THE LATTICE-GAS AND LATTICE BOLTZMANN METHODS: PAST, PRESENT, AND FUTURE

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ABSTRACT. An comprehensive overview of the lattice gas automata (LGA) and lattice Boltzmann equation (LBE) is presented in this article. The mathematical foundation of the LGA and LBE methods are discussed in detail. The connections between the LGA and LBE methods and other kinetic methods are pointed out. Future development of the LGA and LBE method concerning issues in the areas of hardware, modeling, and applications are also discussed.

1. Brief History. More than a decade ago, the lattice-gas automata (LGA) and the lattice Boltzmann equation (LBE) were proposed as alternatives for computational fluid dynamics (CFD). Since their inception, the lattice-gas and lattice Boltzmann methods have attracted much interest in the physics community. However, it was only very recently that the LGA and LBE methods started to gain the attention from CFD community. There exists a significant amount of literature on the lattice-gas and lattice Boltzmann methods (see proceedings [Doolen 1987, Monaco 1989, Doolen 1990, Doolen 1991, Alves 1991, Lebowitz *et al.* 1995, Lawniczak & Kapral 1996, Boghosian *et al.* 1997, Boghosian 1998, Ohashi & Chen 2000], collections of papers [Doolen 1990, Talia & Sloot 1999], reviews [Benzi *et al.* 1992, Chen & Doolen 1998], and monographs [Monaco & Preziosi 1991, Rothman & Zaleski 1997, Chopard & Droz 1998, Wolf-Gladrow 2000]). The lattice-gas and lattice Boltzmann methods have been particularly successful in simulations of fluid flow applications involving complicated boundaries or/and complex fluids, such as turbulent external flow over structures with complicated geometries [Strumolo & Viswanathan 1997], the Rayleigh-Taylor instability between two fluids [He *et al.* 1999a, He *et al.* 1999b], multi-component fluids through porous media [Martys & Chen 1996, Chen & Doolen 1998], free boundaries in flow systems [Clavin *et al.* 1988], and particle suspensions in fluid [Qi 1998, Qi 1999, Qi *et al.* 1999], chemical reactive flows [Chen *et al.* 1995, Boon *et al.* 1996] and combustions [Filippova & Hänel 2000], magnetohydrodynamics [Chen & Matthaeus 1987, Chen *et al.* 1991], crystallization [Miller *et al.* 2000], and others [Rothman & Zaleski 1997, Chen & Doolen 1998, Boghosian 1999].

Although the potential of the lattice-gas and lattice Boltzmann methods as viable CFD tools has been demonstrated in direct numerical simulations of complex fluids, laminar flows at low Reynolds number [Hou *et al.* 1995, Luo 1997, He & Doolen 1997a, He & Doolen 1997b] and turbulent flows at moderate Reynolds numbers [Amati *et al.* 1997a, Amati *et al.* 1997b], there is not sufficient evidence to show that the method can be applied to aerodynamic turbulent flows in the presence of a streamlined body at high Reynolds number [Lockard *et al.* 2000]. At present time, one weakness of the lattice-gas and lattice Boltzmann methods for CFD is the lack of turbulence modeling. Although there have been some preliminary results [Hou *et al.* 1996, Chen *et al.* 1999] in this direction, application of the LBE or LGA methods to turbulent flows at high Reynolds number remains as an area of future development [Succi 1997, Luo 1998a].

Before the methods of lattice-gas automata and lattice Boltzmann equation were invented, there were similar models: the discrete velocity models (DVM) [Broadwell 1964a, Broadwell 1964b], the beam scheme [Sanders & Prendergast 1974], and the Hardy-Pomeau-de Pazzis (HPP) single speed lattice-gas automaton model on a two-dimensional square-lattice space [Hardy *et al.* 1973a, Hardy *et al.* 1973b]. Although these

theoretical models have the mathematical germs of, and close connections to the LGA and LBE methods [Luo 2000a, Xu & Luo 1998, Junk 1999, Frisch *et al.* 1986], most of them were not intended to be used as computation or simulation tools. They were mostly used as theoretical models to study analytical properties of gases or fluids, such as analytic solutions of the Boltzmann equation for simple flows [Broadwell 1964a] or shocks [Broadwell 1964b], or statistical mechanical properties of two-dimensional fluids, such as the divergence of two-dimensional transport coefficients [Hardy *et al.* 1973a, Hardy *et al.* 1973b].

In 1986, Frisch, Hasslacher, and Pomeau [Frisch *et al.* 1986], and Wolfram [Wolfram 1986] proposed the first two-dimensional lattice-gas automaton model for the specific purpose of computational fluid dynamics. A three-dimensional 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, Higuera *et al.* 1989]. 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, and computational fluid dynamics in particular. Some of the key ideas of the LGA and LBE methods may indeed be revolutionary.

The kinetic nature of the LGA and LBE methods leads to the following features that distinguish the LGA and LBE methods from any other conventional CFD methods to solve the Navier-Stokes equations. First, the convection operator of the LGA or LBE models is linear in phase space, similar to that of the Boltzmann kinetic equation, but different than the Euler or the Navier-Stokes equations. Second, the pressure is obtained through an equation of state, as opposed to solving a Poisson equation in the incompressible Navier-Stokes equations. Third, the LGA and LBE methods have the capability to include model interactions such that they can simulate complex fluids. Fourth, the LGA and LBE methods utilize a minimal set of discrete velocities such that the conserved quantities are preserved up to machine accuracy in the calculations. In addition, the LGA and LBE methods have the following computational characteristics:

1. Intrinsic parallelism due to nearest neighbor data communications of the streaming (convection) process and purely local calculation of the collision process;
2. Ability to handle complex boundaries without compromising computational speed.

The intrinsic parallelism of the LGA and LBE methods is an essential feature in light of the clear trend to use massively parallel computers. The ability to handle complex boundaries is important to practical applications such as flow through porous media. The capability to include model interactions is crucial to simulations of some physical systems such as multi-phase or multi-component flows. Furthermore, the LGA method has the following features in addition to the above, due to its Boolean nature:

1. Exact preservation of the conservation laws;
2. Unconditional stability;
3. Memory efficiency;
4. Suitability for special-purpose computers.

The theoretical advantages of the LGA and LBE methods are still largely untested in the realm of CFD. Hence, precisely what advantages the LGA and LBE methods exhibit over conventional methods of solving the Navier-Stokes equations are problem-dependent. The areas where the LGA and LBE methods are more suitable depend on the physical nature of the problems. Unfortunately, due to the lack of research effort in this area, a sufficient amount of numerical evidence to verify the theoretical advantages of the LGA and LBE methods does not exist, especially in the areas where the conventional CFD methods have proven to be useful, such as in the field of aerodynamics.

Before we move on to the technical discussion of the LGA and LBE methods, it would be appropri-

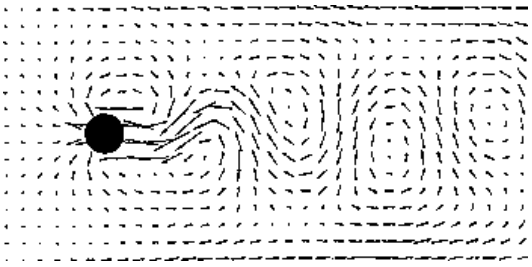

FIG. 1. *LGA simulation of flow past a 2D cylinder. Shown in the Figure are velocity vectors. The Reynolds number of the system is approximately* 100. *(From [Wolfram 1988]. Copyright 1988 by the Board of Trustees of the University of Illinois. Used with the permission of University of Illinois Press.)*

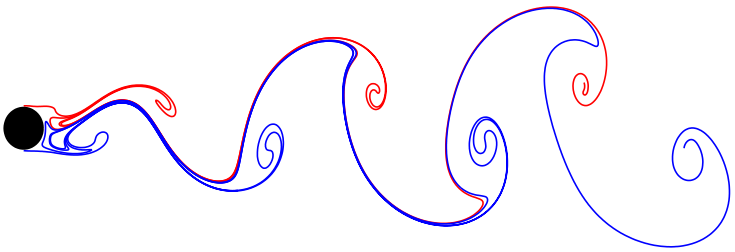

FIG. 2. *LBE simulation of flow past a 2D cylinder. Shown in the Figure are streak lines. Re* = 100. (Courtesy of He.)

ate 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 two-dimensional flow past a cylinder, a classic problem 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, it was demonstrated that the LBE method can faithfully and quantitatively simulate hydrodynamics — Figs. 2 shows the von Kármán vortex street behind a cylinder with a Reynolds number of 100. Various quantities, such as the drag coefficient C_D and the lift coefficient C_L, 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 conventional methods of solving Navier-Stokes equations. The two-dimensional 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 hydrodynamic systems 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.* 1997a, 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 LGA and LBE hydrodynamic equations are derived in detail. An *a priori* derivation of the lattice Boltzmann equation directly from the continuous Boltzmann equation is presented. The boundary conditions of the LBE method, the generalized lattice Boltzmann equation, the lattice Boltzmann model for complex fluids, and gas-kinetic

scheme are also briefly discussed. Sec. 3 addresses the issues concerning the future development of the methods, including hardware, modeling, and applications. Sec. 4 concludes this the article.

2. Theory of the Lattice Gas Automata and the Lattice Boltzmann Equation.

2.1. Philosophy of LGA and LBE Methods. It is a well known fact that a fluid is 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 should be stressed that the continuum treatment of fluid is an approximation. This approximation works extremely well under many circumstances.

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 such as inhomogeneous multiphase or multicomponent flows, or granular flows. In the case of multiphase or multicomponent flows, interfaces between different fluid components (*e.g.* oil and water) or phases (*e.g.* vapor and water) cause the numerical difficulties. 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, neither 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 solution of 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

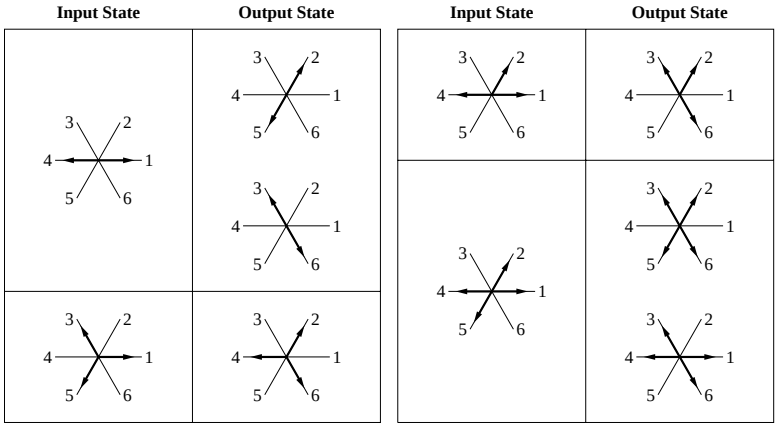

FIG. 3. *Collisions of FHP LGA model.*

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 the 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 the Hardy-Pomeau-Pazzis (HPP) model [Hardy *et al.* 1973a, Hardy *et al.* 1973b] that a two-dimensional square lattice does not possesses sufficient symmetry for hydrodynamics, Frisch, Hasslacher, and Pomeau [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 two-dimensional Frisch-Hasslacher-Pomeau (FHP) model was immediately generalized to a three-dimensional LGA model [Frisch *et al.* 1987].

The LGA model proposed by Frisch, Hasslacher, and Pomeau, and Wolfram evolves on a two-dimensional triangular lattice space. The particles have momenta that 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-velocity 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° clockwise or counter-clockwise with equal probability. In Fig. 3, we do not list those configurations which can 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:

$$n_\alpha(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta_t,\, t + \delta_t) = n_\alpha(\boldsymbol{x},\, t) + C_\alpha\,, \tag{2.1}$$

where n_α is the Boolean particle number with the velocity $\boldsymbol{e}_\alpha$, C_α is the collision operator, $\boldsymbol{x}$ is a vector in the lattice space with lattice constant δ_x, t denotes discrete time with step size δ_t. We usually set both δ_x and δ_t to unity. The subscript α is an index for velocity; as illustrated in Fig. 3, for the FHP model, α runs

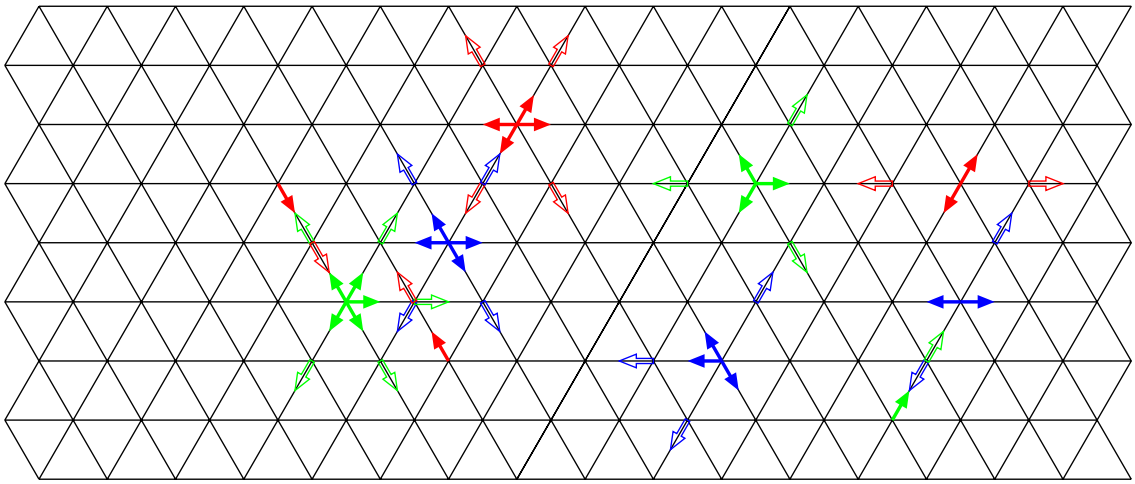

FIG. 4. *Evolution of FHP LGA model. Solid and hollow arrows represent particles with corresponding velocity at time t and $t+1$, respectively. That is, the hollow arrows are the final configurations of the initial configurations of solid arrows after one cycle of collision and advection.*

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_α, can be written as follows:

$$C_\alpha(\{n_\alpha(\boldsymbol{x},\,t)\}) = \sum_{\boldsymbol{s},\,\boldsymbol{s}'} (s'_\alpha - s_\alpha)\,\xi_{ss'} \prod_\sigma n_\sigma^{s_\sigma}\,(1-n_\sigma)^{(1-s_\sigma)}\,, \tag{2.2}$$

where $\boldsymbol{s} \equiv \{s_1,\, s_2,\, \ldots,\, s_6\}$ and $\boldsymbol{s}' \equiv \{s'_1,\, s'_2,\, \ldots,\, s'_6\}$ are possible incoming and outgoing configurations at a given site $\boldsymbol{x}$ and time t, respectively; $\xi_{ss'}$ is a Boolean random number in space and time which determines the transition between state $\boldsymbol{s}$ and $\boldsymbol{s}'$ satisfying the following normalization condition:

$$\sum_{\boldsymbol{s}'} \xi_{ss'} = 1\,, \qquad \forall\, \boldsymbol{s}\,. \tag{2.3}$$

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

$$n_\sigma^{s_\sigma}\,(1-n_\sigma)^{(1-s_\sigma)} = \delta_{n_\sigma s_\sigma}\,, \tag{2.4}$$

where $\delta_{n_\sigma s_\sigma}$ is the Kronecker delta symbol with two indices. Therefore, Eq. (2.2) can be written as

$$C_\alpha(\{n_\alpha(\boldsymbol{x},\,t)\}) = \sum_{\boldsymbol{s},\,\boldsymbol{s}'} (s'_\alpha - s_\alpha)\,\xi_{ss'}\,\delta_{\boldsymbol{n}\boldsymbol{s}}\,, \tag{2.5}$$

where $\delta_{\boldsymbol{n}\boldsymbol{s}} \equiv \delta_{n_1 s_1}\delta_{n_2 s_2}\cdots\delta_{n_b s_b}$. Eq. (2.2), or (2.5), is rather abstract, and the following is a specific example of the collision operator for the two-body collision:

$$\begin{aligned} C_\alpha^{(2)} = {} & \xi_R^{(2)}\, n_{\alpha+1} n_{\alpha+4} \bar{n}_\alpha \bar{n}_{\alpha+2} \bar{n}_{\alpha+3} \bar{n}_{\alpha+5} + \xi_L^{(2)}\, n_{\alpha+2} n_{\alpha+5} \bar{n}_\alpha \bar{n}_{\alpha+1} \bar{n}_{\alpha+3} \bar{n}_{\alpha+4} - \\ & (\xi_R^{(2)} + \xi_L^{(2)})\, n_\alpha n_{\alpha+3} \bar{n}_{\alpha+1} \bar{n}_{\alpha+2} \bar{n}_{\alpha+4} \bar{n}_{\alpha+5}\,, \end{aligned} \tag{2.6}$$

Input State	Output State
	010010
001001	
	100100
010101	101010
001011	100110
	110110
011011	
	101101

Table 2.1

Collision table for 6-Bit FHP model.

where $\bar{n}_\alpha \equiv 1 - n_\alpha$ is the complement of n_α, $\xi_R^{(2)}$ 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 the two-body collision. Obviously, for the collision operator to satisfy the complete lattice symmetry group statistically (on average), they must satisfy

$$\langle \xi_R^{(2)} \rangle = \langle \xi_L^{(2)} \rangle \,, \tag{2.7}$$

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:

$$\sum_\alpha (s'_\alpha - s_\alpha) = 0 \,, \tag{2.8a}$$

$$\sum_\alpha (s'_\alpha - s_\alpha) \boldsymbol{e}_\alpha = 0 \,, \tag{2.8b}$$

$$\sum_\alpha (s'_\alpha - s_\alpha) \frac{1}{2} (\boldsymbol{e}_\alpha - \boldsymbol{u})^2 = 0 \,. \tag{2.8c}$$

In practice, the collision can implemented with various algorithms. One can either use logical operation [as indicated by Eq. (2.6)], or by table-lookup. The collision rules shown in Fig. 3 can also be represented by the a collision table, as shown by Table 2.1. In Table 2.1, each bit in a binary number represents a particle number n_α, $\alpha = 1, 2, \ldots, 6$, 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 velocities (bits) of the model. Table lookup of the LGA models can be directly on a custom made processor [Lee *et al.* 1990, Lee 1993], and both logic operation and table lookup can be extremely fast on digital computers, especially so on dedicated computers [Toffoli & Margolus 1987, Adler 1995].

2.3. Hydrodynamics of Lattice Gas Automata. The ensemble average of Eq. (2.1) leads to a lattice Boltzmann equation:

$$f_\alpha(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta_t, \, t + \delta_t) = f_\alpha(\boldsymbol{x}, \, t) + \Omega_\alpha \,, \tag{2.9}$$

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

$$\langle n_\alpha n_\beta \cdots n_\gamma \rangle = \langle n_\alpha \rangle \langle n_\beta \rangle \cdots \langle n_\gamma \rangle \,. \tag{2.10}$$

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

$$\Omega_\alpha(\{f_\alpha(\boldsymbol{x},\,t)\}) = \sum_{\boldsymbol{s},\,\boldsymbol{s}'} (s'_\alpha - s_\alpha)\, A_{ss'} \prod_\sigma f_\sigma^{s_\sigma} (1-f_\sigma)^{(1-s_\sigma)}\,, \tag{2.11}$$

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

$$\rho = \sum_\alpha f_\alpha\,, \qquad \rho\boldsymbol{u} = \sum_\alpha \boldsymbol{e}_\alpha f_\alpha\,, \qquad \rho\varepsilon = \sum_\alpha \frac{1}{2}(\boldsymbol{e}_\alpha - \boldsymbol{u})^2 f_\alpha\,, \tag{2.12}$$

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

Eq. (2.9) can be expanded in a Taylor series of δ_t up to the second order:

$$(\partial_t + \boldsymbol{e}_\alpha\cdot\nabla) f_\alpha + (\partial_t + \boldsymbol{e}_\alpha\cdot\nabla)^2 f_\alpha = \Omega_\alpha\,. \tag{2.13}$$

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,

$$f_\alpha^{(0)} = \frac{1}{1+\exp(a + b\,\boldsymbol{u}\cdot\boldsymbol{e}_\alpha)}\,, \tag{2.14}$$

where coefficients a and b are functions of ρ and $\boldsymbol{u}^2$ 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 $\boldsymbol{u}$ — 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]:

$$\partial_t \rho + \nabla\cdot\rho\boldsymbol{u} = 0\,, \tag{2.15a}$$

$$\partial_t \rho\boldsymbol{u} + \nabla(g\,\rho\boldsymbol{u}\boldsymbol{u}) = -\nabla P + \nu\nabla^2\rho\boldsymbol{u}\,, \tag{2.15b}$$

where g is a function of ρ,

$$P = c_s^2\,\rho\left[1 - g\frac{\boldsymbol{u}^2}{c^2}\right], \qquad c_s = c/\sqrt{2}\,, \tag{2.16a}$$

$$\nu = -\frac{1}{8}(2\lambda^{-1}+1)c\,\delta_x\,, \tag{2.16b}$$

c_s is the sound speed, $c = \delta_x/\delta_t$, and λ is an eigenvalue of the linearized collision operator corresponding to a shear mode [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_α;
2. The factor $g(\rho)$ is not unity, thus Galilean invariance is destroyed;
3. It is difficult to increase the Reynolds number Re;
4. The equation of state depends on $\boldsymbol{u}^2$ (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 either 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 automata. Eq. (2.9) is the first 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 [Bhatnagar *et al.* 1954] is used in the following analysis. The Boltzmann BGK equation [Bhatnagar *et al.* 1954] can be written in the form of an ordinary differential equation:

$$D_t f + \frac{1}{\lambda} f = \frac{1}{\lambda} f^{(0)} \,, \tag{2.17}$$

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

$$f^{(0)} \equiv \frac{\rho}{(2\pi RT)^{D/2}} \exp\left[-\frac{(\boldsymbol{\xi} - \boldsymbol{u})^2}{2\theta}\right] \,, \tag{2.18}$$

in which D is the dimension of the space; ρ, $\boldsymbol{u}$ 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 $\boldsymbol{\xi}$:

$$\rho = \int f \, d\boldsymbol{\xi} \,, \qquad \rho \boldsymbol{u} = \int \boldsymbol{\xi} \, f \, d\boldsymbol{\xi} \,, \qquad \rho\theta = \frac{1}{2} \int (\boldsymbol{\xi} - \boldsymbol{u})^2 \, f \, d\boldsymbol{\xi} \,. \tag{2.19}$$

Equation (2.17) can be formally integrated over a time interval δ_t:

$$f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \boldsymbol{\xi}, t + \delta_t) = e^{-\delta_t/\lambda} f(\boldsymbol{x}, \boldsymbol{\xi}, t) + \frac{1}{\lambda} e^{-\delta_t/\lambda} \int_0^{\delta_t} e^{t'/\lambda} f^{(0)}(\boldsymbol{x} + \boldsymbol{\xi} t', \boldsymbol{\xi}, t + t') \, dt' \,. \tag{2.20}$$

Assuming that δ_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. (2.20), we obtain

$$f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \boldsymbol{\xi}, t + \delta_t) - f(\boldsymbol{x}, \boldsymbol{\xi}, t) = -\frac{1}{\tau}[f(\boldsymbol{x}, \boldsymbol{\xi}, t) - f^{(0)}(\boldsymbol{x}, \boldsymbol{\xi}, t)] \,, \tag{2.21}$$

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 $\boldsymbol{u}$. By retaining the Taylor expansion up to $\boldsymbol{u}^2$, we obtain:

$$f^{(\mathrm{eq})} = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{\boldsymbol{\xi}^2}{2\theta}\right) \left[1 + \frac{(\boldsymbol{\xi} \cdot \boldsymbol{u})}{\theta} + \frac{(\boldsymbol{\xi} \cdot \boldsymbol{u})^2}{2\theta^2} - \frac{\boldsymbol{u}^2}{2\theta}\right] \,. \tag{2.22}$$

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:

$$\int \boldsymbol{\xi}^m \, f^{(\mathrm{eq})} \, d\boldsymbol{\xi} \,, \tag{2.23}$$

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

$$I = \int \exp(-\boldsymbol{\xi}^2/2\theta) \psi(\boldsymbol{\xi}) \, d\boldsymbol{\xi} = \sum_\alpha W_\alpha \, \exp(-\boldsymbol{\xi}_\alpha^2/2\theta) \, \psi(\boldsymbol{\xi}_\alpha) \,, \tag{2.24}$$

where $\psi(\boldsymbol{\xi})$ is a polynomial in $\boldsymbol{\xi}$, and W_α and $\boldsymbol{\xi}_\alpha$ are the weights and the abscissas (or discrete velocities). Accordingly, the hydrodynamic moments of Eqs. (2.19) can be computed by quadrature as well:

$$\rho = \sum_\alpha f_\alpha\,, \qquad \rho \boldsymbol{u} = \sum_\alpha \boldsymbol{\xi}_\alpha\, f_\alpha\,, \qquad \rho\theta = \frac{1}{2}\sum_\alpha (\boldsymbol{\xi}_\alpha - \boldsymbol{u})^2\, f_\alpha\,, \tag{2.25}$$

where $f_\alpha \equiv f_\alpha(\boldsymbol{x},\, t) \equiv W_\alpha\, f(\boldsymbol{x},\, \boldsymbol{\xi}_\alpha,\, t)$. We shall use the nine-velocity isothermal LBE model on a square lattice space as a concrete example to illustrate the derivation of LBE models: the evolution equation (2.21) on a discretized phase space and time with a proper equilibrium distribution function leads to the Navier-Stokes equations.

To derive the nine-velocity LBE model, a Cartesian coordinate system is used, and accordingly, we set $\psi(\boldsymbol{\xi}) = \xi_x^m\, \xi_y^n$. The integral of Eq. (2.24) becomes:

$$I = (\sqrt{2\theta})^{(m+n+2)}\, I_m\, I_n\,, \tag{2.26}$$

where

$$I_m = \int_{-\infty}^{+\infty} e^{-\zeta^2}\, \zeta^m\, d\zeta\,, \tag{2.27}$$

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 nine-velocity LBE model, *i.e.*, $I_m = \sum_{j=1}^{3} \omega_j \zeta_j^m$. The three abscissas (ζ_j) and the corresponding weights (ω_j) of the quadrature are:

$$\begin{aligned} &\zeta_1 = -\sqrt{3/2}\,, \qquad \zeta_2 = 0\,, \qquad\quad \zeta_3 = \sqrt{3/2}\,, \\ &\omega_1 = \sqrt{\pi}/6\,, \qquad \omega_2 = 2\sqrt{\pi}/3\,, \qquad \omega_3 = \sqrt{\pi}/6\,. \end{aligned} \tag{2.28}$$

Then, the integral of Eq. (2.26) becomes:

$$I = 2\theta\,[\omega_2^2 \psi(\boldsymbol{0}) + \sum_{\alpha=1}^{4} \omega_1\omega_2 \psi(\boldsymbol{\xi}_\alpha) + \sum_{\alpha=5}^{8} \omega_1^2 \psi(\boldsymbol{\xi}_\alpha)]\,, \tag{2.29}$$

where $\boldsymbol{\xi}_\alpha$ 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 $(m + n) \leq 5$.

Now momentum space is discretized with nine discrete velocities $\{\boldsymbol{\xi}_\alpha | \alpha = 0,\, 1,\, \cdots,\, 8\}$. To obtain the nine-velocity 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 θ has no physical significance here because we are only dealing with an isothermal model. We can therefore choose δ_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. (2.24) and (2.29), we can identify the weights defined in Eq. (2.24):

$$W_\alpha = 2\pi\,\theta\, \exp(\boldsymbol{\xi}_\alpha^2/2\theta)\, w_\alpha\,, \tag{2.30}$$

where

$$w_\alpha = \begin{cases} 4/9, & \alpha = 0, \\ 1/9, & \alpha = 1,\, 2,\, 3,\, 4, \\ 1/36, & \alpha = 5,\, 6,\, 7,\, 8. \end{cases} \tag{2.31}$$

Then, the equilibrium distribution function of the nine-velocity model is:

$$f_\alpha^{(\mathrm{eq})} = W_\alpha\, f^{(\mathrm{eq})}(\boldsymbol{x},\, \boldsymbol{\xi}_\alpha,\, t) = w_\alpha\, \rho\, \left\{1 + \frac{3(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})}{c^2} + \frac{9(\boldsymbol{e}_\alpha \cdot \boldsymbol{u})^2}{2c^4} - \frac{3\boldsymbol{u}^2}{2c^2}\right\}\,, \tag{2.32}$$

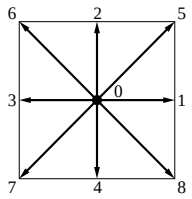

FIG. 5. *Discrete velocities of the nine-velocity model on a square lattice.*

where

$$\boldsymbol{e}_\alpha = \begin{cases} (0,\,0), & \alpha = 0\,, \\ (\cos\theta_\alpha,\,\sin\theta_\alpha)\,c, & \alpha = 1,\,2,\,3,\,4, \\ (\cos\theta_\alpha,\,\sin\theta_\alpha)\,\sqrt{2}c, & \alpha = 5,\,6,\,7,\,8, \end{cases} \tag{2.33}$$

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:

$$\rho\partial_t\boldsymbol{u} + \rho\boldsymbol{u}\cdot\nabla\boldsymbol{u} = -\nabla P + \rho\nu\nabla^2\boldsymbol{u}\,, \tag{2.34}$$

with the ideal gas equation of state

$$P = c_s^2\rho\,, \tag{2.35}$$

where the sound speed $c_s = c/\sqrt{3}$, and the viscosity

$$\nu = \frac{1}{3}(\tau - 1/2)c\,\delta_x = (\tau-1/2)c_s^2\,\delta_t\,. \tag{2.36}$$

It should be noted that the factor $-1/2$ in the above formula for ν accounts for the numerical viscosity due to the second order derivatives of f_α [see Eq. (2.13)]. This correction in ν formally makes the LGA and LBE methods second order accurate.

Similarly, we can derive two-dimensional six-velocity, seven-velocity, and three-dimensional twenty-seven-velocity 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_α at one mesh grid point, say $\boldsymbol{X}$, 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 $f_\alpha(\boldsymbol{X},\,t)$ on each and every mesh grid point

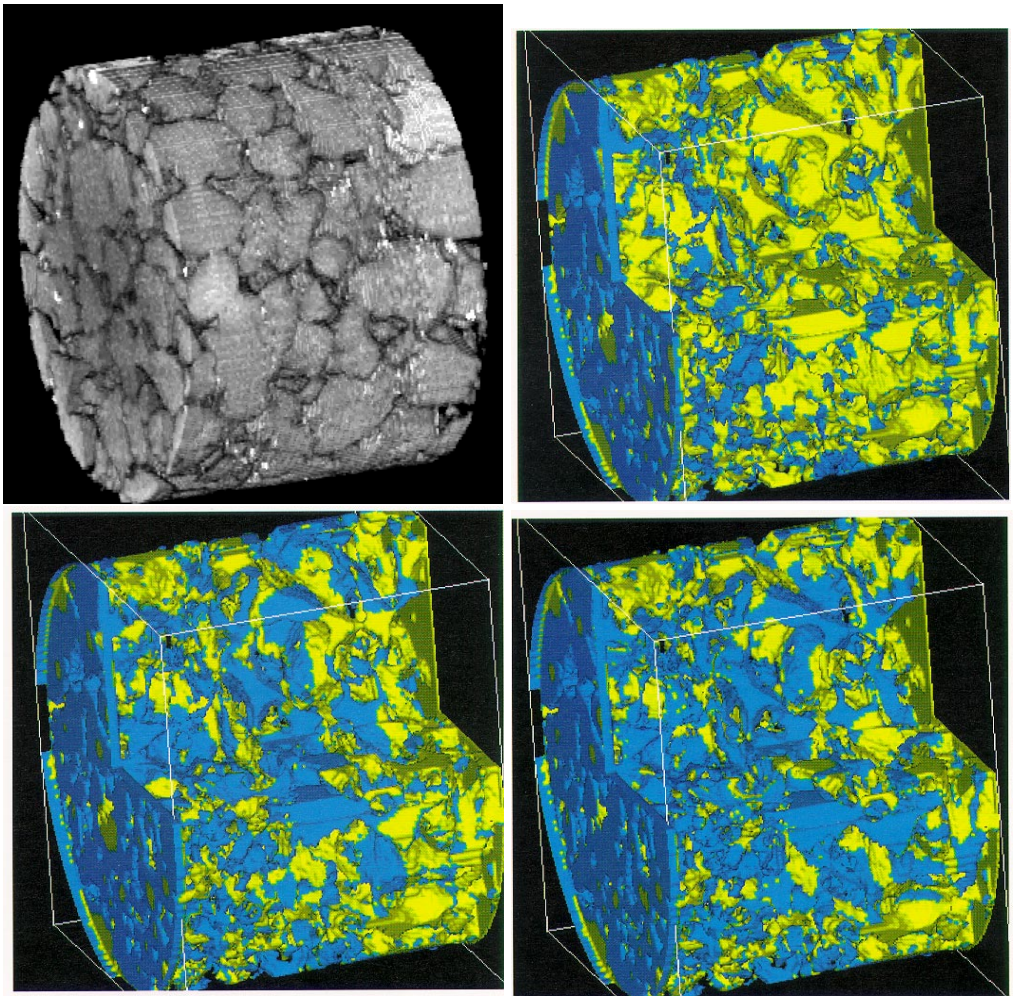

FIG. 6. *LBE simulation of binary fluid mixture through porous media. Top left panel shows the image of a digitized tomography sandstone sample (20μm resolution) used in the simulation. Other panels display the two-component fluid flow through the sandstone at different times* (top right, bottom left, bottom right). *The blue color indicates invading water and the yellow color indicates oil. The sandstone is transparent.* (Courtesy of Chen).

from $f_\alpha(\boldsymbol{X} + \boldsymbol{e}_\alpha\delta_t, t)$ 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 τ [He *et al.* 1996]. In other words, the limitation posed by the lattice Reynolds number is completely overcome [He *et al.* 1997b] and the stability of the LBE method is greatly improved [He *et al.* 1996, He *et al.* 1997b].

2.5. Boundary Conditions. In lattice-gas automata, no-slip boundary conditions can be realized by the bounce-back scheme: a particle colliding with the wall simply reverses its momentum. Also, slip boundary conditions 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 and reflection schemes can be implemented in the lattice Boltzmann equation with some variations [Chen *et al.* 1996, Zou & He 1997, Filippova & Hänel 1998, Mei *et al.* 1999, Mei *et al.* 2000, Bouzidi *et al.* 2000]. It is well understood now that the bounce-back scheme can achieve second order accuracy if one is careful about the location of the boundary [Ginzbourg & d'Humières 1996, He *et al.* 1997c]. The ease of handling boundary conditions with complicated geometries is a very important feature of the lattice-gas and lattice Boltzmann methods. As an example, Figure 6 shows a lattice Boltzmann simulation of a binary fluid through a porous medium [Buckles *et al.* 1994]. As seen in the Figure, the lattice Boltzmann simulation preserves the fundamental phenomena observed in experiments that the water phase (dark fluid) forms long fingers through the porous medium because of the wettability properties of the water. The sandstone sample is obtained from a Mobil offshore oil reservoir. The numerical results obtained the LBE simulation agree well with the experimental measurements.

Another example is particulate suspensions in fluid flows [Qi 1998, Qi 1999, Qi *et al.* 1999, Qi 2000]. Figure 7 shows a three-dimensional lattice Boltzmann simulation of sedimentation of sixteen cylindrical particles in a fluid [Qi 2000]. Note that formation of "invert T" configurations in the evolution process. This phenomenon has also been observed experimentally [Joseph 1993]. One reason that the LBE method can be effectively used to simulate particulate suspensions in fluid flows is because it easily handles fluid-solid boundary conditions. The capability of the LBE method to handle fluid-solid interactions and complicated boundaries makes the LBE method an excellent simulation tool for particulate suspensions in fluid flows.

2.6. Generalized Lattice Boltzmann Model. The BGK model has some inherent shortcomings such as fixed Prandtl number because all the modes have the same relaxation time λ in Eq. (2.17). In addition, the LBGK are numerically unstable when τ is close to $1/2$. This instability of the LBGK model also depends on initial conditions, boundary conditions, the Reynolds number.

The generalized lattice Boltzmann equation [d'Humières 1992] can remove the problem of the fixed Prandtl number due to the single relaxation time approximation and drastically improve the numerical stability of the LBE method [Lallemand & Luo 2000]. The basic idea of the generalized lattice Boltzmann equation is the following. Given a set of discrete velocities $\{\boldsymbol{e}_\alpha | \alpha = 1,\ 2, \ldots,\ b\}$, the corresponding distribution functions $\{f_\alpha\}$ can be mapped into a set of b moments $\{\varrho_\alpha\}$ by an invertible matrix M, and *vice versa*, *i.e.*,

$$|\varrho\rangle = \mathsf{M}|f\rangle\,, \tag{2.37a}$$

$$|f\rangle = \mathsf{M}^{-1}|\varrho\rangle\,. \tag{2.37b}$$

where

$$|\varrho\rangle = (\varrho_1,\ \varrho_2, \ldots,\ \varrho_b)^{\mathsf{T}}\,, \tag{2.38a}$$

$$|f\rangle = (f_1,\ f_2, \ldots,\ f_b)^{\mathsf{T}}\,, \tag{2.38b}$$

are two b-dimensional vectors in $\mathbb{R}^b$. The first $(D+2)$ moments are conserved quantities or hydrodynamic modes (*i.e.*, density ρ, momentum $\rho\boldsymbol{u}$, and energy ϵ), and the rest of $[b-(D+2)]$ moments are (non-conserved) fluxes or kinetic modes, (such as stresses p_{ij}, *etc.*) In the BGK model, all the kinetic modes are relaxed with one parameter, hence the Prandtl number is fixed to be unity. In the generalized lattice Boltzmann equation, all the kinetic modes are relaxed independently with different relaxation parameters, constrained only by the symmetry considerations. Thus, the generalized lattice Boltzmann equation can be written as

$$|f(\boldsymbol{x}_j + \boldsymbol{e}_\alpha\delta_t,\ t+\delta_t)\rangle - |f(\boldsymbol{x}_j,\ t)\rangle = -\mathsf{M}^{-1}\mathsf{S}\mathsf{M}\left[|f(\boldsymbol{x}_j,\ t)\rangle - |f^{(\mathrm{eq})}(\boldsymbol{x}_j,\ t)\rangle\right], \tag{2.39}$$

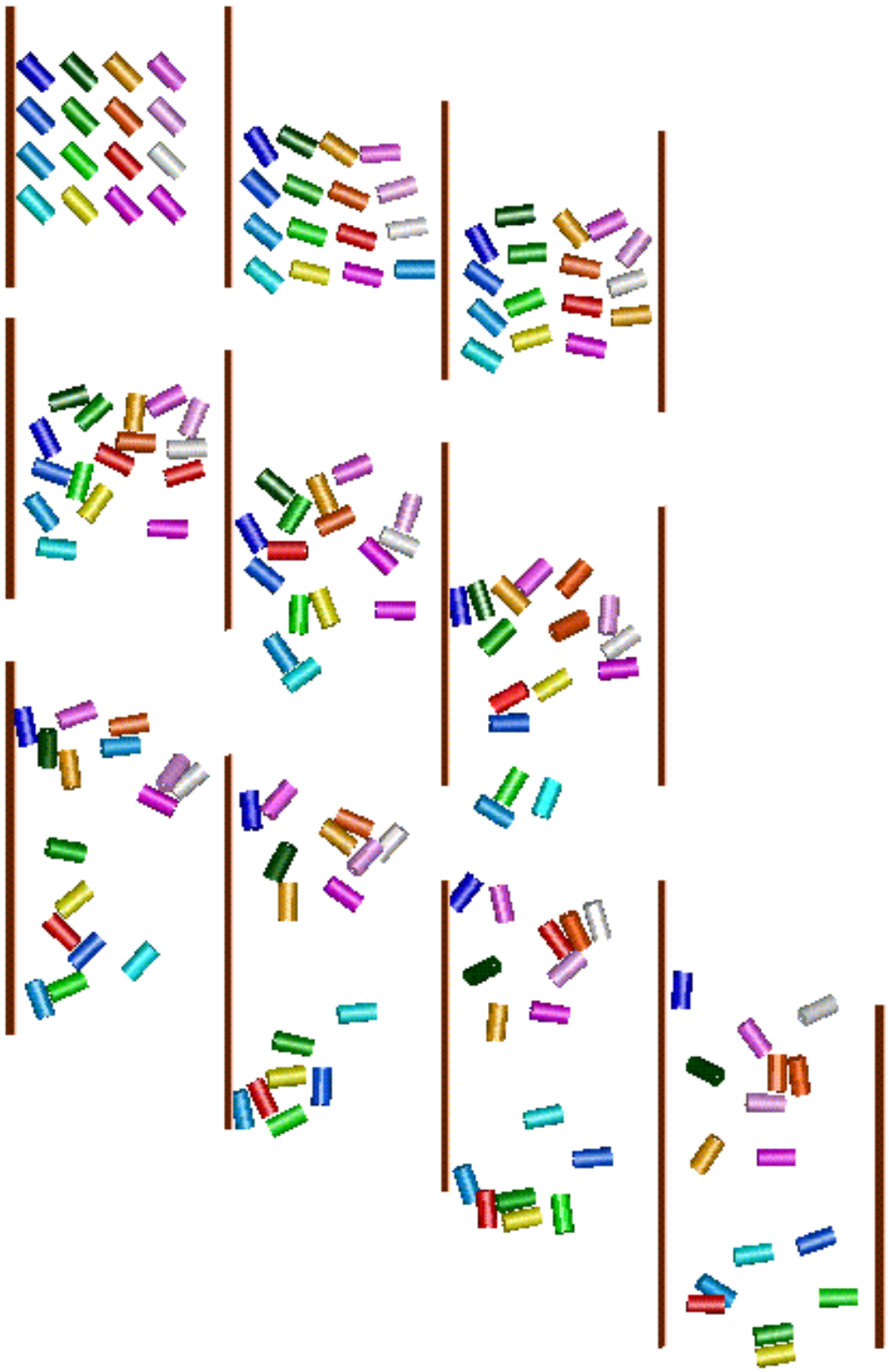

FIG. 7. *LBE simulation of particles sedimentation in fluid. Particle dimensions are* $D = 12$ *and* $L = 24$. *System size is* $N_x \times N_y \times N_z = 140 \times 150 \times 35$. *The averaged single-particle Reynolds number is* $\mathrm{Re} \approx 16.9$. *Time evolution of the system, from left to right and top to bottom. Note that formation of "invert* `T`*" configurations in the evolution process.* (Courtesy of Qi).

where S is a diagonal matrix with $(D+2)$ zero diagonal elements for the conserved hydrodynamic modes, and $[b-(D+2)]$ nonzero diagonal elements which are the relaxation frequencies for the kinetic modes [Lallemand & Luo 2000]. The computational cost of two linear transformations M and M^{-1} is rather insignificant — it is about 10% of the total computation. However, the stability of the generalized lattice Boltzmann equation is significantly superior to the normal lattice Boltzmann equation [Lallemand & Luo 2000].

Figure 8 shows an LBE simulation of a sphere moving downwards inside a cylinder by using a thirteen-velocity generalized LBE model proposed by Lallemand and d'Humières. The drag coefficient obtained from the LBE simulation agrees very well with theoretical prediction and numerical results obtained by other methods.

2.7. Lattice Boltzmann Models for Complex Fluids. One distinguishing feature of the lattice-gas and lattice Boltzmann methods is the easy treatment of complex fluids such as multiphase fluids [Luo 1998b, Luo 2000b] interface dynamics [He *et al.* 1999a, He *et al.* 1999b], droplet collisions [Schelkle & Frohn 1995, Schelkle *et al.* 1999], multicomponent fluids (miscible or immiscible fluid mixtures) [Martys & Chen 1996, Boghosian 1999], viscoelastic fluids in two and three dimensions [Giraud *et al.* 1997, Giraud *et al.* 1998, Lallemand *et al.* 2000]. The LBE model for nonideal gases can be derived for the Enskog equation which explicitly considers the volume exclusion effect in dense gases [Luo 1998b, Luo 2000b]. The LBE model can be used to simulate interfacial dynamics in multiphase fluids, such as Rayleigh-Taylor instability [He *et al.* 1999a, He *et al.* 1999b].

Figure 9 and 10 show the lattice Boltzmann simulations of Rayleigh-Taylor instability in two- and three-dimensions, respectively [He *et al.* 1999a, He *et al.* 1999b]. Such simulations could be rather difficult for front tracking type of techniques in the late stage of the mixing. The lattice Boltzmann method is a capturing technique. The interface thickness is about $2-3$ lattice grids and the interfaces are well sustained by interparticle interactions. The numerical diffusion in the lattice Boltzmann method does not seem to suffer the problem due to numerical diffusivity.

Another area of complex fluids in which the lattice-gas and lattice Boltzmann methods and other mesoscopic methods (*e.g.*, dissipative particle dynamics [Hoogerbrugge & Koelman 1992]) have attracted much attention is simulation of soft materials including emulsions, colloids, liquid crystals, gels and forms, and other complex fluids [Boghosian *et al.* 1996, Starr *et al.* 1996, Emerton *et al.* 1997a, Emerton *et al.* 1997b, Emerton *et al.* 1997c, Boghosian 1999, Denniston *et al.* 2000a, Denniston *et al.* 2000b, Care *et al.* 1999]. Hydrodynamic equations for these complex fluids are either unknown or ill-posed, so that the conventional CFD methods cannot be applied in a straightforward fashion. The LGA and LBE methods become effective alternatives in comparison to molecular dynamics, which is computationally too expensive.

The key idea in the LGA and LBE models for complex fluids is that the model interactions can be easily included in the methods. Figures 11, 12, and 13 show the lattice-gas simulations of various complex fluids. Figure 11(top) shows a lattice-gas simulation of a binary mixture of water and amphiphile in three dimensions. The self-organizing wormlike micelle phase is observed in the mixture. Figure 11(bottom) shows growth of lamellar phase in three-component mixture (oil, water, and surfactant) in three-dimensions.

Figures 12 and 13 illustrate the two-dimensional lattice-gas simulations of self-assembled structures in mixtures under different conditions [Boghosian 1999]. In Figure 12, the three-component mixture of water, oil and amphiphile with random initial conditions forms sponge-like structures. When the same system is subjected to an applied shear, a sponge-to-lamellar phase transition takes place, as shown in Figure 13. Note that all of these applications involve nonequilibrium or dynamical processes that have previously been difficult to address. The most lengthy molecular dynamic simulations to date are barely able to see the

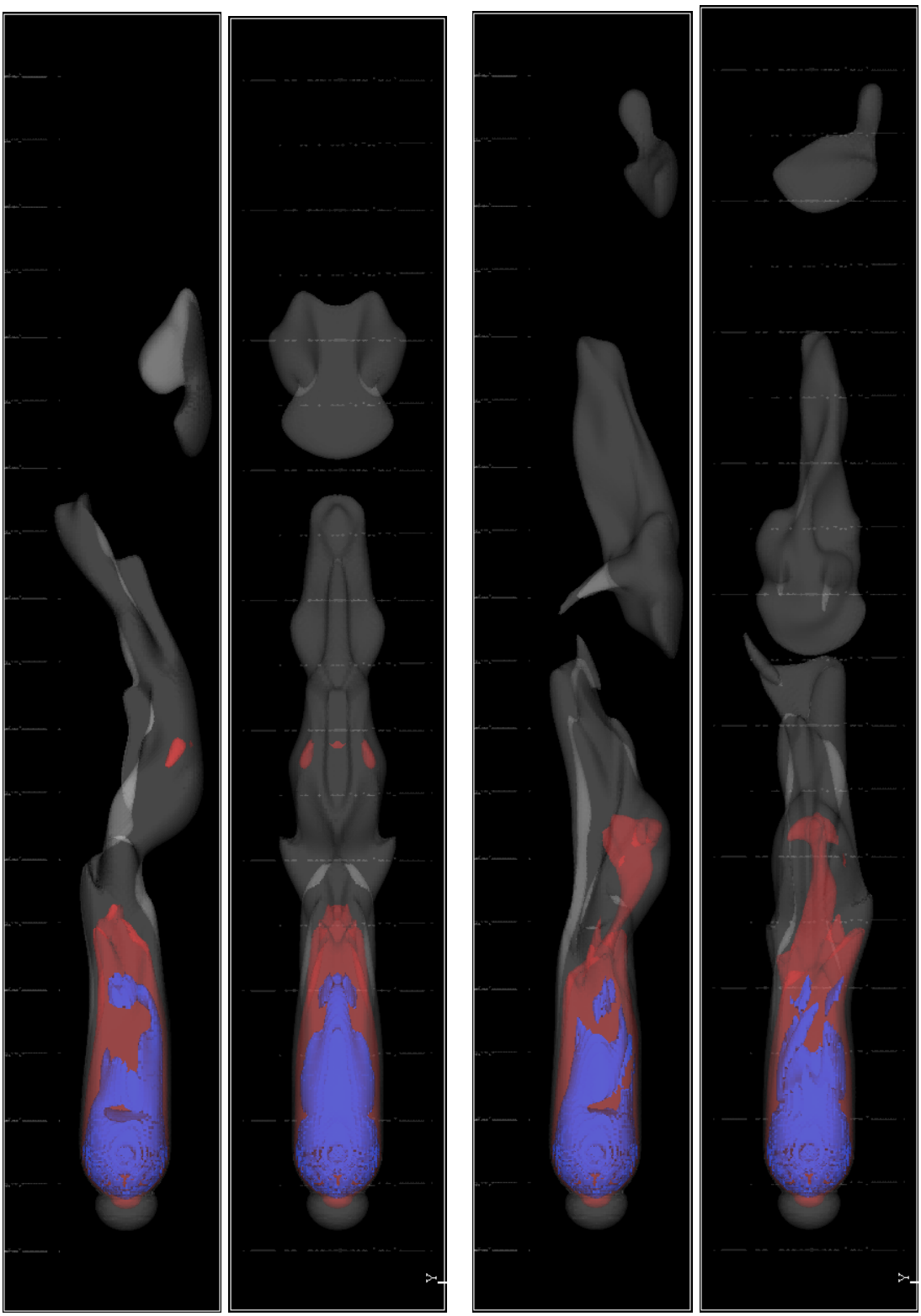

FIG. 8. *LBE simulation of a sphere moving downwards inside a cylinder. The system size is* $N_x \times N_y \times N_z = 500 \times 85 \times 85$. *The center of the sphere is fixed at* $(62, 43, 48)$. *The diameter of the sphere is* 16.10. *The Reynolds number* $\mathrm{Re} = 504$ *based on the diameter of the sphere.* $U_{\max} = 0.08$. *Isosurfaces of* $\|\boldsymbol{u}\|$. *From left to right,* $t = 40,000$, *x-z plane and x-y plane view;* $t = 100,000$, *x-z plane and x-y plane view.* (Courtesy of Lallemand and d'Humières).

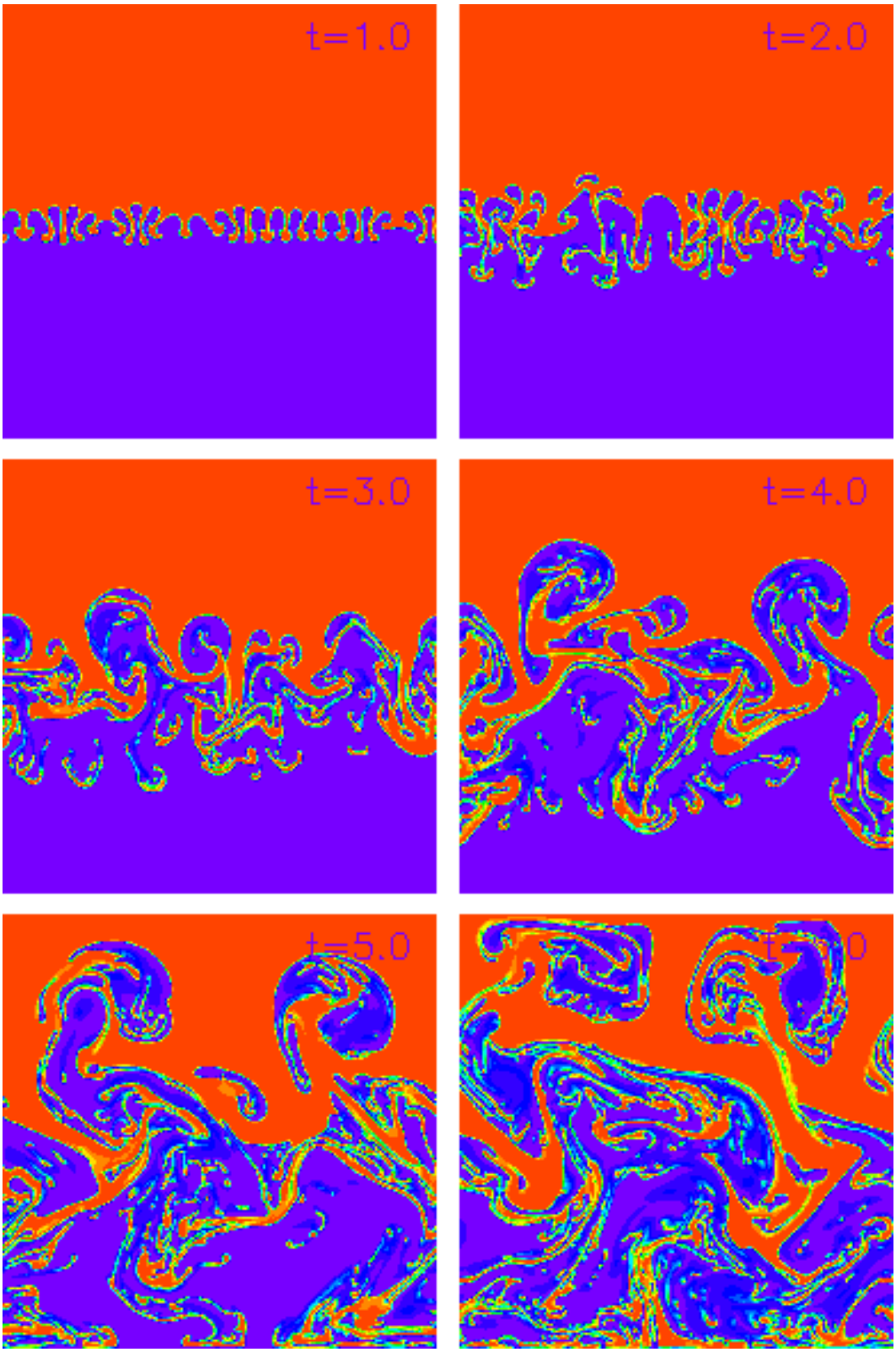

FIG. 9. *Lattice Boltzmann simulation of Rayleigh-Taylor instability in two-dimensions. Rayleigh-Taylor instability from a multiple mode initial perturbation. The Atwood number is* 0.5 *and the Reynolds number is* 4096. *The time is normalized by* $\sqrt{W/g}$. (Courtesy of He).

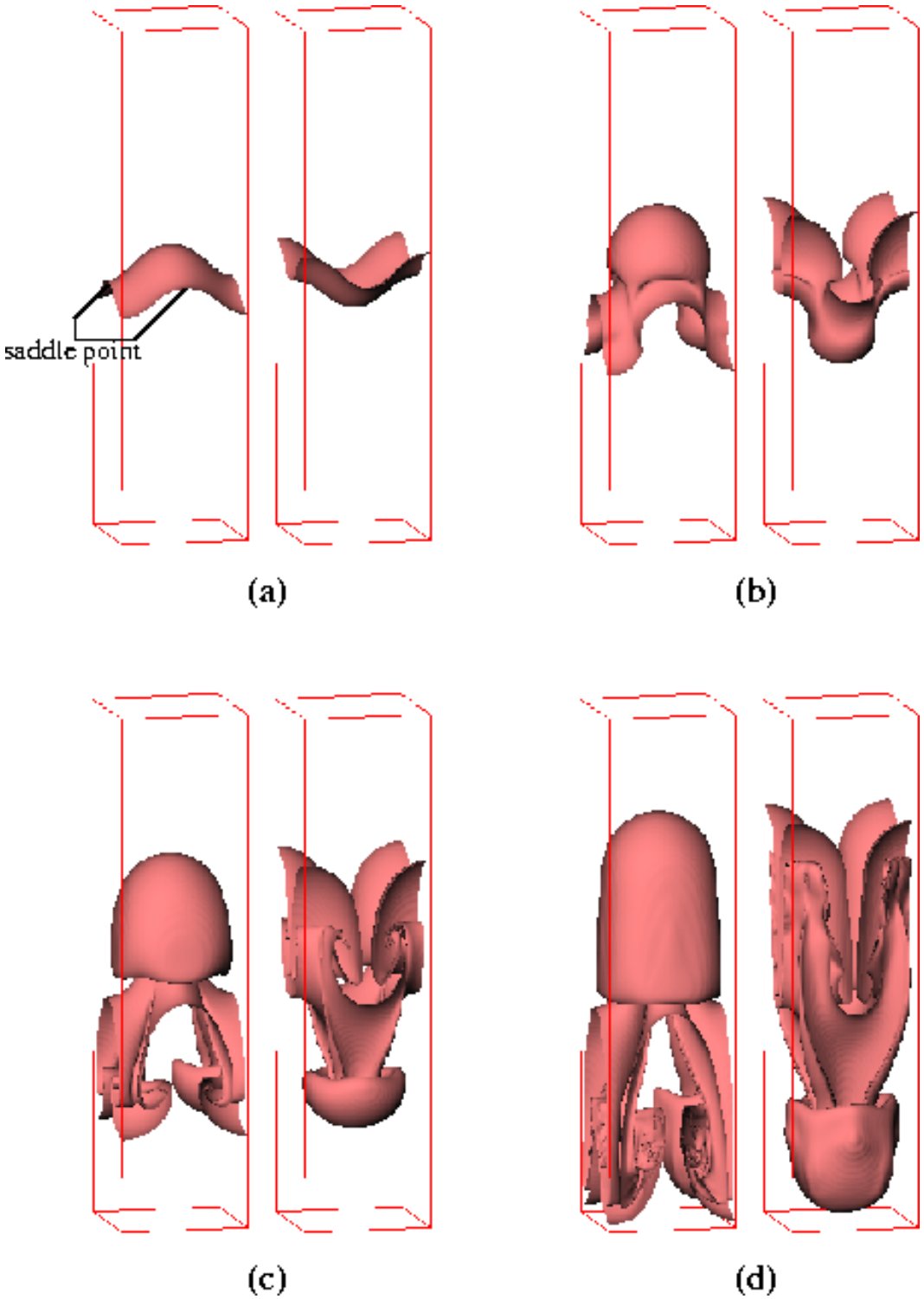

FIG. 10. *Lattice Boltzmann simulation of Rayleigh-Taylor instability in three-dimensions. Evolution of the fluid interface from a single-mode perturbation at* (a) $t = 1.0$, (b) $t = 2.0$, (c) $t = 3.0$, *and* (d) $t = 4.0$. *The Atwood number is* 0.5 *and the Reynolds number is* 1024. *The time is normalized by* $\sqrt{W/g}$. *The interface is viewed from the heavy-fluid side* (left panel) *and from light-fluid* (right panel). *The interfaces in the left panel are shift* $W/2$ *in both* x *and* y *directions for a clearer view of the bubble.* (Courtesy of He).

self-assembly of a single emulsion droplet. The lattice-gas method, by contrast, is able to study the growth and saturation of many such droplets and larger structures, as can be seen in these figures. Undoubtly in time these models will become useful to various chemical and pharmaceutical industries for real applications.

2.8. The Gas Kinetic Scheme for the Compressible Navier-Stokes Equations. There are two approximation made in the lattice Boltzmann equation which prevent the simulation of compressible flows: (1) discretization of (particle) velocity space, and (2) low Mach number expansion of the equilibrium distribution function [Luo 2000a]. One can make incremental improvements by including more discrete velocities and higher order terms ($\boldsymbol{u}$) in the equilibrium distribution function. However, to circumvent the problem all together, one need to abandon the aforementioned approximations.

One can formulate a finite volume scheme based one the BGK equation by using the integral solution given by Eq. (2.20). The Maxwellian equilibrium function $f^{(0)}$ is expanded in space and time, but not in particle velocity space. The particle velocity space is integrated out to obtained the moments. The scheme is called gas-kinetic scheme [Prendergast & Xu 1993, Xu & Prendergast 1993, Xu 1998]. The gas-kinetic scheme is a shock capturing scheme, and is capable of simulating high Mach number flows. It can also be used to simulate interfaces subjected to shocks [Xu 1999], such as Richtmyer-Meshkov instability [Xu 1997, Kotelnikov & Montgomery 1997, Xu 1999, Lian & Xu 2000].

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, $\boldsymbol{u}\cdot\nabla\boldsymbol{u}$; 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-Friedrichs-Lewy (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 δ_t/δ_x, where δ_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 methods, 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 second order in space and time. In contrast to

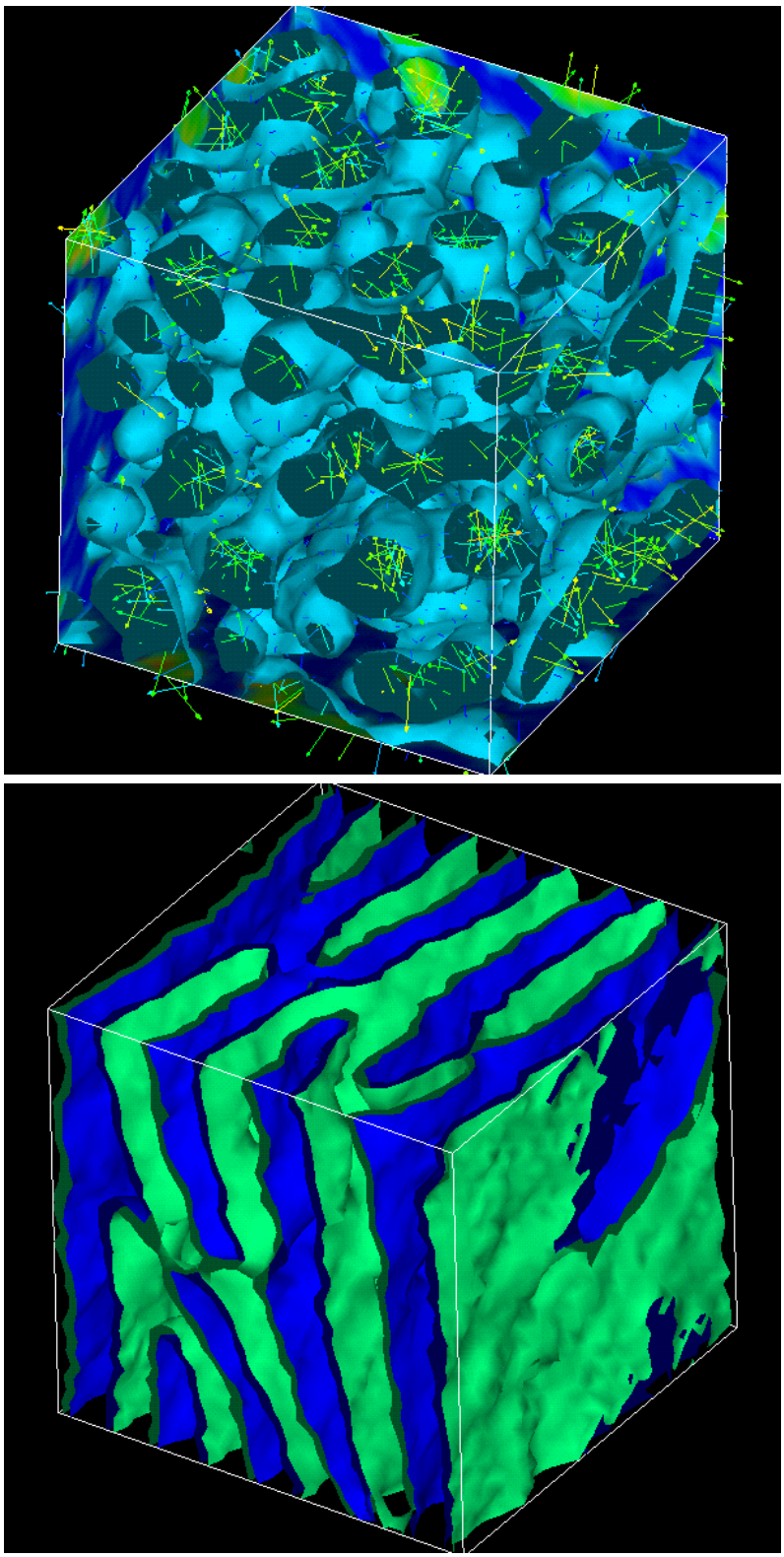

FIG. 11. *Lattice-gas simulations of complex fluids in three-dimensions.* (top) *Growth of wormlike micelle phase in binary mixture of water and amphiphile in three dimensions. The arrows denote the direction of orientation of individual amphiphile particles. This structure self-organized from randomly homogenized initial conditions.* (bottom) *Growth of lamellar phase in three-component mixture in three dimensions. Only the interface is rendered for clarity.* (Courtesy of Boghosian).

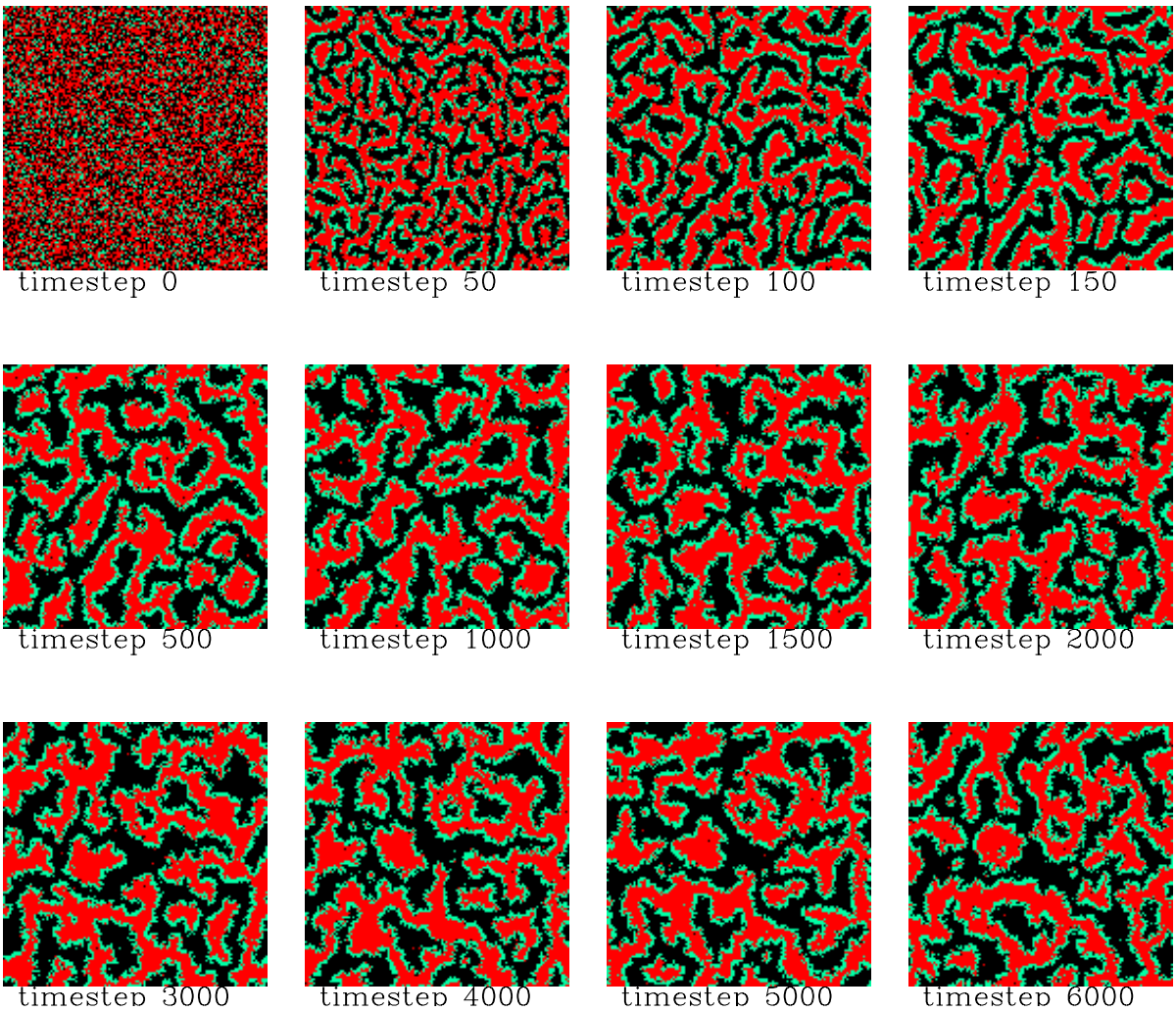

FIG. 12. *Lattice-gas simulations of complex fluids in two-dimensions. Growth of sponge phase in three-component mixture of water, oil and amphiphile in two dimensions. Again, this structure self-organized from random initial conditions.* (Courtesy of Boghosian).

the Navier-Stokes solvers, the LGA and LBE methods usually need comparable, or finer resolutions, depending on specific problems.

9. The spatial discretization in the LGA and LBE methods is dictated by the discretization of the particle velocity space. This coupling between discretized velocity space and configuration space leads regular Cartesian grids. This is a limitation of the LGA and LBE methods, especially for aerodynamic applications.

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. One pressing issue in the LGA and LBE methods is lack of systematic numerical analysis of the models. In addition, the numerics of the LBE method at present time is rather primitive – it is an explicit, first order finite difference form with second order corrections. Many numerical techniques, such implicit method and multigrid method, *etc.*, have just been applied to the LBE method recently [Tölke *et al.* 1998, Verberg & Ladd 1999]. In what follows, we

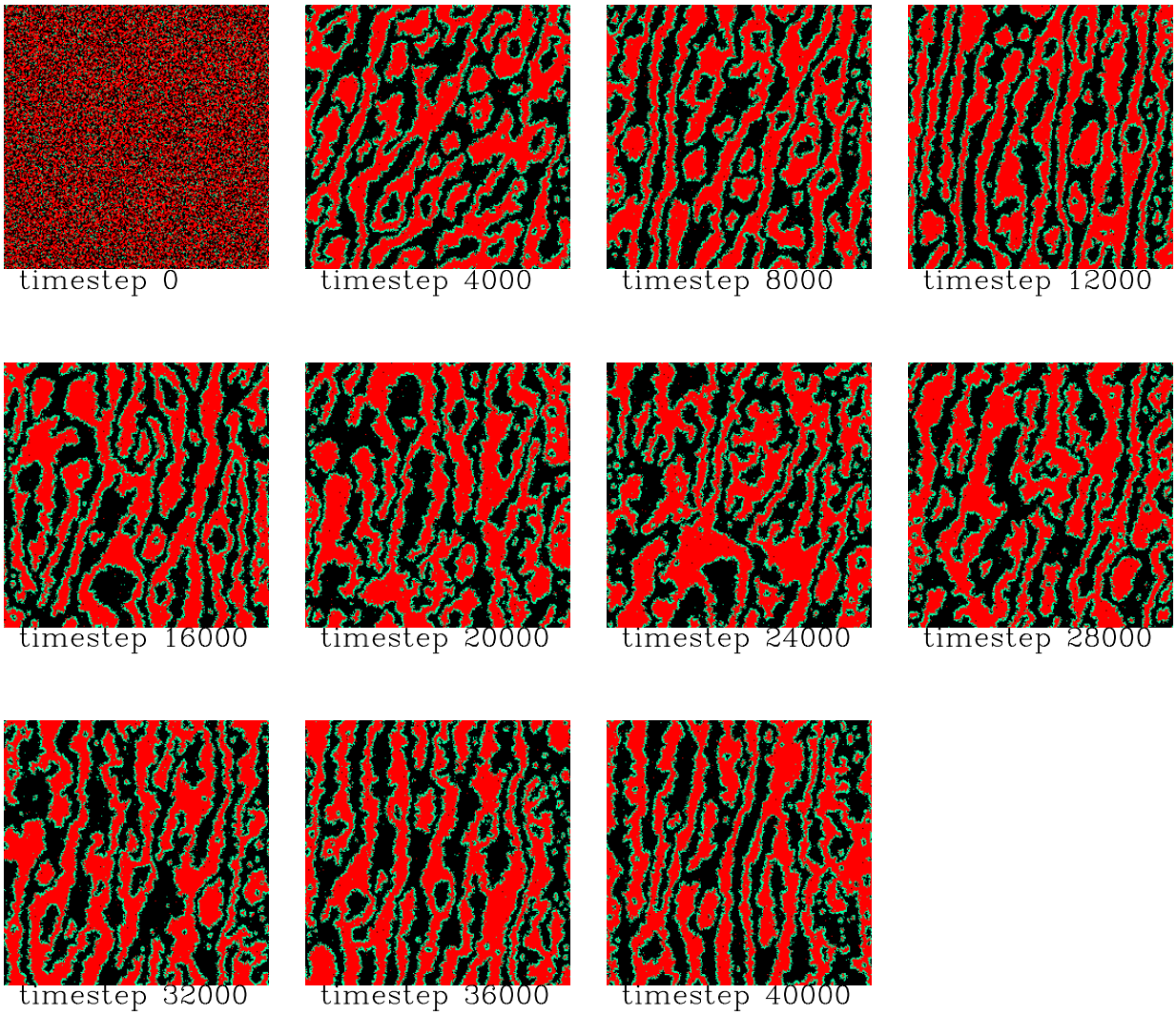

FIG. 13. *Lattice-gas simulations of complex fluids in two-dimensions. Shear-induced sponge-to-lamellar phase transition in a three-component mixture in two dimensions, with an applied shear.* (Courtesy of Boghosian).

briefly discuss the issues concerning hardware, modeling, and applications of the LGA and LBE methods.

3.1. Hardware. Because the LGA algorithms can be implemented with logical (binary) operations or table-lookups. These algorithms can be directly implemented on a custom made microprocessor [Lee *et al.* 1990, Lee 1993], hence they can be extremely fast on special-purpose computers [Clouqueur & d'Humières 1987, Toffoli & Margolus 1987, Despain *et al.* 1990]. A recent study showed that a special-purpose computer Cellular-Automata-Machine-8 (CAM-8) [Toffoli & Margolus 1987] with 8 nodes achieved a speed of 7 million site updates per second for a three-dimensional LGA algorithm [Adler 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 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.

It is also worthwhile to point out that due to ready availability of commodity microprocessors, there is a growing trend to build parallel computer clusters (Beowulf clusters) with commodity microprocessors. The lattice Boltzmann method performs very well on Beowulf clusters. The computational speed of the LBE algorithms scales linearly with the number of 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 Ångströms to a few tens of nanometer. 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 is now possible.

The most recent development in this area is application of a quantum lattice-gas model for computational fluid dynamics [Yepez 1999a, Yepez 1999b, Yepez 1999c, Yepez *et al.* 2000]. The key idea here is to construct a (large) array of quantum computers connected by classical networks with an external control so that the "qubits" (the quantum mechanical wave functions) within the system mimics the behavior of a system of massive quantum particles moving and colliding on a discrete space-time lattice. Consequently the macroscopic behavior of the system can mimics the behavior of a corresponding classical system (such as a fluid system). This is a specific application of quantum computing. A prototype of such quantum computer array has been made [Yepez *et al.* 2000]. These new ideas will have profound impact on the applications of the lattice gas and the lattice Boltzmann methods.

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 ∇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.* 1997a, Palmer & Rector 1999];
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. Simulations of complex fluids such as viscoelastic fluids also require the consideration of internal degrees of freedom of particles [Lallemand *et al.* 2000].
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, certain 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 [Miller *et al.* 2000].
6. Turbulence modeling. Turbulence modeling is a mature subject and it has not been utilized 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. The methods have be successfully applied to simulate interfacial dynamics [Buick & Greated 1998, He *et al.* 1999a, He *et al.* 1999b], even with very complicated boundaries [Martys & Chen 1996, Chen & Doolen 1998], and particle-fluid interactions [Qi 1998, Qi 1999, Qi 2000]. In additional 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). Aeroelasticity is a typical example of such a problem [Strumolo & Viswanathan 1997]. 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 re-

cently. 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. Complex Fluids and 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, consequently, hydrodynamics for such systems are either unknown or ill-posed. The LGA or LBE models which directly use model interactions among particles can be effective to study such systems [Giraud *et al.* 1997, Giraud *et al.* 1998, Boghosian 1999, Lallemand *et al.* 2000].
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, Kometer *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 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.

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