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Lattice gas automata: A tool for exploring dynamical processes

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Abstract. The lattice gas automata (LGA) technique as an alternative to the partial differential equation (PDE) approach for studying dynamical processes, including those in reaction-diffusion systems, is reviewed. The LGA approach gained significance after the simulation of Navier–Stokes equation by Hardy *et al* (1976). In this approach, the dynamics of a system are simulated by constructing a microlattice on each node of which Boolean bits are associated with the presence or absence of particles in *distinct* velocity states. A complete description involves the composition of an *elastic collision operator*, a *reactive collision operator* and a *propagation operator*. The Hardy, de Pazzis and Pomeau (HPP) model does not have the desired isotropy, but its subsequent modification in 1986, known as the Frisch, Hasselacher and Pomeau (FHP) model (Frisch *et al* 1986), has been applied to a variety of nonequilibrium processes. Reaction–diffusion systems have been simulated in a manner analogous to the master equation approach in a continuum framework. The Boltzmann kinetic equation as well as the expected complex features at the macroscopic level are obtained in LGA simulations. An increasing trend is to use real numbers instead of Boolean bits for the velocity states. This gives the lattice Boltzmann (LB) model which is not only less noisy than LGA but also numerically superior to finite-difference approximations (FDAs) to PDEs. The most significant applications of LGA appear to be in the molecular-level understanding of reactive processes.

Keywords. Lattice gas automata; dynamical processes; dynamics; Navier–Stokes equation.

1. Introduction

Complex macroscopic processes owe their genesis to nonlinear geometric relationships in the laws of motion. Such nonlinearity enters either through interactions in space between neighbouring particles or through the mixing of nearby initial conditions. Both situations may arise in the dynamics of chemical systems. Usually one assumes almost perfect knowledge of the laws of motion and the initial conditions as well as the states of the system regarded as points evolving along trajectories in an appropriate space. Properties on the macroscopic scale are then obtained by averaging over an ensemble of such dynamical systems. The functional relations necessary for such averaging depend on the dynamical coordinates (degrees of freedom). Recent breakthroughs in the study of complex systems have arisen from a general class of approaches where such a system is regarded as a conglomeration of small sets of interactions which behave in a simple deterministic manner and yet generate complex features when treated in cooperation (Stein 1989; Jen 1990; Stein and Nadel 1991; Nadel and Stein 1992).

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Conventionally, a dynamical system is formulated through a partial differential equation (PDE). Nonlinear PDEs are extremely difficult to solve analytically and even numerical methods for their solution have to reach a high level of sophistication. Data-level parallelism (Ceperley and Alder 1986) and parallel processing machines have now become essential tools for the numerical analysis of reasonably large microscopic systems. Typically, phenomenological equations like the heat conduction equation or the diffusion equation are simulated as finite difference approximations (FDA) of PDEs, in which discretization of both space and time is utilized, but the dependent variable is continuous. State-to-state transitions in molecular systems can also be described in terms of discrete Boolean variables. This has the advantage of an *in-built* parallelism. Thus, a lattice of points or sites, each with an associated Boolean integer, is allowed to evolve from one dynamical state to another in such a manner that the 'bits' change their values chosen from a defined field. If the interactions describing the rules of evolution are local, then this approach is called the cellular automaton (CA) approach (Wolfram 1983, 1986; Toffoli 1984; Margolus *et al* 1986; Jen 1990). Over the last decade, this approach has emerged as a powerful technique applied to dynamical systems of many different types, ranging from crystal growth to oscillating processes in excitable media (Vichniac 1984; Winfree *et al* 1985; Gerhardt *et al* 1990, 1991; Jen 1990; Weimar *et al* 1992; Singh *et al* 1994). While the applications to excitable media are primarily addressed towards mimicking the complex features in the phase space, the fundamental equations of nonequilibrium thermodynamics are simulated through the lattice gas automata (LGA) which are constructed by using a CA-based formulation of the interactions at the molecular level. These approaches and applications have opened up enormous possibilities for realistic molecular-dynamics simulations of large systems, with the promise of yielding deep insights into the foundations of kinetic theory in particular and nonequilibrium statistical mechanics in general.

The LGA technique is now accepted as an efficient and powerful alternative to the PDE approach for describing evolving physical systems. It has been applied to simulate fluid-dynamical equations like the Navier–Stokes equation, kinetic Boltzmann equation and the associated transport relationships (Frisch *et al* 1986, 1987; Boghosian and Levermore 1987; d'Humieres and Lallemand 1987; Chen *et al* 1989; Kadanoff *et al* 1989; Boghosian 1990; Doolen 1990; Kometer *et al* 1992). Of particular interest to chemists is the simulation of reaction–diffusion systems (Dab *et al* 1990, 1991; Doolen 1990; Kapral *et al* 1991).

In this article we review the formulation and applications of LGA. First, we briefly describe the basic concepts of CA and some of its applications in section 2. Then, LGA and a floating-point limit called the lattice Boltzmann (LB) approach are described in section 3. Some applications of the approach to reaction–diffusion systems are next reviewed in section 4. Finally, section 5 makes a few concluding remarks on the present status of and future directions in this field of research.

2. Cellular automata as an alternative to the PDE approach for studying dynamical problems

The advent of the CA approach has dramatically transformed the modelling and simulation of physical systems (Toffoli 1984; Vichniac 1984; Winfree *et al* 1985;

Margolus *et al* 1986; Gerhardt *et al* 1990, 1991; Jen 1990; Weimar *et al* 1992; Singh *et al* 1994). Conventionally, the modelling of evolving systems is done by using the notion of a continuous variable in an approximate space. This necessitates various details, e.g. the concepts of continuity, locality, etc. for a physical system, that are not always realizable in practice with systems exhibiting complex features. The requirement of continuity also obstructs the fast processing of jobs and is thus computationally expensive. In the CA approach, the problem is defined in terms of a look-up table which provides the rules for the evolution of a lattice of points with prescribed realization of Boolean variables. Collectively, the set of lattice points (or the 'universe') evolve into complex dynamical features characteristic of nonlinear systems. Since the operations in a computer are performed by using Boolean logic, the CA approach offers the advantage of a natural or in-built parallelism. It is also quite attractive because natural systems undergoing nonlinear, nonequilibrium processes seem to follow logical networks. Furthermore, unlike the floating-point description, the CA simulations do not involve any round-off errors. Although CA may be regarded as a reduced or limiting case of a neural network, the former has been applied to fairly complex phenomena such as reaction–diffusion systems (Oono and Kohmoto 1985; Gerhardt *et al* 1990, 1991; Tadic *et al* 1992; Weimar *et al* 1992), artificial life (Langston 1988), etc. The LGA models to describe flow systems have shown that the approach is remarkably powerful and far more efficient than the FDAs to PDEs.

For a one-dimensional problem involving only nearest-neighbour interactions, bits chosen from a binary field give rise to $2^{2^3} = 256$ possible rules of evolution (the binary set, $\{0, 1\}$, has two members, and for nearest-neighbour interactions we consider three sites, namely the evolving site and its two nearest neighbours). Symmetry restrictions and other considerations reduce this number to only 32. Thus, all meaningful one-dimensional problems with nearest--neighbour interactions can be described using one of these 32 rules. For higher dimensions, the possibilities are immense; still truth tables can be designed to mimic a realistic evolution without much numerical complexity.

Although early applications (Oono and Kohmoto 1985) involving CA were rather simplistic in terms of numerical details, recent works have designed more realistic and elaborate models. For instance, an excitable system is modelled (Gerhardt *et al* 1990, 1991; Weimar *et al* 1992) by using a rectilinear grid of cells with zero-flux boundary conditions. The dynamics of the cells reflect the typical phase portrait. This is achieved by introducing two distinct state variables. One of them is an excitation variable (u) and the other a recovery variable (v). While u has a binary field, v acquires values chosen from a higher logic, the maximum value corresponding to the physical jump from an excited state to a recovery state typical of bistable reactive systems.

The requirement of *local* rules does *not* prohibit the modelling of *global* phenomena. Thus, collective oscillatory, solitary wave-like or turbulent behaviour is seen to result from a purely local set of interactions (Oono and Kohmoto 1985; Gerhardt *et al* 1990, 1991). Similarly, for a distribution of electrons around a nucleus, evolving from a nonequilibrium initial density to an equilibrium density, two of us have observed complex features like oscillations of the electron density around the nucleus (Singh *et al* 1994). This is an example of a physical problem where the interactions are global and yet locality is maintained in designing the truth table. The flow of the electron

density was determined by using the criterion of flow from higher to lower chemical potential in the Thomas–Fermi framework (Parr and Yang 1989).

In the next section, we discuss lattice gases as a special case of CA.

3. Lattice gas automata (LGA)

The LGA model is a special type of CA involving a set of particles which move about on a lattice of points. The term LG refers to the particles on the lattice behaving like gas molecules as far as dynamical properties are concerned. The importance of these models was realized widely since the discovery by Frisch *et al* (1986) that the Navier–Stokes equation can be simulated by using such an approach. Essentially, LGA provides an efficient alternative to the conventional PDE formalism with special reference to flow systems.

Since they are specialized CA, LGA have the property of being represented by a number of bits at every site. Usually, it is a finite number of bits (for example a binary, ternary, quaternary or a special higher-order logic like $\{0, 1\, M(>1)\}$. In principle, the number of bits can also be infinite, but then there will be no essential difference between a floating-point description and a CA. Thus, it is sensible to focus one's attention on mostly those types of LG problems where the number of bits from which a value is chosen for a variable at a site is finite. The rules of evolution are local and are based on interactions with neighbours. The interactions generate dynamics with an inherent time dependence.

LG represents a typical example of excitable media where some sites may be forever at rest while some are continually excited and, after reaching a threshold excitation, are driven into a refractory stage. Unlike a usual CA description for, e.g., a diffusion system where the interactions between neighbouring sites change the 'bit' at a particular site, in the LGA approach a bit is conventionally thought of as a particle undergoing collisions while being subjected to a flow dynamics (say like a Hamiltonian fluid).

The evolution of LGA in a single time step is analogous to the formulation of classical kinetic theory describing the dynamics in the phase space. It can be seen as a combination of steps the first of which is an advection or streaming phase and the second a collision phase. In the flow or streaming process, the value moves to the neighbour to which it is associated (through interactions); all bits other than those corresponding to the 'rest' will move. The analogue of streaming in the conventional kinetic theory is the Hamiltonian phase flow which may evolve into complex features if the interactions are nonlinear in nature (Chirikov 1979). In the collision phase, the newly arrived bits change their values.

Usually, such a formulation is deterministic. However, stochasticity is introduced in the rules of evolution if the bits are changing randomly.

It is worth noting that corresponding to the conservation principles (balance equations) in continuum mechanics, analogous relationships exist in the CA framework. For instance, in some LG the total number of particles is a conserved quantity. This can be obviously maintained in the flow phase. The collision rules can be chosen in ways that conserve appropriate quantities. In fact, the LG method can be applied only to such PDEs that are consistent with the assumed conservation principles. The number and type of conserved quantities differ for the LGA equivalents

of the Navier–Stokes equation, Burgers' equation and diffusion equation (Boghosian 1990). For the Navier–Stokes equation, only mass balance and momentum balance are required; in the corresponding LG the quantities conserved are obviously mass and momentum. Likewise, the Fourier heat conduction requires an energy balance and the corresponding LGA model has only one scalar quantity conserved. These constraints do pose a problem in formulating the rules of evolution of the LGA, but it can be solved by skillfully designing the rules.

In a binary logic if '0' indicates particles at rest, then the transformation at every time step involves only the bits with value '1'. Thus, a map from the initial number of bits to the final number of bits conserves particles as long as the number of bits with value '1' is unchanged by the collision. Similar considerations are also valid for higher levels of logic. Reactive collisions require further modifications because the number of bits of a particular value changes in such cases.

3.1 *LGA and lattice Boltzmann (LB) techniques*

The rules of interaction determining the evolution of the set $\{b_i\}$ of bits $b_i(\mathbf{x}, t)$ for $i = 1, \ldots, n$ are chosen such that (a) the Liouville equation (LE) giving $b_i(\mathbf{x}, t+1)$ in terms of b_i^s at time t and (b) the Boltzmann equation are satisfied. While the first requirement implies that one is considering dissipative processes with conserved quantities, the second implies that the *stosszahl* (chaos at the molecular level) assumption of Boltzmann with no prior correlations between colliding molecules is incorporated. As long as the density of particles is small, the latter assumption is known to be valid in the continuum framework. To develop a discrete analogue of the Boltzmann H-theorem, one requires to establish equilibria by using the collision rules. An exclusion principle is established to this effect by allowing one particle per velocity state. This corresponds to a Fermi–Dirac distribution. This becomes clear if we consider the directions towards which a particle points, somewhat akin to the spin of an electron.

In the last five years, there has been an increasing trend of using a real-number description for the particle distribution and ignoring particle–particle correlations completely. This procedure, known as the lattice Boltzmann (LB) method, reduces the noise considerably compared to the LGA approach (McNamara and Zanetti 1988; Higuera *et al* 1989; Alexander *et al* 1992; Chen *et al* 1992). This is, in a sense, a coupled-lattice-map version of the LGA method; here the discretization of time and space are retained, but the state variable is allowed to take on continuous values (Kaneko 1989; Moon 1992). In the LGA approach, there is an inherent statistical noise due to the fact that the dependent variable is retrieved from the microlattice dynamics by an ensemble averaging (round-off errors are not present in the *evolution* of a particular system). The dynamic range of floating-point methods is also higher than discrete methods at the cost of reduced speed and enhanced redundancy. However, it should be realized that using floating-point numbers as opposed to Boolean variables destroys the CA nature of the method, although the lattice structure is retained as a numerical advantage. Being more accurately a discretized Boltzmann equation-type description (microscopic) rather than a discretized Navier–Stokes (macroscopic) equation-type picture, the LB methods are much better than FDAs of PDEs. LB methods may be regarded as combining the best features of both LGA and floating-point methods.

It is well known that microscopic conservation laws give rise to macroscopic hydrodynamic equations. We now elaborate on this point by first discussing the discrete analogue of the Chapman–Enskog method for lattice gases.

3.2 *The Chapman–Enskog method*

3.2.1 *The derivation of the Boltzmann equation.* In continuum mechanics, the balance equations are derived from fundamental laws of motion of the particles. The relationships between the forces and the evolution of dynamical variables, as specified by classical laws of mechanics, comprise the laws of motion. The analogous formulation in the LGA approach is to write an expression for the bit at time $t + \Delta t$ in terms of that at time t at a particular site $\mathbf{x}$ having undergone a displacement described by a lattice vector $\mathbf{r}_i$:

$$b_i(\mathbf{x} + l\mathbf{r}_i, t + \Delta t) = b_i(\mathbf{x}, t) + \Delta[\{b(\mathbf{x}, t)\}]. \tag{1}$$

There are different ways to define $[\{b(\mathbf{x}, t)\}]$. If there were no collisions and the particles arriving at a site moved along without any interactions, then the dynamics are described by $\Delta = 0$. This would be called *propagation* and an operator describing this dynamics, called the *propagation operator* P, is designed.

The presence of collisions defines other operators. The collisions may be elastic or inelastic. Elastic collisions have the effect of changing the orientations of the velocities of the particles. Such changes are incorporated by a *rotational operator* R, while the inelastic (reactive) collisions are described using an operator C (Dab *et al* 1990).

Thus the complete updating or description of the rule of evolution of the LGA is given by the composition $R \circ C \circ P$, of the propagation, inelastic (e.g. reactive) transformations and the rotation operators (the symbol $\circ$ denotes the composition of operators).

The earliest significant model proposed for the elastic collisions is known as the Hardy, de Pazzis and Pomeau (HPP) model (Hardy *et al* 1976). In this model exactly two particles are assumed to arrive at a node from opposite directions and they experience a head-on collision (figure 1). They leave the node immediately in the two other, perpendicular, previously unoccupied directions. These are deterministic collision laws obviously conserving mass (number of particles) as well as momentum locally and are the only nontrivial ones with these properties.

Thus, each of the cells (lattice points or sites) connected by the unit vector $\mathbf{r}_i$ to its four nearest neighbours has two states (codes) described by the values of a Boolean variable.

$$b_i(\mathbf{x}) = \begin{cases} 1 & \text{'if occupied'} \\ 0 & \text{'if unoccupied.'} \end{cases} \tag{2}$$

Equation (1) for this system (no reactive or inelastic collisions) can be described in two steps:

(i) *Effect of the operator R*: At each node, the four state bits are exchanged, $R(1,0,1,0) \leftrightarrow (0,1,0,1)$, all other states being left unchanged.

(ii) *Propagation*: $Pb_i(\mathbf{x}) = b_i(\mathbf{x} - \mathbf{r}_i)$.

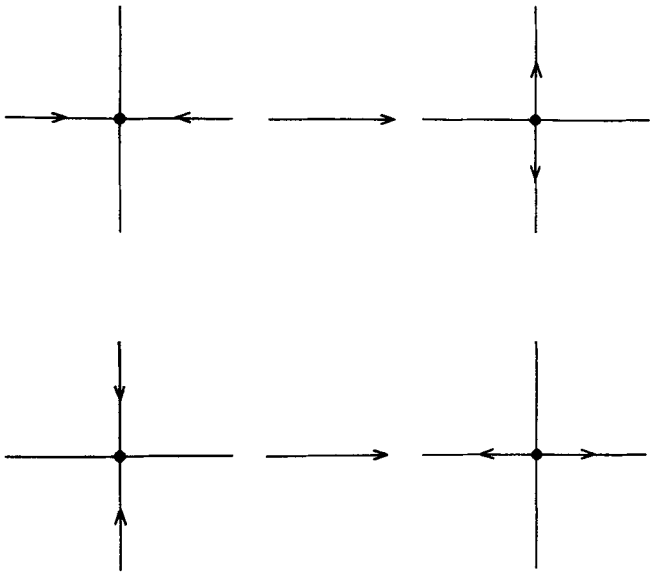

Figure 1. Schematic depiction of collision rules in the HPP model.

The propagation operator conserves mass globally. Thus, the HPP model yields dynamics invariant under all discrete transformations as well as under duality (i.e. exchange of 1s and 0s).

When the dynamical variables are varied slowly (effectively varying density and momentum in space and time) and an ensemble averaging is performed, the macroscopic equations obtained differ from the Navier–Stokes equation. However, Galilean invariance is not preserved because of the lattice structure. The symmetry of invariance under rotations by $\pi/2$ leaves an undesired anisotropy in the tensor relating the momentum flux with the quadratic terms in velocity.

In the Frisch, Hasselacher and Pomeau (FHP) model (Frisch *et al* 1986), a larger invariance group is utilized. Instead of a rectangular (Cartesian) 2-D grid, one has a triangular residing lattice with unit lattice constant (figure 2a). Each node is now connected with six neighbours by the vector $\mathbf{r}_i$ which thus brings in a six-bit state (figure 2b). As before, the rules of evolution are determined by the collision and

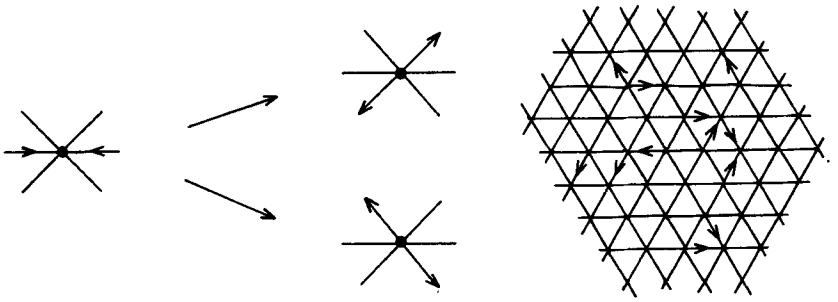

Figure 2. (**a**) Schematic depiction of collision rules in the FHP model. (**b**) Schematic representation of a lattice with a few particles.

propagation steps. There are now many more collision rules involving binary, ternary and quaternary collisions. There may also be some binary collisions with a third particle at rest.

The rules of evolution may also involve non-deterministic components. For instance, for every head-on collision, there are two output channels for the particles to move out and either of the two can be used; this could be done deterministically or by using a probabilistic description.

The 2-D models give rise to a crossover dimension problem. The effect of this is seen in the viscosity developing a logarithmic scale dependence. This problem disappears in higher dimensions. The extension of the FHP model to 3-D, hypercentric 4-D and pseudo-4-D models has been discussed by Rivet (1987).

Once the collision rules are finalized, one can write down $[\{b_i\}]$ explicitly. The conservation constants can then be verified. Finally, an ensemble of such lattice gas simulations, on grids of the same size, is constructed. The macroscopic initial conditions are identical for each LGA, but the molecular-level configurations are distinct. An ensemble averaging is performed in this ensemble.

Unlike a typical ensemble averaging, the LG is simulated on a very fine *microlattice*. A local spatial averaging is done and the dependent variables are defined on a *macrolattice*. These are the quantities subjected to the ensemble averaging. It can be shown that the averaged quantities

$$n_i(\mathbf{x}, t) = \langle b_i(\mathbf{x}, t) \rangle, \tag{3}$$

when subjected to the *Stosszahl* ansatz of Boltzmann, satisfy a relation

$$n_i(\mathbf{x} + \delta/1\, \mathrm{lr}_i, t + \Delta t) = n_i(\mathbf{x}, t) + c_i(\{n_i\}), \tag{4}$$

where c_i is the collision operator (here it includes rotations) with the property

$$\langle c_i\{b_i|\}\rangle \simeq c_i\{\langle b_i\rangle\} = c_i\{n\}. \tag{5}$$

Equation (4) is the LB equation corresponding to the integro-differential Boltzmann equation in the kinetic theory. It is fundamentally different from (1) in that it involves macro-averaged quantities and hence real numbers as opposed to bits. It is developed from a Boolean master equation at the microscopic level and yet, as a macroscopic equation, it does not have any Boolean variables.

3.2.2 *Solution of the Boltzmann equation.* In the continuum framework, the Chapman–Enskog procedure utilizes a Taylor expansion of a reduced distribution function in the phase space. This function has implicit spatial and temporal dependence described through the local density, flow density and temperature (McQuarrie 1984). The zeroth order solution for the distribution and the higher-order terms describe various stages of relaxation of a dilute gas to its equilibrium state.

Since (4) involves real numbers, one can use Taylor expansion here also and a formal perturbation expansion can be written as

$$\{n\} = \{n\}^{(0)} + \varepsilon\{n\}^{(1)} + \varepsilon^2\{n\}^{(2)} + \ldots. \tag{6}$$

Perturbation analysis then provides us with the solutions

$$\{n\}^{(0)} = \{n\}^{(0)}(\Gamma_1, \ldots, \Gamma_n), \tag{7}$$

where the Γ_is are the conserved densities (mass, momentum, etc.). For instance, for the HPP gas ($N = 3$), the zeroth-order distribution turns out to represent a local Fermi–Dirac equilibrium, as expected from the assumed exclusion principle for the velocities.

One can likewise obtain the higher-order terms in $\{n\}$ and express conservation equations by retaining these terms.

Once the distribution of bits is obtained, any other relevant property can now be obtained by summing over the distribution function. This is analogous to molecular-dynamics calculations. We will briefly discuss examples of these in the next section.

4. Applications

Once the fundamental equation of kinetic theory, namely the Boltzmann equation, is obtained and the solution for the reduced distribution function to a desired order is achieved, the method can be applied to a large number of dynamical problems, including reaction–diffusion systems. All the hydrodynamical equations can be obtained by using the distribution function. In particular, the mass balance (conservation of number of particles), momentum balance and the composite Navier–Stokes equation can be obtained. The solution of these equations with appropriate boundary conditions provides the dynamics of transport phenomena, e.g. that for a diffusion system, heat conduction, Poiseuille flow, Couette flow, etc. The LGA approach has been used by various workers to simulate fluid flow (Frisch *et al* 1986, 1987; Boghosian and Levermore 1987; d'Humieres and Lallemand 1987; McNamara and Zanetti 1988; Chen *et al* 1989, 1992; Higuera *et al* 1989; Kadanoff *et al* 1989; Boghosian 1990; Doolen 1990; Alexander *et al* 1992; Kometer *et al* 1992). Kadanoff *et al* (1989) have simulated a forced two-dimensional channel flow and shown that the LGA is a very efficient tool for simulative verification of a linear growth for kinematic viscosity with the linear size of the system; only with a significant reduced density this growth rate is reduced to a low value. They also showed that the noisy behaviour of the LGA is an advantage in the simulation of fluid flow, as long as the fluid is compressible and the actual equations obtained are far more complex than the Navier–Stokes equation. From a knowledge of the kinematic shear viscosity in terms of the density, one can calculate the Reynolds number associated with a large-scale flow (Frisch *et al* 1987). Kometer *et al* (1992) applied an LGA algorithm to an efficient treatment of complex scattering kernels and geometries. They showed that the technique is robust and works well even with coarse discretization. They used it for simulating the semiclassical Boltzmann equation for transport in semiconductors.

Perhaps the most significant applications of LGA are in the molecular-level understanding of reactive processes and simulation of phenomenological results starting from dynamical expressions at the molecular level. The statistical-mechanical treatment of chemical processes is done by investigating the reaction–diffusion system at the microscopic level and then by ensemble averaging the relevant dynamical properties. The PDE appropriate for such systems is the class of Ginzberg–Landau equations:

$$\partial_t x = \phi(x) + \nabla^2 x, \tag{8}$$

where x is a real number, a concentration (or number of particles). When $\phi(x) = 0$,

we obtain the ordinary Fickian diffusion. Nonzero values of $\phi(x)$ correspond to contributions from changes in chemical potentials arising from factors other than diffusion, namely reactive terms. In the automata analogue, $\phi(x)$ appears as a polynomial whose highest degree is set by the lattice symmetry.

The automata approach to reaction–diffusion systems has been applied to purely temporal situations as well as for situations where $\phi(x)$ is nonzero. Dab *et al* applied the LGA approach to the Schlögl model (Dab *et al* 1990, 1991; Lawniczak *et al* 1991):

$$A + 2X \rightleftharpoons 3X,$$
$$X \rightleftharpoons A.$$

This set of reactions is known to exhibit complex features like bistability, domain formation, etc. (Schlögl *et al* 1983). It was shown that the LGA approach to this typical reactive scheme produces all expected phenomenological features. More remarkably, it provides a microscopic approach which indicates the limits of validity of the phenomenological results. In Dab *et al*'s formulation, the particle number at a node may change in a local reaction of the type $\alpha X \rightarrow \beta X$ $(\alpha, \beta = 0, \ldots, 4)$, each reaction being assigned a probability $P_{\alpha\beta}$ regardless of the velocity state of the X species. The off-diagonal elements of this matrix P carry the information about the reactive processes.

Considering the kinetic regime, where the Knudsen number is of the order of unity, and decoupling the random fields for every α and β at all times, it can be shown that with standard projection operator techniques, the LB equation can be converted to a reaction–diffusion equation. Thus, in simulations starting with an LGA in a homogeneous unstable steady state, after 100 time steps, significant domain formation was seen for the Schlögl model and after an even larger number of time steps (300), the domain formation is the prominent feature of the automata lattice.

In a later work Dab *et al* (1991) have used the LGA approach to a two-species reaction–diffusion system:

$$\partial_t x = \psi(x, y) + D_x \Delta x,$$
$$\partial_t y = \phi(x, y) + D_y \Delta y.$$

Such systems are known to exhibit interesting features like oscillations and Turing bifurcations in space, and are thus useful for explaining various biological pattern formations such as morphogenesis (Prigogine 1980). With the variations now occurring due to diffusive transport and reactive processes, the macroscopic behaviour of the automata is described by a set of coupled PDEs.

The coupled-lattice formalism was used to deal with a set of reaction–diffusion equations known as the Maginu model:

$$\psi(x, y) = x - x^3/3, \tag{9}$$
$$\phi(x, y) = \frac{x - ky}{c}.$$

This problem is known to exhibit oscillatory behaviour and Turing structures (patterns in space) (Maginu 1975, 1978). The LGA simulation of the Maginu model

on a lattice of 64 × 64 nodes produced limit cycles. It is seen that the cycle is smaller in size (in the X–Y concentration phase space) as the ratio of reactive to elastic collisions is increased. A linear stability analysis performed on this system shows that the homogeneous steady state becomes unstable by spatial destabilization when $\sqrt{D_x/D_y} \leqslant (1-\sqrt{1-k})\sqrt{c}/k$, for $0 < c < k$ (Li 1990). In these limits, worm-like spatial structures are formed with characteristics of Turing bifurcations.

The method has been extended to n reactive species and illustrated with the Selkov model (Kapral *et al* 1991),

$$A \rightleftharpoons X$$

$$X + 2Y \rightleftharpoons 3Y$$

$$Y \rightleftharpoons B,$$

for which oscillations and spiral waves of diverse nature are generated. The speed with which LGA generates these complex features is in contrast to the enormous computations required due to the long distance and time scales that need to be explored even in approximate molecular-dynamics simulations of macroscopic reaction–diffusion phenomena.

These few applications of LGA make it abundantly clear that for the statistical mechanics of far-from-equilibrium systems, the former does have the promise of an efficient and powerful alternative to the PDE-based approaches.

5. Conclusions

We have presented here a summary of developments in one of the most exciting areas of frontier chemical physics, namely lattice gas automata approach to explore dynamical processes. Based on the general principles of CA modelling, LGA offers a far more efficient method of simulating phenomenological observations numerically than the conventional PDE approach. In particular, using the LGA approach one can obtain the Boltzmann kinetic equation and, at the macroscopic level, the Navier–Stokes and related balance equations. The method can be applied to reaction–diffusion systems and, for special classes of reactions like the Schlögl model, the remarkable agreement between the features obtained separately by using the PDE and the LGA master equations represents a great success of the method. The floating-point limit of LGA known as the LB model is gaining popularity in recent years. It has the best characteristics of the LGA and FDA to PDE approaches.

The statistical mechanics of fluids, flow systems and nonequilibrium systems has reached a revolutionary threshold with the advent of the LGA methods. While on the one hand computational ease has reduced the numerical difficulties, a much deeper insight about the microscopic dynamics leading to the complex macroscopic features is also achieved. At the same time, LGA methods are inherently noisier because the ensemble averaging is performed over a reasonably large microlattice to obtain the local functions. The fluid equations simulated by using the LGA are more complicated than the hydrodynamical equations.

In future, much greater activity is anticipated in the area of lattice gas automata

and their applications to far-from-equilibrium processes. Especially in areas such as investigations of biological processes, e.g. intercellular communication, etc., nonlinearity is known to play a dominant role, and LGAs offer a natural model for the evolution of these phenomena. Likewise, many other well-known problems of nonlinear dynamics are still understood in the PDE-based continuum framework and investigations of these by using LGAs are expected in the near future.

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References

Alexander F J, Chen H, Chen S and Doolen G D 1992 *Phys. Rev.* **A46** 1967
Boghosian B M 1990 in *1989 Lectures in complex systems*. Vol. II, Santa Fe Institute Studies in the Sciences of Complexity, (ed.) E Jen (New York: Addison-Wesley)
Boghosian B M and Levermore C D 1987 *Complex Systems* **1** 17
Ceperley D M and Alder B J 1986 *Science* **231** 555
Chen H, Chen S, Doolen G D, Lee Y C and Rose H A 1989 *Phys. Rev.* **A40** 2850
Chen H, Chen S and Matheus W, 1992 *Phys. Rev.* **A45** 5339
Chivikov B V 1979 *Phys. Rep.* **52** 463
Dab D, Boon J P and Li Y X 1991 *Phys. Rev. Lett.* **66** 2535
Dab D, Lawniczak A, Boon J P and Kapral R 1990 *Phys. Rev. Lett.* **64** 2462
Doolen G D (ed.) 1990 *Lattice gas method for PDEs: Theory, application and hardware. Physica* **D45** 1
Frisch U, Hasselacher B and Pomeau Y 1986 *Phys. Rev. Lett.* **56** 105
Frisch U, d'Humieres D, Hasselacher B. Lallemand P, Pomeau Y and Rivet J P 1987 *Complex Systems* **1** 649
Gerhardt M, Schuster H and Tyson J J 1990a *Physica* **D46** 416
Gerhardt M, Schuster H and Tyson J J 1990b *Science* **247** 1563
Gerhardt M, Schuster H and Tyson J J 1991 *Physica* **D50** 189
Hardy J, de Pazzis O and Pomeau Y 1976 *Phys. Rev.* **A13** 1949
Higuera F, Succi S and Benzi R 1989 *Europhys. Lett.* **9** 345
d'Humieres D and Lallemand P 1987 *Complex Systems* **1** 598
Jen E (ed.) 1990 *1989 Lectures in complex systems* (New York: Addison-Wesley)
Kadanoff L P, McNamara G R and Zanetti G 1989 *Phys. Rev.* **A40** 4527
Kaneko K 1989 *Prog. Theor. Phys., (Suppl.)* **99** 263
Kapral R, Lawniczak A and Masiar P 1991 *Phys. Rev. Lett.* **66** 2539
Kometer, Zandler G and Vogel P 1992 *Phys. Rev.* **B46** 1382
Langston C (ed.) 1988 *Artificial life: Proceedings of Interdisciplinary Workshop in the Synthesis and Simulation of Living Systems*, (Santa Fe: Santa Fe Institute)
Lawniczak A, Dab D, Kapral R and Boon J P 1991 *Physica* **D47** 132
Li Y X 1990 *Phys. Lett.* **A147** 204
McNamara G and Zanetti G 1988 *Phys. Rev. Lett.* **61** 3232
McQuarrie D 1984 *Statistical mechanics*, (New York: Harper and Row)
Maginu K 1975 *Math. Bio. Sci.* **27** 17
Maginu K 1978 *J. Differ. Equ.* **31** 130
Margolus N, Toffoli T and Vichniac G 1986 *Phys. Rev. Lett.* **56** 1694
Moon F C 1992 *Chaotic and fractal dynamics* (New York: John Wiley)
Nadel L and Stein D (eds) 1992 *1991 Lectures in complex systems* Vol. IV, Santa Fe Institute Studies in the Sciences of Complexity, (New York: Addison-Wesley)
Oono Y and Kohmoto M 1985 *Phys. Rev. Lett.* **55** 2927

Parr R G and Yang W 1989 *Density-functional theory of atoms and molecules* (New York: Oxford University Press)
Prigogine I 1980 *From being to becoming* (San Francisco: Freeman)
Rivet J P 1987 Ph D thesis, Universite de Nice, Nice, France
Schlögl F, Escher C and Berry R S 1983 *Phys. Rev.* **A27** 2693
Singh H, Sukumar N and Deb B M 1994 (to be published)
Stein D 1989 (ed.) *1988 Lectures in complex systems*, Vol. I, Santa Fe Institute Studies in the Sciences of Complexity (New York: Addison-Wesley)
Stein D and Nadel L 1991 (eds) *1990 Lectures in complex systems*, Vol. III, Santa Fe Institute Studies in the Sciences of Complexity (New York: Addison-Wesley)
Tadic B, Nowak U, Usadel K D, Ramaswamy R and Padlewski S 1992 *Phys. Rev.* **A45** 8536
Toffoli T 1984 *Physica* **D10** 117
Vichniac G 1984 *Physica* **D10** 96
Weimar J R, Tyson J J and Watson L T 1992a *Physica* **D55** 309
Weimar J R, Tyson J J and Watson L T 1992b *Physica* **D55** 328
Winfree A, Winfree E and Seifert H 1985 *Physica* **D17** 109
Wolfram S 1983 *Rev. Mod. Phys.* **55** 601
Wolfram S 1986 (ed.) *Theory and applications of cellular automata* (Singapore: World Scientific)