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LETTER TO THE EDITOR

Pattern formation in reversible cellular automata

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Abstract. We analyse the dynamics of pattern formation in two examples of reversible cellular automata which have been argued to belong to the critical dynamics universality class of the kinetic Ising model. The results obtained suggest that their dynamical evolution is different from the analogous kinetic Ising model.

Cellular automata have been introduced as simple mathematical models capable of generating very complex behaviour. They consist of a set of identical units—described by a discrete variable—that interact locally through prescribed rules (von Neumann 1966; for recent reviews see Wolfram (1983, 1984a)), where space and time are discretised. They have been introduced as models for many different processes, ranging from physics to biology and computer science. Starting from random initial states, the rules (which can be either stochastic or deterministic) iterate into stationary patterns that fall into four broad categories (Wolfram 1984a): the evolution leads to (i) a final homogeneous state, (ii) a set of separated simple states or periodic structures, (iii) a chaotic pattern and (iv) complex localised structures. Extremely simple rules can thus lead to self-organisation in the system, displaying qualitatively different behaviour for different choices of the rule.

One-dimensional cellular automata have been extensively analysed (see, for instance, Wolfram 1984b), but less attention has been paid to the higher-dimensional counterparts. Such a study is significant for comparisons with many experimental results on pattern formation in physical systems (Packard and Wolfram 1985). In addition, it seems interesting to us to analyse how cellular automata develop spatial structure as opposed to the more conventional analysis of the structure of the stationary patterns given by a certain rule. The time development of such spatial structure could also be of interest to experimentalists.

In fact, similar problems have arisen in connection with the dynamical evolution of kinetic models defined by conventional master equations on a lattice (Wu 1982). Such models were originally introduced to analyse spin systems (e.g. kinetic Ising models) and their cooperative phenomena in thermal equilibrium. Of particular interest to us is their application to the problem of pattern formation during a first-order phase transition (Gunton *et al* 1983, Binder 1985, San Miguel 1985). Although these models also discretise space and time and are formulated in terms of local rules, the constraint that the system must eventually reach thermal equilibrium for any given initial state leads to the restriction that the change in the local variables has to be in accordance with the Boltzmann weight (Glauber 1963, Kawasaki 1972).

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Consequently, the fundamental difference between kinetic Ising models and cellular automata is the existence or not of invariance under time reversal or, equivalently, the existence of an underlying microscopic Hamiltonian dynamics. Secondly, although it is not strictly essential, cellular automata are synchronous, i.e. all the variables defining a given state are updated simultaneously whereas spins in a kinetic Ising model are updated sequentially (usually in a random sequence through the lattice). Although the significance of this distinction will be made more quantitative below, synchronous updating in cellular automata raises some interesting questions concerning the determination of the underlying Hamiltonian or the very ergodic behaviour of reversible rules (see, e.g., Vichniac (1984); Pomeau (1984) actually discusses the definition of invariants for reversible rules and, in particular, he studies one of the rules considered below; Grinstein *et al* (1985) derived the more general reversible rule that would admit an underlying Hamiltonian, a rule that will also be analysed below).

We analyse in this letter the dynamics of pattern formation in different examples of a subclass of reversible cellular automata that seem to have the same critical behaviour as the Ising model. In particular, we are interested in to what extent they also belong to the same dynamical universality class away from the critical point. More precisely, we calculate the rate at which domains of one of the degenerate stationary states of the model grow from an originally completely random state and compare our results to the standard kinetic Ising model in a similar context.

We consider a two-dimensional cellular automaton on a square lattice with N sites, each occupied by an Ising spin $s_i = \pm 1$. If $P(\{s_i\}, t)$ is the probability of a given configuration at step ('time') t, the rule which defines the cellular automaton can be written as a discrete master equation:

$$P(\{s_i'\}, t+1) = \sum_{\{s_i\}} Q(\{s_i'\}|\{s_i\}) P(\{s_i\}, t) \tag{1}$$

where $Q(\{s_i'\}|\{s_i\})$ is the conditional probability of finding the cellular automaton in state $\{s_i'\}$ at $t+1$ given that it was in state $\{s_i\}$ at t. The conditional probability is normally chosen to be of the form

$$Q(\{s_i'\}, \{s_i\}) = \prod_i Q(s_i'|s_i, \{s_{i'}\}) \tag{2}$$

where $Q(s_i'|s_i, \{s_{i'}\})$ is again a conditional probability in the same sense as before. The product is taken over all individual spins and we have made explicit the dependence on the neighbourhood of spin s_i: $\{s_{i'}\}$.

Detailed balance requires the existence of a Hamiltonian $H(\{s_i\})$ such that

$$\prod_i \frac{Q(s_i'|s_i, \{s_{i'}\})}{Q(s_i|s_i', \{s_{i'}'\})} = \exp[-(H(\{s_i'\}) - H(\{s_i\}))] \tag{3}$$

for any given pair of states.

In the cases where we refer to the Ising model, the Hamiltonian considered is

$$H(\{s_i\}) = \tfrac{1}{2} K \sum_{i \neq j} s_i s_j \tag{4}$$

where the sum is restricted to the four nearest neighbours in the square lattice. Let us now briefly present the three models used in our study.

In the first place, we will include the results corresponding to the standard kinetic Ising model whose Hamiltonian is given by (4). We note that the algorithm which is

actually used in a Monte Carlo simulation can be written as follows:

$$P(\{s_i'\}, t+1) = \sum_{\{s_i\}} \prod_i{}' Q(s_i'|s_i, \{s_{i'}\}) P(\{s_i\}, t+(i-1)/N) \tag{5}$$

where the unit of time is one Monte Carlo step (N attempts to update a spin). The prime in the product means that the spins are updated sequentially in some prescribed order. We will consider the common procedure of selecting the spins to be updated at random. We want to emphasise that equation (5) has an additional time dependence on the right-hand side which is not in the general equation (1). Consequently, in a practical sense, the algorithm used is defining the master equation that is being simulated (further details on this issue can be found in Choi and Huberman (1984), Gawlinski *et al* (1985) and Ceccatto (1986)). Notice, however, that different updating procedures can generate very different dynamical behaviour although they will all eventually lead to the same final canonical distribution, if detailed balance is satisfied. The origin of such a difference is the existence of additional correlations that can be introduced by the updating procedure.

On the other hand, conventional cellular automata are synchronous. The first example of cellular automata which we wish to investigate has been introduced by Domany and others (Domany (1984), Vichniac (1984); the problem of the determination of the invariants associated with this rule has been discussed by Pomeau (1984)), who consider an Ising model of the type given by equation (4). In order to both update spins simultaneously and also preserve detailed balance for the specified Hamiltonian, the lattice is divided into two sublattices in such a way that the spins belonging to each sublattice do not interact among themselves. Under that condition, all the spins belonging to the same sublattice are updated simultaneously, with the various sublattices being updated in a sequential manner. In our particular case we divide the square lattice into two interpenetrating square sublattices α and β. Given the nearest-neighbour Hamiltonian (4), each spin in the sublattice α only interacts with spins in the sublattice β and vice versa. The master equation which is being simulated can be written as

$$P(\{s_i'\}, t+1) = \sum_{\{s_i\}} \left(\prod_{i\in\alpha} Q(s_i'|s_i, \{s_{i'}\}) P(\{s_i\}, t) \right.$$
$$\left. \times \prod_{i\in\beta} Q(s_i'|s_i, \{s_{i'}\}) P(\{s_i\}, t+\tfrac{1}{2}) \right). \tag{6}$$

Note that with this definition of the updating rule, detailed balance is trivially satisfied. A closely related model (defined on a different lattice) has been analysed by Domany and Gubernatis (1985) in order to obtain the dynamical critical exponent. It is then implicitly assumed that the model defined by such a master equation will have the same critical behaviour as the conventional Ising model defined by equations (4) and (1) or (5).

The third model we wish to investigate is related to the work of Grinstein *et al* (1985) which deals with the critical behaviour of probabilistic cellular automata (both reversible and irreversible). They derive the most general form of a transition probability that satisfies the requirements of detailed balance and simultaneity in updating the spins. The only restrictions on the rule are its totalistic character, i.e.

$$Q(s_i'|s_i, \{s_{i'}\}) = Q\left(s_i'|s_i, \sum_{i'} s_{i'}\right)$$

where $(1/z)\,\Sigma_{i'}\, s_{i'}$ is the average magnetisation of the neighbourhood i, where z is the number of neighbours considered, and one has the up-down symmetry

$$Q\left(s_{i'}|s_i, \sum_{i'} s_{i'}\right) = Q\left(-s_{i'}|-s_i, -\sum_{i'} s_{i'}\right).$$

This general form can be written as

$$Q\left(s_i'|s_i, \sum_{i'} s_{i'}\right) = \frac{1}{2}\left[1 + s_i s_i' \tanh\left(a + bs_i \sum_{i'} s_{i'}\right)\right] \tag{7}$$

where a and b are arbitrary constants. Given the symmetries in the problem and the normalisation of Q, a rule is completely specified by

$$f(M) \equiv Q(-1|1, M) = \tfrac{1}{2}[1 - \tanh(a + bM)] \tag{8}$$

where $M = \Sigma_{i'}\, s_{i'}$. Note that in spite of the fact that the rule is quite similar to the Glauber choice for the transition probability in the spin-flip Ising model, the underlying Hamiltonian for the rule defined by equations (1), (2) and (7) involves first-, second- and third-neighbour interactions whose strength is, in general, a complicated function of a and b.

In the three cases which we have studied the simulation procedure has been identical. We start from an initial random state and consider the evolution of the cellular automaton in the region of its parameter space in which the final stationary states are homogeneous. In the case of the Ising model (defined by (4) and (5)) and for the model defined in (6), the system evolves at $K^{-1} = 0.2$ (where $K = J/k_B T$ in the standard Ising notation). The choice of the suitable parameters in the third model (equation (8)) has been made in the following way. Starting from the master equation (1), a recursive relation for the average magnetisation $\langle s\rangle(t)$ can be written in the mean-field limit (Grinstein *et al* 1985) as

$$\langle s\rangle(t+1) = \langle s\rangle(t) - 2[f_o(\langle s\rangle(t)) + \langle s(t)\rangle f_e(\langle s\rangle(t))] \tag{9}$$

where f_o and f_e are the odd and even parts of $f(M)$ as defined in (8). By choosing $a = 0$, the recursion relation reduces to

$$\langle s\rangle(t+1) = \tanh(b\langle s\rangle(t)) \tag{10}$$

and has two fixed points: $\langle s\rangle^* = 0$ *for* $b > 0$ (a 'paramagnetic' state) and $\langle s\rangle^* \neq 0$ for $b < 0$ (a 'ferromagnetic' state). Consequently, we start with a random initial configuration and use a rule with $a = 0$, $b < 0$. We note that this general model equation (7) has also been argued to belong to the Ising universality class at the critical point.

Consequently, in all three cases we have studied the evolution of the state of the system from a random state towards any of its competing degenerate stationary states. The details of the simulation are as follows. We use a square lattice of $N = 100^2$ spins with periodic boundary conditions. In the case of the kinetic Ising model, we choose Glauber's Q:

$$Q(-s_i|s_i, \{s_{i'}\}) = \tfrac{1}{2}(1 - \tanh \tfrac{1}{2}\Delta H) \tag{11}$$

where $\Delta H = H(-s_i, \{s_i\}) - H(s_i, \{s_i\})$ and $H(\{s_i\})$ is defined in (4). We used the standard master equation as defined in (5) where the spins which are to be updated are chosen at random. The evolution was followed for the first 100 MCS and the results were averaged over 100 independent runs. The same Hamiltonian has been used to study the second model, as defined in (6). We have analysed two different choices for

the transition probability: the first given by equation (11) and the second by the usual Metropolis algorithm:

$$W(-s_i|s_i, \{s_{i'}\}) = \min(1, \exp(-\tfrac{1}{2}\Delta H)) \tag{12}$$

(note that W is a transition rate and is not normalised). For both choices the process was monitored for 100 MCS (a Monte Carlo step is defined as above). The results have also been averaged over 100 independent runs. Finally, in the third model analysed (equations (7) and (8)) we have used

$$f(M) = \tfrac{1}{2}[1 - \tanh(bM)] \tag{13}$$

with $b = -10$. In this case the evolution has been analysed for 1000 MCS (where one MCS now corresponds to updating the whole lattice simultaneously) and the results have been averaged over 50 independent runs.

In order to characterise the development of spatial structure, we use as a characteristic length the amplitude of the Bragg peak ($\boldsymbol{k}_0$) of the structure factor (Sadiq and Binder 1984, Gawlinski *et al* 1985):

$$\bar{R}^2(t) = S(\boldsymbol{k}_0, t) = N\langle s^2\rangle(t). \tag{14}$$

In our first two models (equations (5) and (6)), a unique peak develops at $\boldsymbol{k}_0 = 0$. However, in the third model (equation (7)), two distinct peaks develop at $\boldsymbol{k}_1 = (0, 0)$ and $\boldsymbol{k}_2 = (\pi/a, \pi/a)$ and grow in time (the lattice constant a is taken equal to one). Consequently we have analysed in the third model the following three quantities:

$$\begin{aligned} \bar{R}_F^2 &= S(\boldsymbol{k} = (0, 0), t) \\ \bar{R}_A^2 &= S(\boldsymbol{k} = (\pi/a, \pi/a), t) \\ \bar{R}^2 &= \bar{R}_F^2 + \bar{R}_A^2. \end{aligned} \tag{15}$$

In the case of the ferromagnetic kinetic Ising model with non-conserved order parameter, theoretical studies (Allen and Cahn 1979, Kawasaki *et al* 1978, Ohta *et al* 1982, Mazenko and Valls 1983, Viñals *et al* 1985) and computer simulations (Gawlinski *et al* 1985) agree that the average size $\bar{R}(t)$ of the growing domains follows the Allen-Cahn growth law:

$$\bar{R}(t) \propto t^n \qquad n = \tfrac{1}{2}. \tag{16}$$

Universality classes are commonly defined in terms of the growth exponent n. We present in figures 1 and 2 the results we have obtained for the different cellular automata considered. We also include the results for the kinetic Ising model for comparison.

The results indicate that significant qualitative differences exist between the models studied despite the fact that they are claimed to have the same dynamical critical behaviour. In the case of the cellular automata defined by equation (6), the fact that one sublattice is always updated before the other introduces memory effects at the interfaces. With this rule, the spins belonging to the sublattice which is updated last will systematically experience a different local curvature since both neighbouring spins have always been updated first. (Note that in this model, where the order parameter is not conserved, the motion of the interfaces separating the different domains is driven by the local curvature.) This subtle effect is not noticeable (within the precision of our study) for the Galuber dynamics, equation (11). This fact can be interpreted as a consequence of the symmetry of the rule about $\Delta H = 0$ (the probability of flipping a spin with no cost in energy is 0.5). In this particular case we obtain the same exponent

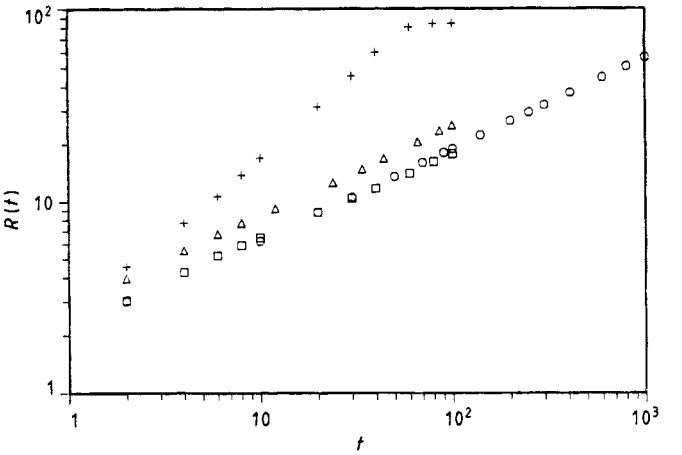

Figure 1. Average size of the domains $\bar{R}(t)$ as a function of discrete time for the different rules defined. □ represents the standard kinetic Ising model (equation (4)); △ and + correspond to the rule defined in equation (6) with transition probabilities given by (11) and (12) respectively and ○ is the total average domain size given by (7).

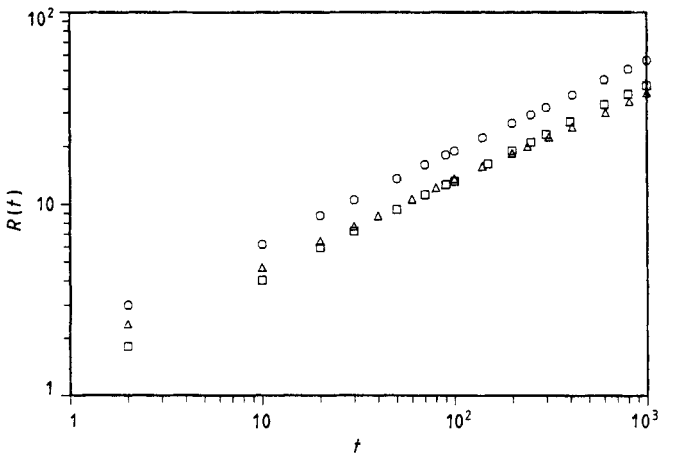

Figure 2. This figure represents the three measures of length defined in the text for the rule given in (7), where all the spins are updated simultaneously. □, △ and ○ correspond to $\bar{R}_F(t)$, $\bar{R}_A(t)$ and $\bar{R}(t)$ respectively.

$n = \frac{1}{2}$ as for the kinetic Ising model. On the other hand, the Metropolis algorithm breaks this symmetry (now the probability of flipping one spin when $\Delta H = 0$ is 1) and the growth clearly displays this memory effect. In fact, as seen in figure 1, the growth is faster than a power law.

The dynamics of the third rule (equation (7)), although we obtain the same growth exponent $n = \frac{1}{2}$ for the lengths defined, is considerably more complicated. In fact, although the mean-field ground state is ferromagnetic if b in equation (13) is less than zero, the rule favours local antiferromagnetic order. As a consequence, during the ordering process the system contains domains of four kinds: two ferromagnetic and two antiferromagnetic. The growth at interfaces is still driven by local curvature, which is consistent with the Allen-Cahn growth law that we observe for the three characteristic

lengths defined (figure 2 shows the results for these three lengths). Nevertheless, the ferromagnetic domains change sign at each step and flat interfaces between ferromagnetic and antiferromagnetic domains are stable. Thus, the behaviour of the system for later times could be more complicated.

To conclude, our results suggest that, although reversible cellular automata may belong to the same universality class as the Ising model at their respective critical points, the dynamics of pattern formation exhibits new features, all depending on the local action of the rule. In the first case (equation (6)), even with the same Hamiltonian, the particular transition probability in the cellular automata rule introduces different additional correlations at the interfaces which give rise to a different growth law. In the third model (equation (7)), the restriction that all the lattice must be updated simultaneously leads to a complicated Hamiltonian, producing a very different dynamical behaviour. Interestingly enough, the growth is still curvature driven and the classical Allen-Cahn result is still valid for early times.

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References

Allen S M and Cahn J W 1979 *Acta Metall.* **27** 1085
Binder K 1985 *Condensed Matter Research Using Neutrons, Today and Tomorrow* (New York: Plenum) p 1
Ceccatto H A 1986 *Phys. Rev.* B **33** 4734
Choi M Y and Huberman B A 1984 *Phys. Rev.* B **29** 2796
Domany E 1984 *Phys. Rev. Lett.* **52** 871
Domany E and Gubernatis J E 1985 *Phys. Rev.* B **32** 3354
Gawlinski E T, Grant M, Gunton J D and Kaski K 1985 *Phys. Rev.* B **31** 281
Glauber R J 1963 *J. Math. Phys.* **4** 294
Grinstein G, Jayaprakash C and He Y 1985 *Phys. Rev. Lett.* **55** 2527
Gunton J D, San Miguel M and Sahni P S 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (New York: Academic) p 267
Kawasaki K 1972 *Phase Transitions and Critical Phenomena* vol 2, ed C Domb and M S Green (New York: Academic) p 443
Kawasaki K, Yalabik M C and Gunton J D 1978 *Phys. Rev.* A **17** 455
Mazenko G F and Valls O T 1983 *Phys. Rev.* B **27** 6811
Ohta T, Jasnow D and Kawasaki K 1982 *Phys. Rev. Lett.* **49** 1223
Packard N H and Wolfram S 1985 *J. Stat. Phys.* **38** 901
Pomeau Y 1984 *J. Phys. A: Math. Gen.* **17** L415
Sadiq A and Binder K 1984 *J. Stat. Phys.* **35** 517
San Miguel M 1985 *Stochastic Processes Applied to Physics* ed L Pesquera and M A Rodriquez (Singapore: World Scientific)
Vichniac G Y 1984 *Physica* **10D** 96
Viñals J, Grant M, San Miguel M, Gunton J D and Gawlinski E T 1985 *Phys. Rev. Lett.* **54** 1264
von Neumann J 1966 *Theory of Self-Reproducing Automata* ed A W Burks (Urbana University of Illinois Press)
Wolfram S 1983 *Rev. Mod. Phys.* **55** 601
—— 1984a *Physica* **10D** 1
—— 1984b *Nature* **311** 419
Wu F Y 1982 *Rev. Mod. Phys.* **54** 235