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Lattice Gas Simulations of One and Two-Phase Fluid Flows Using the Connection Machine-2

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ABSTRACT

In this paper, we report recent lattice gas simulations for single-phase and two-phase fluid flows for two dimensional problems using the Connection Machine-2. For the single-phase fluid problem, we use the standard 7-bit lattice gas model with the maximum collision rules. The velocity and vorticity field of the Kelvin-Helmholtz instability is studied. It is shown that the lattice gas method preserves the main properties of the flow patterns observed in other numerical simulations. Using colored particles and holes, the lattice gas method is extended to simulate immiscible fluids with adjustable surface tension, using a purely local collision scheme. The locality of this model allows us to implement a very fast and parallel algorithm on the Connection Machine-2. Because this new model correctly describes short-range particle-particle interactions between liquids and also particle-solid interactions between the fluid and the wall, cohesion and wettability can be simulated. Applications of the current model to several physical systems including spinodal decomposition, Rayleigh-Taylor flows and wettability in two-phase flows through porous media are discussed.

1 Introduction

At the microscopic level, the lattice gas method is based on simple, local, logical and parallel operations in discrete space and time. The coarse-grained macroscopic statistical properties of a lattice gas reproduce very complex physical phenomena which satisfy partial differential equations, including the Navier-Stokes equations.

Coupled with locality, the parallelism of the lattice gas guarantees rapid computation of flow fields. This is one reason why the development of the lattice gas methods has had a close relationship with the recent development of parallel computers, including the Connection Machine 2 and the CAM-8.

The single-phase lattice gas model proposed by Frisch, Hasslacher and Pomeau (FHP)[1] has been extensively used in a wide variety of problems. It has proved to be especially successful for describing flows through porous media[3,4]. Lattice gas models can accurately simulate flows in complex geometry at low Reynolds numbers, agreeing with experimental measurements of porosity within a few percent[4]. Nonslip and slip velocity conditions are easily treated for complex boundaries using lattice gas methods; whereas these boundaries are quite difficult for traditional numerical methods.

On the other hand, even for simple flow problems, most lattice gas simulations are still restricted to low Reynolds numbers because high Reynolds numbers (Re) require large computer memory and long running times. The Reynolds number for lattice gas models is defined as follows: $Re = g(n) \frac{UL}{\nu}$. Here $g(n)$ is the coefficient of the advection term in the Navier-Stokes equations for lattice gas models, U and L are the characteristic velocity and length of the system and ν is the kinematic viscosity. Because the kinematic viscosity is completely determined by the collision rules and particle density and because the characteristic velocity is required to be small in order for the Navier-Stokes equations to be valid[5], the Reynolds number for a given system is determined mainly by the system size in lattice units. On the CM-2 with 8 gigabytes of memory, it is possible to simulate in two dimensions, Reynolds numbers of the order of 30,000.

Lattice gas models for two-phase immiscible fluids including surface tension have been studied by several authors[6] [7] [8]. Rothman and Keller [6] first used a colored-particle algorithm to represent this system. To model short-range attractive interactions between particles of the same color, a color density gradient was required, using nearest-neighbor information. Their model demonstrated promising results for several applications. Models including colored particles and colored holes were proposed by Somers and Rem[8]. The introduction of the colored holes into the model was a crucial step; it makes the collision operation completely local and it efficiently utilizes memory. Usually, models including colored holes require less memory for the collision operation and are easier to implement on parallel machines.

Recently, we proposed a new two-phase lattice gas model which extends the approach incorporating colored particles and holes. The main advantage of our model over the model of Somers and Rem is that we force colored particles to move in a direction opposite to that of the local, colored-hole flux. In our model, a colored hole is created every time a particle is scattered. The hole propagates in the direction the particle had before scattering. When the hole encounters a pair of scattering particles, it preferentially causes particles with its color to be scattered in the direction from which the hole came. After the hole causes this preferential scattering, the hole is annihilated. Unlike other models, the colored holes in the present model are created and annihilated deterministically. Our model has a relatively small collision table. It may also be easier to analyze theoretically.

In Section 2, we present lattice gas simulations of one-phase flows undergoing a Kelvin-Helmholtz instability. We present the spatial velocity and vorticity patterns. Section 3 is devoted to a brief review of our two-phase lattice gas model. The Con-

tion Machine 2 program structure for our model is discussed in Section 4. Numerical simulations of two-phase flows for three different problems will be shown in Section 5. In Section 6, some conclusions are presented.

2 Single Phase Flows: Kelvin-Helmholtz Instability

In this section, a 7-bit lattice gas model with saturated collisions[9] is used to simulate a Kelvin-Helmholtz instability. The Reynolds number, Re , is expressed in terms of the reduced Reynolds number, Re^* , as follows:

$$Re = Re^* M L,$$

where M is the Mach number, $\frac{U}{c_s}$, and c_s is the sound speed. In order to simulate high Reynolds number flows, we prefer the density, $d = 0.3$. This gives an $Re^* = 2.78$, almost the maximal value. A system of 8192×8192 lattice sites and a maximum velocity of 0.3 are used. The Reynolds number, based on the velocity difference and the total box size, is about 20,000.

Initially, we assign the particle distributions from a Fermi-Dirac equilibrium for all sites. As shown in the first plot of Fig. 1, the middle region of half space has a velocity of 0.3. The top and bottom portions of the figure have a velocity of -0.3. The total momentum of the system is zero. Periodic boundary conditions are used for all sides. The vorticity, ω , is defined as follows:

$$\omega = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x},$$

where u and v are the velocity in the x - and y -direction, respectively. The initial vorticity has a nonzero distribution only near $y = 2048$ and $y = -2048$ (in lattice units), forming two vorticity sheets.

Fluctuations in the initial flow are automatically included in the initial particle distribution. This system is unstable without any stirring force and no additional wave-dependent perturbation is required to initiate the instability. The evolution of this system is characterized by the redistribution of vorticity in space. A good physical understanding of the vortex dynamics is given in Batchelor[10].

In Figs. 1 and 2, we present the velocity vector field and vorticity scalar field at various times during the lattice gas simulation. We observe that the initial vortex sheet is separated into discrete vortices by the shear force. Gradually, vortices with the same sign merge and eventually two large, oppositely rotating vortices are formed. During the merging process, one observes typical spiral vortex patterns. The viscous term in the Navier-Stokes equation dissipates the vorticity. Usually, viscosities in lattice gas models are not very small, and vorticity dissipates rapidly. Because our simulation has a high Reynolds number, the convection term still dominates. The vortex dynamics consists mainly of vortex mixing and convection.

The phenomena observed in this and other lattice gas simulation for vortex dynamics are qualitatively similar to other numerical simulations[11]. It is difficult to

quantify agreement between any pair of simulations for this highly unstable flow. Quantitative studies of the Kelvin-Helmholtz vortex dynamics could provide useful accurate comparisons between the lattice gas method and other methods.

3 Lattice gas models for two-phase immiscible fluids

As others have done before, we use a 14-bit hexagonal lattice gas model for two mixed fluids, distinguished by their colors, red and blue. For each of the six directions of motion and for the rest state, we assign two bits (f_i, N_i) to distinguish four possible states: (0,0) for blue hole, (0,1) for blue particle, (1,0) for red hole and (1,1) for red particle. This representation makes maximal use of two bits. Exclusion rules apply to particles and holes in each direction. A particle and a hole cannot occupy the same state. The lattice gas algorithm has two operations during each time step: streaming and collision. During the streaming process, particles or holes (f_i, N_i) move to their nearest-neighbor sites, without change of color, along $\vec{e}_i$, $i = 1, 2, \dots, 6$, the unit velocity in the i -direction. Rest particles and rest holes do not move. Let (f, N) be the initial state before a collision at site $\vec{x}$ and time t , where $f = (f_1, f_2, \dots, f_7)$ and $N = (N_1, N_2, \dots, N_7)$. Define (f', N') to be the state after the collision. Then, to ensure that the two-phase fluids satisfy the Navier-Stokes equations, we require conservation of particle number for each color and conservation of total momentum for each collision:

$$\begin{aligned}\sum_i N_i f_i &= \sum_i N'_i f'_i, \\ \sum_i N_i (1 - f_i) &= \sum_i N'_i (1 - f'_i),\end{aligned}$$

and

$$\sum_i N_i \vec{e}_i = \sum_i N'_i \vec{e}_i. \quad (1)$$

Colored holes are created and destroyed as follows: when a particle changes direction due to a collision, a hole of the same color is created, moving in the original direction. A particle annihilates any hole if one exists in its new direction. One consequence of this rule is that information describing the local particle color flux is carried by hole and transmitted by the streaming process through a distance of the order of a mean free path. To obtain an interface surface tension, the color flux must have a preferred direction (and consequently semi-detailed balance is violated) with the colored particles moving along the opposite direction of local colored hole flux. We define the local hole flux and particle color flux using:

$$\begin{aligned}\vec{G} &= \sum_i (2f_i - 1) N_i \vec{e}_i, \\ \vec{F} &= \sum_i (2f_i - 1) (1 - N_i) \vec{e}_i.\end{aligned} \quad (2)$$

Note that in the Somers and Rem model, the total color flux was used for $\vec{F}$. Our new rules for particle collisions are as follows:

(i) Choose the output state to maximize the quantity: $Q = -\vec{F} \cdot \vec{G}'$, where F is calculated from the given input hole state before collisions and G' is calculated for the output particle state. This rule ensures that colored particles move in the opposite direction to their local color gradient.

(ii) If there are several configurations which have the same maximum value of Q , we choose the output having the minimum $|G'|$. This step directs the colored particles as close as possible to the direction opposite to the local color flux.

In Fig. 3, we show a typical site configuration. The collision rule will pick the configuration (b) as the output. One can see that this rule enhances the particle flux in the direction opposite to the local hole color flux. This step also enhances the isotropy of the surface tension[12].

(iii) If there are still several equivalent configurations, then we chose the output state with a rest particle. This reduces the fluid motion and enhances phase separation. This step violates the semi-detailed balance[5], which is required in order to have a Fermi-Dirac equilibrium distribution. This step increases surface tension and reduces the degeneracy for the output state.

(iv) If several configurations satisfy the above restrictions, then choose the output which minimizes the viscosity. This step requires that the output state be different from input state.

Following these rules for our present lattice gas model, we still have a choice of 6 possible output states for a few of the input states. We pick among the remaining states at random.

This simple lattice gas model produces a surface tension described by: $\Delta P = \frac{\epsilon}{R}$, where ΔP is the pressure difference between the pressure inside a drop and the pressure outside the drop. In Fig. 4a, we present our measurements of pressure drop cross a circular interface; In Fig. 4b, we show the tension σ as a function of the radius of the drops, R , for densities 0.4. We see that the surface tension does not depend on the radius of the drops.

Similar hole emission models can be used at walls to generate an attractive force between a fluid and a wall, simulating wettability. If a particle collides with a solid wall, it simply reverses its velocity and changes color. A zero-velocity condition is then produced at the wall. If a hole collides with a wall, it also reverses velocity but it then has a probability, P_r , of having red color.

The mechanism for walls to attract the color particles is similar, in spirit, to the attractive force between the same color particles described above. Here the probability, P_r , determines the intensity of the attraction between the wall and red particles.

Fig. 5 presents a computer measurement of the contact angle of the red particle versus probability, P_r , for an ideal solid wall. The measurements are obtained by drawing a tangential line through the contact point. The data is obtained by averaging 12 realizations (with different initial conditions) after the systems equilibrate. We see that the contact angle can vary from 26° to 180° . It is important to be able to simulate a wide range of contact angles. We will use this capability to demonstrate

the dependence on wettability for flows through porous media.

4 The Connection Machine 2 and Lattice Gas Simulators

The simulations in this paper were performed on a Connection Machine-2 supercomputer. The CM-2 is a single-instruction, multiple-data (SIMD) system with up to 65,536 bit-serial processors. Thirty-two bit-serial processors are ganged together to form a "sprint node", named after the Sprint chip, which handles data manipulations on-node. In addition to the custom-designed chips, there is a commercial memory chip and (Weitek) floating-point accelerator at each node. The bit-serial processors are all driven in lock-step by the front-end processor, which provides a familiar C or Fortran computing environment—usually a SunOS or Ultrix operating system. The CM-2 has its own framebuffers, providing high-speed visualization of simulation results.

We have chosen to perform single-phase and two-phase lattice gas calculations using table lookup rather than logical operations. While single-phase collisions might be implemented to run slightly faster with logical operations, we prefer using table lookup to simplify the code. For two-phase collision rules, it is clear that table lookup is most efficient. Table lookup, the bottleneck of the calculation, is performed in hardware by the indirect-addressing capability of the Sprint chip. Although the distributed-memory architecture of Connection Machine systems requires storing many copies of the large lookup table (about 0.3 megabyte per copy), the amount of memory available per sprint node (4 MByte) made this memory overhead negligible. A fully configured CM-2 runs at about 800 million lookups per second. This is an optimal performance for lattice gas codes using table lookup for this architecture.

The collision table was precomputed. Collisions are subject to a variety of constraints (such as conservation of particle number for each color and total momentum) and criteria (such as the maximization of surface tension and the minimization of viscosity as discussed in section 3). Despite these considerations, a number of ambiguities exist among output states and we must pick from among the alternative output states uniformly so that artifacts are not introduced into the simulation. For the collision-saturated single-phase model, output states are either nondegenerate or two-fold degenerate. We treated all cases as two-fold degenerate, where both output states could be identical. Similarly, we were able to reduce output states for the two-phase model to be nondegenerate or two-fold, three-fold, or six-fold degenerate. We implemented table lookup treating all cases to be six-fold degenerate.

For the single-phase model, at each lattice site we assign eight bits to describe the local particle state. Six bits describe the moving particles; one bit describes the rest particle; and one bit determines the existence or nonexistence of a wall. For the two-phase model, fourteen bits are used for particle and hole states with colors; and two bits describe the wall state. For one of the wall bits, unity represents the existence of the wall and zero indicates a normal flow field. The other wall bit supplies the wall color information. At the wall, nonslip velocity boundary conditions were chosen for

both single-phase and two-phase simulations. For the two-phase model, there are two possible outcomes for colored holes for each input state. One outcome corresponds to maximal "red" wettability, the other to maximal "blue" wettability. These two output states may be identical for some input states. The wettability of the wall site is controlled by biasing the choice between these two output states determined by the probability, P_r .

A performance rate of roughly 700 million site updates per second on a 65,536-processor CM-2 for large lattices was obtained.

We also optimized forcing for the SIMD architecture. For example, forcing flow by applying a pressure differential across a system can be costly since it requires boundary operations during which most of the processors, those in the interior of the lattice, are idle. Such pressure differentials are maintained by a high- and a low-pressure reservoir, one at each end of the system. Generating site states at a specified pressure is an expensive operation, involving random-number generation and nontrivial bit manipulations. Thus, we generate large caches of fluid using all machine processors. Then, these caches are streamed over the pressure reservoirs from time to time to replenish the reservoirs. Low processor utilization is limited to this relatively inexpensive replenishing step.

The code was written in Connection Machine Fortran, which is roughly equivalent to the evolving Fortran 90 standard. Most of the low-level routines are currently written with Parallel Instruction Set (Pis) commands.

5 Some Simulation Results for Two-Phase Fluids

5.1 Spinodal Decomposition and Correlation Function

One interesting problem in the study of two-phase dynamics is the ordering process involving two mixed phases. Spinodal decomposition is an important example, which exhibits dynamic scaling for the particle density correlation function. Because the current lattice gas model correctly describes the short-range particle-particle interaction potentials, it is expected that the model should give a good approximation to reality for domain growth and for scaling.

In Fig. 6, we show a sequence of framebuffer displays for two-phase separation. The system has 512×512 lattice sites with periodic boundary conditions. The initial particle and hole color configuration is randomly distributed. The density, d , is 0.3 particles per direction. There are an equal number of red particles and blue particles. A short-range attraction exists between identical color particles. A small droplet of like particles grows and spinodal decomposition occurs.

There is an important difference between our model and the model of Rothman and Keller, where the self-diffusivity, κ , has a transition in $\kappa - d$ space. For d less than 0.2, the model of Rothman and Keller has a normal positive diffusion. Our model has negative self-diffusivity for all densities[12], even for very low density, such as $d = 0.02$.

To study the domain growth, we examine the pairwise red particle particle corre-

lation function defined as follows:

$$g^r(\mathbf{x}, t) = \frac{1}{N^2} \sum_{\mathbf{x}'} \langle (n_r(\mathbf{x}' + \mathbf{x}, t) - \langle n_r(\mathbf{x}' + \mathbf{x}, t) \rangle)(n_r(\mathbf{x}', t) - \langle n_r(\mathbf{x}', t) \rangle) \rangle, \quad (3)$$

where $\mathbf{x}$ is a lattice vector, and $\langle \cdot \rangle$ is the ensemble average. The sum is over all lattice sites $\mathbf{x}'$. Assuming homogeneity, the correlation function should only depend on $r = |\mathbf{x}|$, the radial distance. We define the radial correlation function

$$g^r(r, t) = \frac{1}{N_r} \sum_{|\mathbf{x}|=r} g^r(\mathbf{x}, t),$$

where N_r = the number of lattice vectors of length $|\mathbf{x}|$.

The simulation for measuring this correlation function was done in a lattice gas system with 1024×1024 lattice sites and averaged over all space (using a spatial average to replace the ensemble average). The evolution of correlation function for times = 10,000, 20,000 and 30,000 is shown in Fig. 7. $L(t)$ in the plot is the first zero-crossing of $g(r, \tau)$. The interesting feature is that the correlation functions (after being scaled by the characteristic space length) can be described by a single curve, as predicted by the scaling law for domain growth. We will discuss this problem more detail in [12].

5.2 Surface dynamics: Rayleigh-Taylor Instability

To simulate surface dynamics for different densities in a gravitational field, we introduce the forcing for our two-phase lattice gas model. Two-phase forcing schemes are similar to forcing schemes used in one-phase fluids[4].

For the present model, pressure is linearly proportional to the local density and surface tension only can balance a small pressure difference. The density difference between two fluids at equilibrium must be small. To study the interface between light and heavy fluids, we use different forcing rate for each fluid. For the present simulation, we only allow the forcing difference to be small, approximately 0.0048 each time step per site.

In Fig. 8, we present a simulation of the two-dimensional Rayleigh-Taylor instability. The gravitational forcing is from right to left. The dark black fluid is denser than the fluid in white. As time evolves, an instability occurs and fingering emerges. This qualitatively agrees with observations[13] and other numerical simulations[14]. For these instability simulations, no perturbation is initialized. The kinetic fluctuations are sufficient to move the system away from its neutral equilibrium state.

5.3 Two-Phase Fluid Flows Through Porous Media

In this section, we briefly discuss the application of our lattice gas model to flows through porous media. The main result illustrates how the wettability of model affects the saturation of the fluids in the porous media. Saturation is a measure of the amount of one phase trapped in the pore structure after a purging flow of the other phase. The pore geometry used in this simulation is an experimental pore structure scanned from photograph of a thin slice of sandstone. Images of these etched glass micro-models were digitized and used in the simulations[4].

For reservoir simulations, a pressure difference is required. As discussed in Section 4 and elsewhere [4], two reservoirs can be used to generate the pressure difference. Because of surface tension between two fluids and the wettability of the sandstone, the flow rate depends quite strongly upon the wettability of the pushing fluid. We use Fig. 9(a) as our initial condition, where black color represents the wetting fluid, gray color represents for nonwetting fluid and white color represents sandstone. As time evolves, upstream snap-off of the nonwetting phase is observed. This qualitatively agrees with video recordings of the microscopic experiments[15].

The saturation of the wetting fluids and relative permeability of the system very strongly depend on the wettability of the fluids. This wettability can be varied over a wide range using our model. In Fig. 10, we show the effect of the wettability on the saturation of the wetting fluids. In Fig. 10a, the wetting fluids has reached saturation for the given wettability ($P_b = 1$). Fig. 10b is the phase distribution for later time (after another 800,000 time steps) after the wettability is changed to $P_b = 0.3$. One can see that the saturation ratio has totally changed.

6 Discussions and Conclusions

In this paper, we have discussed lattice gas models for one-phase and two-phase fluid flows and their simulation results using the Connection Machine-2. Because of the parallelism of the lattice gas model, it is possible to do rapid computation and to utilize efficiently the computer memory.

A simulation of the single-phase Kelvin-Helmholtz instability has illustrated typical vortex pairing process, as observed in other numerical simulations. This single-phase large system simulation demonstrates the lattice gas capability to simulate high Reynolds numbers on the Connection Machine-2. The simulation results for two-phase fluids confirm the existence of the surface tension between two fluids and wettability between fluids and solids. The surface dynamics in Rayleigh-Taylor instability problem demonstrates the usefulness of the model for front tracking of the two-phase interface. The model described can be generalized to simulate the wettability of oil and brine. It is possible that two-phase flow through porous micro-models will have important applications in enhanced oil recovery problems.

Our current CM-2 will allow systems as large as $2^{13} \times 2^{13}$ to be run. Reynolds numbers up to 30,000 can be simulated. This is adequate to study several two-dimensional turbulent problems and many instability problems, including the transition to turbulence for flows between two parallel plates.

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8 Figure Captions

- Fig. 1** Velocity distribution for the Kelvin-Helmholtz instability at time = 0, 15,000, 20,000, 55,000 and 490,000.
- Fig. 2** Vorticity distribution for the Kelvin-Helmholtz instability at time = 0, 15,000, 20,000, 55,000 and 490,000. One can see the pairing process for like vortices.
- Fig. 3** A typical site configuration: (a) is the input state; (b) and (c) are two possible output states which satisfy (i). Here $\vec{F}_a = (0, 1)$, $\vec{G}_b = (2, -1)$ and $\vec{G}_c = (0, -1)$. The rule (ii) only allows (b) as the output state.
- Fig. 4** (a) A typical pressure distribution as a function of distance, R , from the center of the bubble (in lattice units). (b) Surface tension versus reciprocal of the drop radius. This plot demonstrates that the surface tension is relatively independent of the radius in this model.
- Fig. 5** Contact angle as a function of probability P_r . The error bars represent one standard deviation.
- Fig. 6** A typical spinodal decomposition process caused by surface tension. The initial configuration is a random mixture, with equal densities of 0.3, at time = 1, 300, 1,400, and 3,400.
- Fig. 7** Density fluctuation correlation function as a function of distance. $L(t)$ is the first zero crossing for the correlation function at time, t . $\circ$ is for time = 10000, $\circ$ is for time = 20,000 and $\times$ is for time = 30,000.
- Fig. 8** Typical configurations for the two-dimensional Rayleigh-Taylor instability with a denser fluid (dark black) above a less dense fluid (white) under the influence of gravity. The gray represents sites with zero particle occupation. Times shown are in lattice units.
- Fig. 9** Typical patterns for flow through porous media at time = 0, 70,000, 140,000, and 340,000. Note that drops of nonwetting fluid become trapped in the pores. The pressure drop from left to right is 0.15 in lattice units.
- Fig. 10** The wetting fluid (black) saturation distribution: (a) strong wettability with $P_b = 1$; (b) weak wettability with $P_b = 0.3$ at 800,000 time steps later.

Fig. 1

Fig. 2

Fig. 3

Fig. 6

Fig. 7

$t = 0$

$t = 500$

$t = 1000$

$t = 1500$

$t = 2000$

$t = 2500$

$t = 3000$

Fig. 8

Fig. 9

Fig. 10