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TITLE A BRIEF DESCRIPTION OF LATTICE GAS MODELS FOR MULTIPHASE FLOWS AND MAGNETOHYDRODYNAMICS

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SUBMITTED TO Proceedings of the 1989 Santa Fe Summer School on Complex Systems, held in Santa Fe, NM, June 4-30, 1989

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A Brief Description of Lattice Gas Models for Multiphase Flows and Magnetohydrodynamics

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November 22, 1989

Presented in the 1989 Santa Fe Summer School on Complex Systems

ABSTRACT

Lattice gas models for multiphase fluids and for magnetohydrodynamic fluids are briefly described.

1 Introduction

Lattice gas automata (LGA) are many-body dynamical system with discrete space and time. The microscopic state of the system is completely specified by a few integer quantities at each lattice site. An update of the system is implemented according to the dynamics of the lattice gas automata particles, which are usually determined only by local information. The first LGA model was introduced by Frisch, Hasslacher and Pomeau (FHP)[1]. It exhibits a fluid behavior and, in the low Mach number limit, obeys the incompressible Navier-Stokes equations. Since the creation of the FHP model, lattice gas research has developed rapidly, providing not only further insight into the relation between the microscopic processes and macroscopic properties, but also a new procedure for doing fast computations. Recently there have been new models formulated for improving various properties of the FHP model [2] or for extending it to include other physical processes[3,4,5,6]. As a result, this research has opened up brand new fields. Already this research has had some impact on the understanding of the macroscopic properties of physics, in particular, the properties of multiple fluid systems. Moreover, some important potential industrial applications [7] are now being explored.

There are several reasons for the recent rapid growth in lattice gas research. The method provides very high resolution because it is very memory efficient. In the simplest algorithm, over 10 cells are stored in each CRAY word. Problems with 5 000,000,000 cells can now be run on a CRAY X/MP. The algorithm is quite fast. 300,000,000 cells can be updated each second on a CRAY X/MP using four heads and about an order of magnitude higher speed can be achieved on a Connection Machine 2.

Also, the algorithm is totally parallel. This parallel feature is easily exploited

on existing computers. In addition, an enormous gain can be made by constructing dedicated hardware. Already, inexpensive dedicated boards are available which allow small PCs to run lattice gas problems near CRAY speeds. Dedicated boards are now planned for delivery in 1990 which are expected to be a thousand times more powerful. It is possible to build with existing technology a dedicated machine which has the complexity of existing CRAYs but which would execute lattice gas algorithms many millions of times faster. (One should interpret this impressive gain in computer speed cautiously. For periodic problems on existing machines, lattice gas methods are slower than spectral methods at least by an order of magnitude. But for complicated boundary conditions, lattice gas methods can solve problems which are not solvable by other methods, for example, flow through porous media.)

Other advantages of the lattice gas algorithm include their ability to conserve energy and momentum exactly, their inherent stability with no mesh tangling or time step crashing, and their capability of implementing complex boundary conditions quickly and easily.

2 The FHP Model

The basic 2-D FHP lattice gas model[1] consists of identical particles on a hexagonal lattice with lattice constant $c = 1$. All particles have the same mass and they reside only on the sites of the hexagonal lattice. There are six different particle momentum states at each lattice site which can be associated with the directions $\hat{e}_a = [\cos(2\pi a/6), \sin(2\pi a/6)]$ ($a = 1, \dots, 6$). An exclusion rule is imposed so that no more than one particle at a given site can have a given momentum state. If we use $N_a(\mathbf{x})$ ($a = 1, \dots, 6$) to denote the particle occupation in state a at site \mathbf{x} , then $N_a = 0$ or 1. There are two microscopic updating processes at each time step: advection and collision. In the advection process, a particle in state \hat{e}_a moves from its

present site to nearest neighbor sites in the direction \hat{e}_a ; all particles have the same speed ($= 1$) and the same kinetic energy. In the collision process, particles at each site are redistributed among the 6 momentum states at the same site in such a way that the total particle number ($= \sum_{a=1}^6 N_a$) and the total momentum ($= \sum_{a=1}^6 \hat{e}_a N_a$) are conserved. Since all particles have the same mass and speed, energy conservation is equivalent to mass conservation. The particles behave like hard spheres with zero radii. It can be shown that at equilibrium the FHP lattice gas behaves like an ideal gas [8,9], $p = \rho/2$, where ρ is the average particle density.

The microdynamical evolution of the FHP system is also completely determined by the above two processes, which can be described exactly by the following microscopic equation everywhere on the lattice:

$$N_a(\mathbf{x} + \hat{e}_a, t + 1) = N_a(\mathbf{x}, t) + \Lambda_a; \quad a = 1, \dots, 6;$$

where Λ_a represents the creation or annihilation of the particle occupation $N_a(\mathbf{x}, t)$ at the momentum state \hat{e}_a due to collisions, which only depends on the information at the site \mathbf{x} at time t . The particle and momentum conservations are satisfied by $\sum_{a=1}^6 \Lambda_a = 0$ and $\sum_{a=1}^6 \hat{e}_a \Lambda_a = 0$. The explicit expression of Λ_a depends on the detailed collision rules[8,9]. Ensemble averaging the microscopic equation we obtain the lattice Boltzmann equation for large scale space and time behavior[9],

$$\partial_t f_a(\mathbf{x}, t) + \hat{e}_a \cdot \nabla f_a(\mathbf{x}, t) = \Omega_a,$$

where $f_a \equiv \langle N_a \rangle$ is the distribution function, $\Omega_a \equiv \langle \Lambda_a \rangle$, and " $\langle \quad \rangle$ " denotes the ensemble averaging. Using the standard definition for the fluid density $\rho = \sum_{a=1}^6 f_a$ and velocity $\mathbf{v} = \sum_{a=1}^6 \hat{e}_a f_a$, and after the Chapman-Enskog expansion, it can be shown that the FHP system obeys the following fluid equations[1,8]:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0,$$

$$\begin{aligned}\partial_t(\rho\mathbf{v}) + \nabla \cdot [\rho g(\rho)\mathbf{v}\mathbf{v}] &= -\nabla p + \nu \nabla^2(\rho\mathbf{v}), \\ p &= \frac{1}{2}[\rho - g(\rho)\mathbf{v}^2],\end{aligned}$$

where $g(\rho) = (\rho - 3)/(\rho - 6)$, and ν is the viscosity. Therefore the incompressible Navier-Stokes equations are recovered in the low Mach number limit by rescaling the time, since in the density ρ is a constant in this limit.

3 Realistic Equations of State

Another important development is the formulation of lattice gas models for arbitrary equations of state, including multiphase systems. It is known that the equation of state for FHP system approximates an ideal gas law. To simulate systems with nonideal gas equation of state, the particles must have more than one speed in order to have a realistic energy equation. Also the particle interactions must be generalized to include potential energy, which can depend on density and temperature. A simple model which has these minimal properties was recently proposed[15] and was shown to exhibit first-order phase transitions.

In addition to the FHP rules, this model allows at each site \mathbf{x} another kind of particle (“bound pair”), with occupation $N_0(\mathbf{x})$ ($= 1, 0$). A square-well pairwise potential energy is introduced between any two bound-pairs at distance r :

$$\epsilon(r) = \begin{cases} -\epsilon_0 & \text{if } 0 < r \leq c \\ 0 & \text{otherwise} \end{cases}$$

where $\epsilon_0 = \text{const.} \geq 0$. (This constant can be set equal to unity without loss of generality.) That is, a bound-pair only has non-zero potential energy with those bound-pairs at its 6 nearest neighbor sites. These bound-pairs possess a total potential energy, $E = -\frac{1}{2}\epsilon_0 \sum_{\mathbf{x}, \mathbf{a}} N_0(\mathbf{x})N_0(\mathbf{x} + \hat{a}_i)$, which varies according to the distribution of the bound-pairs. A transition between bound pairs and free pairs process is included, such that the ratio of the probabilities for the system to change from one state to

another is proportional to $\exp(-\beta\Delta E)$, where ΔE is the potential energy difference between the two states. Since the evolution of the system is a Markovian process, it can be shown that the canonical ensemble is an invariant measure for the system in equilibrium with temperature $1/\beta$ [16].

In this simplest model, the following transitions are allowed: 1) a pair of oppositely directed free particles may form a bound-pair with zero net momentum, and 2) a bound-pair may become two oppositely directed free particles. The mass of a bound-pair is twice that of a free particle. The potential energy change associated with a binding transition at a site is $\Delta E(\mathbf{x}) = -\epsilon_o \sum_{i=1}^6 N_o(\mathbf{x} + \hat{e}_i)$. With constant temperature everywhere, the updating rules are specified as follows: To avoid multiple transitions the lattice is divided into 3 independent sublattices, each of them a hexagonal lattice but with the lattice constant $\sqrt{3}c$; particles on the same sublattice are separated by more than one lattice unit and hence not mutually interact. At each time step, the updating of the system associated with the transition process is done in parallel in 3 steps, each step involving only one sublattice. A binding probability $\phi = \lambda \exp(-\beta\Delta E)/(1 + \exp(-\beta\Delta E))$ ($\lambda \leq 1$) is assigned at each site of a sublattice. The unbinding probability $\bar{\phi}$ for particles is $\lambda(1 - \phi)$. A transition is not allowed if it leads to a state which violates the exclusion constraint of no more than one particle per microstate. For example, if $N_o = 1$, $\bar{\phi}$ is sampled and, if successful, one of the three paired momentum directions is chosen with equal probability. An unbinding is allowed only if there are no free particles in the chosen pair of directions. If $N_o = 0$, one of the three paired momentum directions is chosen with equal probability. If the chosen pair of the free particle states is occupied, ϕ is sampled and, if successful, a binding occurs such that the pair of free particles form a bound-pair and N_o becomes one. For fixed β , $\lambda = 1$ leads to the shortest time scale for the system to reach equilibrium. Streaming and elastic collision processes also occur at each time step.

The FHP model is a special case with $\beta = -\infty$.

The microdynamic evolution of this simple system can be formulated as a set of local binary microscopic equations:

$$N_a(\mathbf{x} + \hat{e}_a, t + 1) = N_a(\mathbf{x}, t) + \Lambda_a + \Pi_a; \quad a = 1, \dots, 6,$$

$$N_0(\mathbf{x}, t + 1) = N_0(\mathbf{x}, t) + \Pi_0,$$

where Λ_a represents the usual FHP contribution from pure elastic collisions for the free particles[8,9]. Π_a ($a = 0, \dots, 6$) is the additional contribution from the transition processes:

$$\Pi_a = \mathcal{B}_a^+(1 - N_a(\mathbf{x}, t)) - \mathcal{B}_a N_a(\mathbf{x}, t) \quad (a = 0, \dots, 6)$$

where \mathcal{B}_a^+ and \mathcal{B}_a ($= 0$, or 1) are the creation and annihilation operators for N_a ($a = 0, \dots, 6$) due to the transition processes, respectively. They are functions of the particle occupations at site \mathbf{x} as well as the occupations of the bound pairs at the 6 nearest neighboring sites. This form of Π_a guarantees the particle occupation at every state is either 0 or 1. It can be seen[15], from the explicit expressions for \mathcal{B}_a and \mathcal{B}_a^+ ($a = 0, \dots, 6$), that mass and momentum are conserved: $\sum_{a=1}^6 \Pi_a + 2\Pi_0 = 0$ and $\sum_{a=1}^6 \hat{e}_a \Pi_a = 0$.

Using the mean field approximation, it can be shown that,

$$f_a = \frac{1}{1 + \exp(\alpha + \gamma \hat{e}_a \cdot \mathbf{u})}, \quad a = 1, \dots, 6,$$

and

$$f_0 = \frac{1}{1 + \exp(2\alpha - \beta\epsilon)},$$

where f_a ($a = 1, \dots, 6$), f_0 represent the free particle distribution and bound-pair distributions, respectively. ϵ is the mean-field potential energy per bound-pair. The fluid equation for this model is:

$$\partial_t(\rho \mathbf{u}) + \nabla \cdot (g(\rho) \mathbf{u} \mathbf{u}) = -\nabla(p + h(\rho) \mathbf{u}^2) + \nu \nabla^2(\rho \mathbf{u}).$$

where $g(\rho) = (\rho^2(\rho_f - 3))/(\rho_f(\rho_f - 6))$. ρ_f is the free particle density. The explicit form of $h(\rho)$ has not yet obtained in closed form. p is the kinetic pressure determined from the equation of state. By a simple mapping, it can be shown that the invariant measure of the bound pairs is equivalent to that of the Ising model on a triangular lattice with an external magnetic field dependent on density and temperature. Therefore the equation of state of this model contains first-order phase transitions, with the inverse critical temperature $\beta_c \approx 1.09$. Dynamic properties of this simple model have been studied both analytically and numerically.

Many possible applications and extensions of this simple model can be made. For example, we may be able to study multi-phase flows by extending this model to allow moving bound-pairs. Moreover, unlike FHP and other models[2,8], this simple model provides the important capability of simulating supersonic flows. Near the critical point, the sound speed $c_s (= \sqrt{dp/d\rho}) \approx 0$. This is observed in computer models which show that moderate flow velocity will be supersonic.

Other extensions include generalizing the particle interaction energy to be anisotropic, so that liquid crystal fluids with rodlike particle structures can be simulated. Another extension incorporates an interaction energy which includes a lattice energy; enabling problems related to melting may be studied.

4 Hydrodynamic and Magneto-hydrodynamic LGA.

Since the FHP model[1] was introduced for simulating hydrodynamics, lattice gas research has developed rapidly. Many lattice gas models have been formulated as efforts to simulate various kinds of physical processes[3,4,5,6]. All these were realized by introducing new microscopic degrees of freedom and by modifying the lattice gas micro-dynamical rules. There are also attempts at generalizing the space and time by introducing "dynamical lattices"[11]. By adopting very different microscopic up

dating processes such as the random walk process, it has shown that the 1-D Burgers equation can be simulated[5]. Furthermore, by attaching to the lattice gas particles additional degrees of freedom like color or spin, physical processes such as the evolution of a passive scalar[10], temperature field[2] and others can be simulated. For example, it is possible to use these additional degrees of freedom to simulate fluids consisting multispecies such as the oil and water mixtures[6]. The particle interactions are able to be generalized due to the additional degrees of freedom so that the cohesion force and the chemical reaction can be represented[6,12]. Recently, it is found that this kind of models have important industrial applications. However, the earliest attempt of using lattice gas to model different fluids was due to Montgomery and Doolen for magnetohydrodynamics (MHD)[3].

The incompressible MHD fluid is usually described by the following equations:

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + (\nabla \times \mathbf{B}) \times \mathbf{B} + \nu \nabla^2 \mathbf{v}, \quad (1)$$

$$\partial_t \mathbf{B} + \mathbf{v} \cdot \nabla \mathbf{B} = \mathbf{B} \cdot \nabla \mathbf{v} + \mu \nabla^2 \mathbf{B}, \quad (2)$$

$$\nabla \cdot \mathbf{v} = \nabla \cdot \mathbf{B} = 0, \quad (3)$$

where \mathbf{v} and \mathbf{B} are velocity and magnetic field, respectively. p is the kinetic pressure. The magnetic vector potential \mathbf{A} is related to \mathbf{B} by $\nabla \times \mathbf{A} = \mathbf{B}$. Equation (1) is referred to as the momentum equation while equation (2) is referred to as the magnetic induction equation. The magnetic field modifies the motion of the fluid in the momentum equation through the Lorentz force, $(\nabla \times \mathbf{B}) \times \mathbf{B}$. In the 2-D case, one can choose $\mathbf{A} = A\hat{z}$, and the induction equation can be replaced by a scalar equation for the magnetic vector potential,

$$\partial_t A + \mathbf{v} \cdot \nabla A = \nu \nabla^2 A.$$

The Montgomery and Doolen (MD) lattice gas model for MHD was based on the fact that the magnetic vector potential in the 2-D case can be treated as a scalar.

In order to represent the magnetic vector potential in the lattice gas system, an additional scalar quantity was introduced. In addition to the FHP rules, each lattice gas particle carries a magnetic potential ‘quantum number’ $\sigma = 1, -1, \text{ or } 0$. Particles carrying different quantum numbers are distinguishable. The vector potential A is related to σ by $\rho A = \sum_{\mathbf{a}, \sigma} \sigma f_{\mathbf{a}}^{\sigma}$, where $f_{\mathbf{a}}^{\sigma}$ is the distribution function for particles with quantum number σ at state $\hat{e}_{\mathbf{a}}$. Collisions exactly conserve the net value of σ in each site of the lattice. It has been shown that the evolution of this magnetic vector potential obeys the scalar equation (2). Since, in 2-D case, the Lorentz force in the MHD momentum equation can be expressed as $-\nabla A \nabla^2 A$, this force is included in the model by introducing a force, whose average is constrained to equal the Lorentz force. However, this average requires ‘supercell averaging’. Because of fluctuations, the supercell size must be large enough to have a sufficient smooth representation of the Lorentz force. Their implementation required a finite difference procedure for calculating A .

An alternative lattice gas model for simulating MHD was later introduced by Chen, Matthaeus and Klein using different concept[4,13]. The advantage of their alternative model is that the update of the system, similar to FHP, is local. This is done by generalizing the particle advection, utilizing the symmetry structure of the MHD equations and Elsasser[14] variables $\mathbf{z}^{\pm} = \mathbf{v} \pm \mathbf{B}$. In the Elsasser representation, the MHD equations have the form $\partial_t \mathbf{z}^{\pm} = -\mathbf{z}^{\mp} \cdot \nabla \mathbf{z}^{\pm}$ (ignoring pressure and dissipation). Thus, instead of representing the magnetic field by the vector potential \mathbf{A} , one treats the magnetic field on an equal footing with the velocity field. In order to generalize advection, model introduces six additional unit vectors related to the magnetic field quanta: $\hat{e}_b (= [\cos(2\pi b/6), \sin(2\pi b/6)]$; $b = 1, \dots, 6$). A microstate (a, b) at a site can be defined as a state in each particle has a defined momentum quantum, \hat{e}_a , and a magnetic field quantum, \hat{e}_b . To minimize memory requirements, only one particle at

a site can have the same value for \hat{e}_a and \hat{c}_b . Using $N_{ab}(\mathbf{x})$ to represent the particle occupation at state (a, b) at site \mathbf{x} , we have $N_{ab}(\mathbf{x}) = 1$ or 0 . If the particle occupation everywhere in the lattice is known, the system is completely determined. This model introduces a “bidirectional random walk” process. That is, a particle at state (a, b) will advect from one site to one of its 6 nearest neighboring sites in the direction \hat{e}_a with probability $1 - |P_{ab}|$, or to one of these sites in the direction $\text{sign}(P_{ab})\hat{c}_b$ with probability $|P_{ab}|$. The parameter P_{ab} ($|P_{ab}| \leq 1$) is a function of (a, b) only. As a consequence, the evolution of this MHD lattice gas system is described by the following modified Boltzmann equation:

$$\partial_t f_{ab}(\mathbf{x}, t) + \{(1 - |P_{ab}|)\hat{e}_a + P_{ab}\hat{c}_b\} \cdot \nabla f_{ab}(\mathbf{x}, t) = \Omega_{ab},$$

where $f_{ab} \equiv \langle N_{ab} \rangle$ is the particle distribution. Ω_{ab} is the term associated with collisions, which are chosen to conserve the total mass, momentum and magnetic field at each site.

The macroscopic number density ρ and magnetic field \mathbf{B} are defined

$$\rho = \sum_{a,b} f_{a,b},$$

$$\rho \mathbf{B} = \sum_{a,b} \{Q_{ab}\hat{c}_b + R_{ab}\hat{e}_a\} f_{ab},$$

while the fluid velocity, \mathbf{v} , is defined by

$$\rho \mathbf{v} = \sum_{a,b} \{(1 - |P_{ab}|)\hat{e}_a + P_{ab}\hat{c}_b\} f_{ab}.$$

The parameters P_{ab} , Q_{ab} and R_{ab} are chosen to satisfy such that the MHD equations. Because the system is invariant under a proper or improper rotations, it can be shown that these parameters only depend on $|a - b|$. Because the velocity field is a vector field and the \mathbf{B} is pseudo vector, the time evolution of the magnetic field in the MHD system is unchanged if the velocity field is reversed. This property is guaranteed by

requiring that $P_{ab} = -P_{ab+3}$, $Q_{ab} = Q_{ab+3}$ and $R_{ab} = -R_{ab+3}$. Hence, there are only 6 independent parameters in this model after. These are selected to be P_{aa} , P_{aa+1} , Q_{aa} , Q_{aa+1} , R_{aa} and R_{aa+1} .

Using a Chapman-Enskog, it can be shown that ρ , \mathbf{v} and \mathbf{B} approximately obey the following equations:

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) &= 0, \\ \partial_t (\rho \mathbf{v}) &= - \nabla [C_1 \frac{\rho}{6} - \frac{1}{2} \rho g(\rho) (C_2 \mathbf{v}^2 - C_3 \mathbf{B}^2)] \\ &\quad - \nabla \cdot \rho g(\rho) [C_2 \mathbf{v} \mathbf{v} - C_3 \mathbf{B} \mathbf{B}] + \nu \nabla^2 (\rho \mathbf{v}), \\ \partial_t (\rho \mathbf{B}) &= - (D_1 - D_3) \nabla \cdot [\rho g(\rho) \mathbf{B} \mathbf{v}] + (D_2 + D_3) \nabla \cdot [\rho g(\rho) \mathbf{v} \mathbf{B}] \\ &\quad + D_3 \nabla [\rho g(\rho) \mathbf{v} \cdot \mathbf{B}] + \mu \nabla^2 (\rho \mathbf{B}), \end{aligned}$$

where $g(\rho) = (\rho - 18)/(\rho - 36)$. The coefficients C_1 , C_2 , C_3 , D_1 , D_2 , D_3 , ν and μ depend only the six free parameters. By selecting the values of the 6 parameters under the conditions $C_2 = D_1 = D_2 \geq 0$, $D_3 = 0$ and $C_1 \geq 0$, together with the rescaling of the time by the $g(\rho)$ factor, the MHD equations are obtained in the low Mach number limit[13]. It can be argued that $\nabla \cdot \mathbf{B} = 0$ can be satisfied statistically in the weak magnetic field case[13].

An additional property of this alternative MHD LGA model is that it can easily be extended to three dimensions.

5 Discussion

It is important to generalize the existing lattice gas models to include various kinds of many-body physical systems. Although many models have been formulated such as those mentioned above, there are significant number of physical systems yet to be modeled by lattice gas automata. There are other major research directions in the

lattice gas automata study not mentioned above. For example, it is crucial to have the existing models improved so that they represent more realistic physics. One of the central problems in this regard is to see if the incompressibility condition for FHP and related lattice gas models could be relaxed significantly without increasing too much complications. There are important progresses in this attempt[2], however, it is limited so far to the weak compressible domains.

The success of the FHP model for simulating incompressible Navier-Stokes equations has led to considerable interest in the use of lattice gas automata for the study of fluid and fluidlike systems. There are at least two important reasons for this interest. First, lattice gas models suggest a fundamentally new way of doing numerical computations. It has no roundoff errors and can be massively parallel. Second, by formulating lattice gas models we may find insights into the relationship between the microscopic and the macroscopic world. A successful lattice gas model indicates that the relevant macroscopic behavior critically depends on only a few simple microscopic properties. Therefore, the theoretical importance of lattice gas models may be that they provide simplified but fundamental pictures of the realistic physical systems.

6 Acknowledgements

This work was supported by the United States Department of Energy and by NASA Innovative Research Program under grant NAGW 1648.

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