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A Microcanonical Model for Interface Formation

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We describe a new cellular automaton model which allows us to simulate separation of phases. The model is an extension of existing cellular automata for the Ising model, such as Q2R. It conserves particle number and presents the qualitative features of spinodal decomposition. The dynamics is deterministic and does not require random number generators. The spins exchange energy with small local reservoirs or "demons." The rate of relaxation to equilibrium is investigated, and the results are compared to the Lifshitz–Slyozov theory.

KEY WORDS: Cellular automata; Ising model; phase separation; spinodal decomposition; Monte Carlo algorithm.

The problems posed by the dynamics of phase separation are manifold and complex.[1] The statistical mechanics of spinodal decomposition is involved at the microscopic level, whereas the larger scales exhibit nontrivial hydrodynamics. The latter involves the motion of interfaces, one of the most complicated problems of fluid mechanics. Thus, phase separation in fluids is interesting at both the microscopic and macroscopic scales. A simple model for the computational study of such phenomena would be of great interest and in this paper we attempt a cellular automaton (CA) approach. Recently the hope has been expressed that CA models would help to investigate many problems of physics and represent the phenomena over a wide range of scales.[2,3]

CA models are entirely deterministic and discrete. They have simple dynamics, which involve only a finite number of states per site and only nearest neighbor interactions. For problems of statistical physics of near-equilibrium states, they are a potent competitor to Monte Carlo

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simulations: the dynamics they simulate appear in a way to be more realistic. The CA models used so far for the simulation of phase transitions conserve an interaction energy during the evolution and have been called microcanonical models. Because of the energy conservation, heat transport and diffusion are observed.[4,5]

Cellular automaton rules have been proposed for the simulation of the Ising model,[5,6] and there are also interesting rules for hydrodynamics, as shown by Ref. 7. Some models that separate phases and have hydrodynamic behavior have recently been proposed. Ideally, a realistic model should be able to conserve energy, momentum, and particle number. Conservation of energy is necessary for the construction of a state of thermodynamic equilibrium. Conservation of momentum is required for hydrodynamic behavior, and conservation of particle number will prevent such unrealistic effects as the disappearance of small clusters. No known model has been simulated that obeys all these conservation laws and has a realistic behavior.[3] Obviously a model conserving all of the relevant quantities would be required for problems involving the interplay of spinodal decomposition and hydrodynamic behavior such as the late stages of the decomposition.[10] Partial success has been obtained recently by Rothman and Keller[11] with a rule that conserves particle number and momentum but not energy. Here we report some investigations on rules that conserve particle number and energy but not momentum. The idea of the model is not new: it can be seen as a microcanonical implementation of the model of Kawasaki.[9]

The model consists of spins σ_i that live on the nodes of a square lattice of size $N \times N$, and of auxiliary variables $n_{\langle ij \rangle}$, called "demon numbers" corresponding to the local reservoirs of energy.[5] The variable i ranges over all the sites on the lattice, and $\langle ij \rangle$ ranges over all nearest neighbor pairs. In our simulations periodic boundary conditions were used. The demons live on the links of the lattice, and the maximum demon number allowed on each link is n_D. The demon numbers correspond to units of energy stored by demons residing on each link. The spins may take two values, $\sigma_i = +1$ or $\sigma_i = -1$, and may alternately be described as "red particles" and "blue particles." The interaction energy of the spin configuration is

$$H_I = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \tag{1}$$

To update a configuration we consider all the nearest neighbor pairs of nodes of the lattice in a sequence defined below. For each pair $\langle ij \rangle$ we

[3] A simple momentum-conserving extension of this model on a square lattice has been studied by Rucklidge.[8]

attempt to exchange the spins between the two nodes; this may or may not change the total interaction energy. Let $\Delta H_{\langle ij\rangle}$ be the decrease in energy associated with the swap. If the energy is unchanged, the spins are swapped, otherwise one tries to extract or deposit the energy $\Delta H_{\langle ij\rangle}$ in the local reservoir. It is easy to see that $\Delta H_{\langle ij\rangle}$ must be a multiple of $4J$. Correspondingly, the demon number indicates how much energy is stored in the reservoir prior to the exchange, in units of $4J$. The swap is performed if

$$4Jn_D \geqslant 4Jn_{\langle ij\rangle} - \Delta H_{\langle ij\rangle} \geqslant 0 \tag{2}$$

After the swap the demon number is decreased by $\Delta H_{\langle ij\rangle}/4J$. The total energy of the lattice is hence

$$H = H_I + H_D \tag{3}$$

where

$$H_D = 4J \sum_{\langle ij\rangle} n_{\langle ij\rangle} \tag{4}$$

One notices that the change in energy can be determined from the value of σ_i at the two nodes and at six other neighboring nodes, as shown in Fig. 1.

The sequence in which pairs are investigated is determined in the following way. The lattice is partitioned into 18 sublattices, which are ordered sequentially. A particular sequence is exhibited in Fig. 2. Each of the pairs bearing the same label forms a periodic sublattice of the entire array. These pairs can always be updated in parallel since the exchange

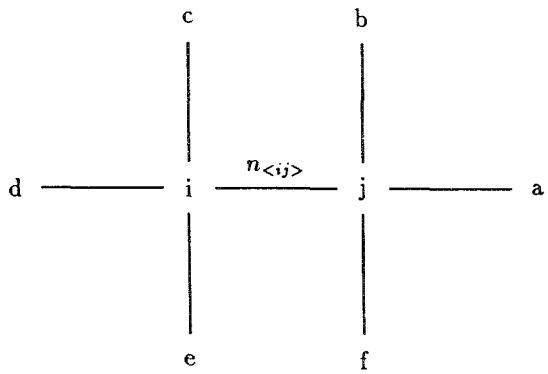


Fig. 1. A link of the lattice and its neighborhood. Information on the states of nodes a–f is required to process the link.

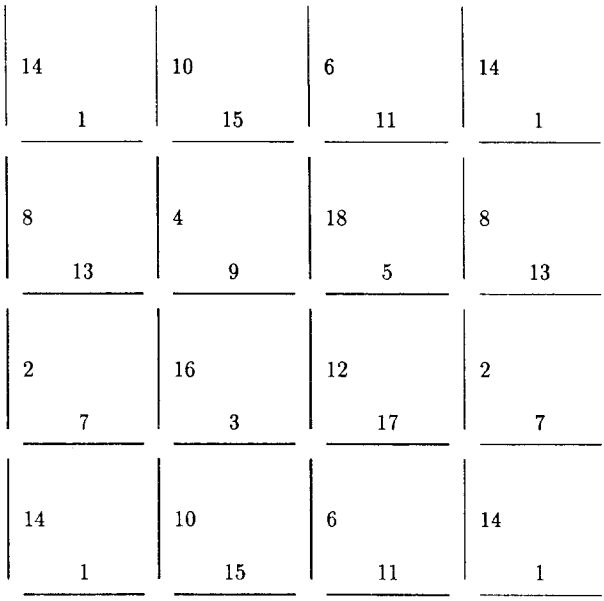


Fig. 2. The 18 sublattices that are used in the updating of the entire lattice. All links with the same number are updated simultaneously in the order of the number.

of their spins does not affect the outcome for any other pair of spins belonging to the same sublattice.

In the course of evolution the temperature T of the distribution can be estimated from the assumption that the demons are distributed according to a Gibbs distribution

$$P(4Jn_{\langle ij\rangle} = E) = \frac{\exp(-E/T)}{Z_D} \tag{5}$$

where

$$Z_D = \sum_{n=0}^{n=n_D} \exp(-4nJ/T) \tag{6}$$

The maximum demon number was 3 in all the simulations reported here, corresponding to an energy change of $12J$.

The actual computations were made using multispin coding: several spin variables were packed into each machine word, and the evolution rule was translated into a sequence of Boolean operations on the words. All our computations were done on Sun 3 type computers, resulting in a speed of

about 10,000 sites updated per second. The demons themselves were allowed to diffuse around the lattice, using a rule for the diffusion of noninteracting particles proposed in Ref. 3. This meant that neighboring reservoirs were allowed to exchange energy at random times. Instead of using random number generators to decide whether to exchange two reservoirs, a CA random bit plane was used.[3]

Simulations were performed with initial conditions consisting of uniformly distributed red and blue particles with a density of $\rho = 0.5$ red particles per site. The spins separated into a pattern of magnetic domains. The separation was quick at first then slowed down as the homogeneous regions grew. Figure 3 presents such a simulation on a 90×90 lattice.

We also made a simulation of a slightly different, next nearest neighbor model. In this model all nearest and next nearest neighbors interact with equal coupling: the interaction energy H_I in Eq. (1) is defined by a sum over all pairs $\langle ij \rangle$ of nearest and next nearest neighbor pairs. In the exchange operation, the interactions with spins c, b, e, and f on Fig. 1 all cancel, while four new spins become relevant. No significant difference from the results with the Ising model (1) was found except that the interfaces appear smoother.

A measure of the speed at which the mixture separated is offered by the measurement of the energy H_I as a function of time. The energy $H_I(t)$ has been fitted to a law of the form

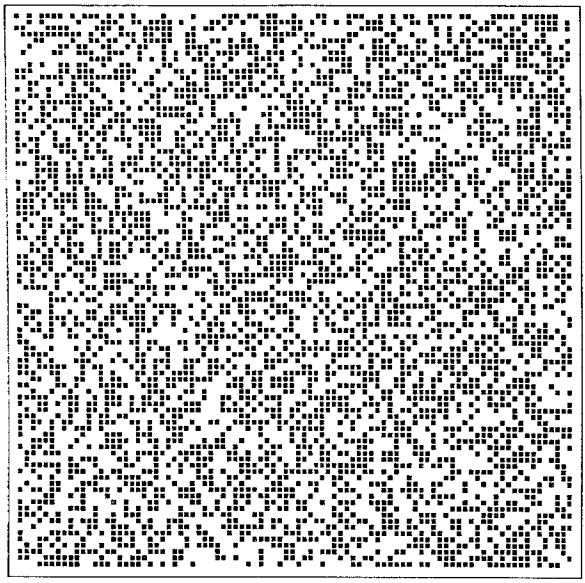
$$H_I(t) = H^{\text{eq}} + Ct^{-a} \tag{7}$$

Thirty simulations of a 90×90 lattice were made, all with a temperature reaching 2.2 at the largest time. For each realization, the constants a, C, and H_I^{eq} were obtained by a least square fit of $H_I(t)$ for $10^2 < t < 10^4$. See, for instance, Fig. 4, where the quantity $H_I(0.5t) - H_I(t) \sim t^{-a}$ is plotted for one realization. The results were averaged over the 30 realizations, yielding

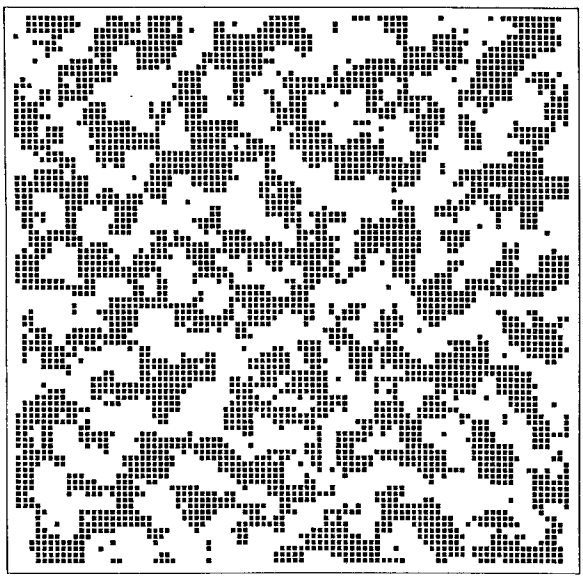
$$a = 0.292 \pm 0.05 \tag{8}$$

where the error is set to two standard deviations. The late stage decay is probably related to the slow growth of the clusters[12]: according to the Lifshitz–Slyozov theory,[12] the size of the clusters grows like $R(t) \sim t^{1/3}$. A simple dimensional argument shows that for monodisperse clusters the length of the interface is proportional to N^2/R. This yields $a = 1/3$. However, an additional complication is that the temperature estimated from the demon number distribution varies in time as the system relaxes slowly. This might complicate the comparison with other Monte Carlo simulations, such as those reported in Ref. 1.

The particular role played by the demons is an important feature dis-

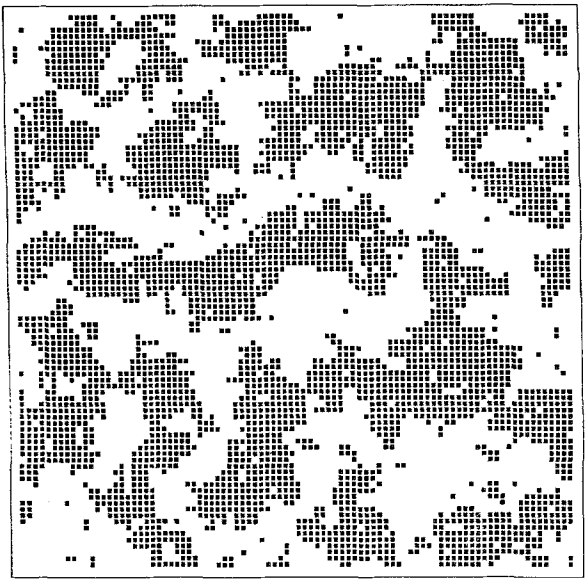


(a)

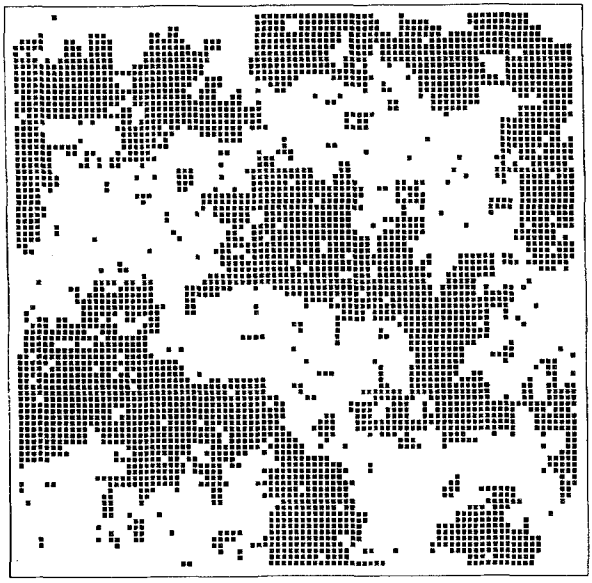


(b)

Fig. 3. A series of snapshots at various times, starting from a random initial configuration. The final temperature was 2.16. (a) $t = 0$, (b) $t = 100$, (c) $t = 1000$, (d) $t = 10000$.



(c)



(d)

Fig. 3 (*continued*)

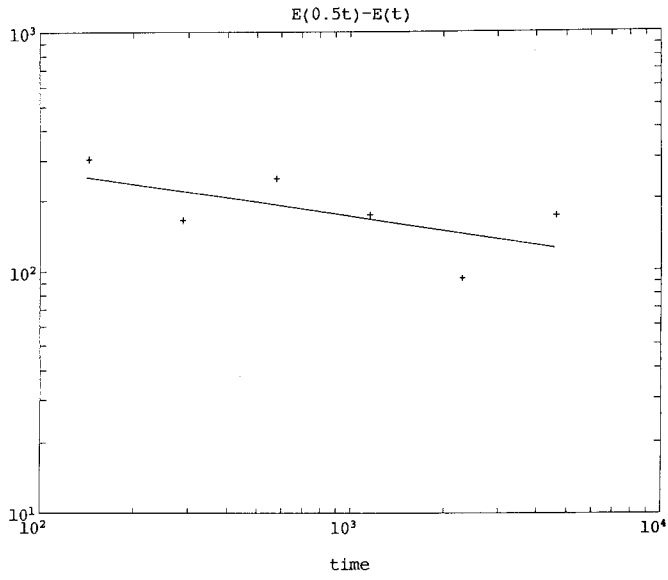


Fig. 4. The decay of the quantity $H_f(0.5t) - H_f(t)$ for one realization.

tinguishing the Q2R model from the various models of Creutz.[5,6] The lack of demon may be responsible for some unusual kinetics in Q2R.[13] Preliminary investigation showed that demons play an important role in this model as well. For instance, if demons are fixed in place instead of diffusing, the relaxation to equilibrium appears much slower.

To conclude, it seems that microcanonical models offer an interesting dynamical modeling of spinodal decomposition. Separation can be achieved using a purely entropically driven motion. A difficulty, however, is that the relaxation is slow and requires thousands of iterations. However, there is no conservation of momentum in our model and this slows down the final stage of separation compared to real fluids. The addition of momentum to a model of this kind would certainly provide a much more realistic model of binary fluid mixtures. Whether it would be practical for simulation probably depends on a fast machine implementation of the kind already existing for simpler cellular automata.[3,7]

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