslip Boundary Conditions for the Lattice Boltzmann BGK Model, *J. Stat. Phys.*, **87**, pp. 115–136.
- Ho, C.-M. and Tai, Y.-C. (1998) Micro-Electro-Mechanical-Systems (MEMS) and Fluid Flows, *Ann. Rev. Fluid Mech.*, **30**, pp. 579–612.
- Hou, S., Zou, Q., Chen, S., Doolen, G. and Cogley, A.C. (1995) Simulation of Cavity Flow by the Lattice Boltzmann Method, *J. Comput. Phys.*, **118**, pp. 329–347.
- Kometer, K., Zandler, G. and Vogl, P. (1992) Lattice-Gas Cellular-Automaton Method for Semiclassical Transport in Semiconductors, *Phys. Rev. B*, **46**, pp. 1382–1394.
- Kotelnikov, A.D. and Montgomery, D. (1997) A Kinetic Method for Computing Inhomogeneous Fluid Behavior, *J. Comput. Phys.*, **134**, pp. 364–388.
- Lent, C.S., Tougaw, P.D., Porod, W. and Bernstein, G.H. (1993) Quantum Cellular Automata, *Nanotechnology*, **4**, p. 49.
- Lent, C.S. and Tougaw, P.D. (1997) A Device Architecture for Computing with Quantum Dots, *Proc. IEEE*, **85**, pp. 541–557.
- Luo, L.-S. (1997) Symmetry Breaking of Flow in 2D Symmetric Channels: Simulations by Lattice-Boltzmann Method, *Int. J. Mod. Phys.*, **8**, pp. 859–867.
- Luo, L.-S. (1998) A Unified Theory of Non-Ideal Gas Lattice Boltzmann Models, to appear in *Phys. Rev. Lett.*
- Margolus, N. (1998) Crystalline Computation, to appear in *Feynman and Computation*, A. Hey ed., Addison-Wesley, New York.
- Martys, N.S. and Chen, H. (1996) Simulation of Multicomponent Fluids in Complex Three-Dimensional Geometries by the Lattice Boltzmann Method, *Phys. Rev. E*, **53**, pp. 743–750.
- McNamara, G.R. and Zanetti, G. (1988) Use of the Boltzmann Equation to Simulate Lattice-Gas Automata, *Phys. Rev. Lett.*, **61**, pp. 2332–2335.
- Mei, R. and Shyy, W. (1997) On the Finite Difference-Based Boltzmann Method in Curvilinear Coordinates, submitted to *J. Comput. Phys.*
- Meyer, D.A. (1997) Quantum Mechanics of Lattice Gas Automata: One-Particle Plane Waves and Potentials, *Phys. Rev. E*, **55**, pp. 5261–5269.
- Nature, (1998) *Quantum Engineering: Selected Papers from Recent Issues of Nature*.

- Nie, X., Doolen, G.D. and Chen, S. (1998) Lattice-Boltzmann Simulations of Fluid Flows in MEMS, submitted to *Phys. Fluids*.
- Pavlo, P., Vahala, G. and Vahala, L. (1998) Higher Order Isotropic Velocity Grids in Lattice Methods, *Phys. Rev. Lett.*, **80**, pp. 3960–3963.
- Qian, Y.H., d’Humières, D. and Lallemand, P. (1992) Lattice BGK Models for Navier-Stokes Equation, *Europhys. Lett.*, **17**, pp. 479–484.
- Rothman, D.H. and Zaleski, S. (1997) *Lattice Gas Cellular Automata*, Cambridge University Press, Cambridge.
- Strumolo, G. and Viswanathan, B. (1997) New Directions in Computational Aerodynamics, *Physics World*, **10**, pp. 45–49.
- Succi, S. (1996) Numerical-Solution of the Schrödinger-Equation Using Discrete Kinetic Theory, *Phys. Rev. E*, **53**, pp. 1969–1975.
- Toffoli, T. and Margolus, N. (1987) *Cellular Automata Machines*, MIT Press, Cambridge.
- Tougaw, P.D. and Lent, C.S. (1996) Dynamic Behavior of Quantum Cellular Automata, *J. App. Phys.*, **80**, pp. 4722–4736.
- Wolfram, S. (1986) Cellular Automaton Fluids 1: Basic Theory, *J. Stat. Phys.*, **45**, pp. 471–526.
- Wolfram, S. (1988) Cellular Automaton Supercomputing, in *High-Speed Computing: Scientific Applications and Algorithm Design*, ed. R.B. Wilhelmson, pp. 40–48, University of Illinois Press, Urbana-Champaign.
- Wolfram, S. (1994) *Cellular Automata and Complexity: Collected Papers*, Addison-Wesley, New York.
- Xu, K. and K. H. Prendergast, K.H. (1993) Numerical Navier-Stokes Solutions from Gas Kinetic Theory, *J. Comput. Phys.*, **114**, pp. 9–17.
- Zou, Q. and He. X. (1997) On Pressure and Velocity Boundary Conditions for the Lattice Boltzmann BGK Model, *Phys. Fluids*, **9**, pp. 1591–1598.