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LETTER TO THE EDITOR

Fast simulation of the Ising model using cellular automata

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Abstract. A totalistic Ising cellular automaton (ICA) is proposed which can reproduce the thermodynamics of the Ising model. The automaton rules are preset in the usual way but some random mixing of these existing rules is subsequently permitted. The model employs a vectorized multispin coding algorithm to reach spin updating speeds comparable with the best Metropolis Monte Carlo performances and is characterized by a nonlinear dynamical critical exponent whose value seems less than two

Since the Ising model and its variants are used to describe many critical phenomena, it is a challenge to discover faster algorithms for its simulation. Deterministic cellular automata have been considered as suitable candidates because the fact that no random numbers must be generated at each step makes them very efficient. The state of a spin is determined from the state of its neighbours on the basis of quenched rules which are determined at the start of the simulation. One such cellular automaton is the Q2R [1-3]. Q2R automata have been studied extensively and these studies have revealed some difficulties with reproducing properly all the thermodynamic properties of Ising systems [3-5].

More recently, the Ising cellular automaton, or ICA [6-8], was proposed for studying the effects of damage spreading in Ising spin systems. However, no detailed examination of the thermodynamic properties of the ICA has been made. The purpose of this letter is to investigate the conditions under which ICAs give the same macroscopic behaviour as the Ising model. Following the experiences we have with Q2R the two essential points to check are if there is a breakdown of ergodicity and how much randomness must be introduced into the model in order to overcome any non-ergodicity and retrieve the exactly known macroscopic properties independent on the initial configurations. Finally, not only the computer speed must be compared to the best existing algorithms (multispin Metropolis reusing random numbers, cluster algorithms, etc) but also the exponent z governing the critical slowing down must be checked.

Let us consider first the cellular automaton known as the Kauffman model [9]. In the nearest-neighbour version on a square lattice, there are 16 possible configurations of the neighbouring spins. The spin update rule for one such configuration is determined as follows. First a probability p is specified for the system. A random number is chosen and compared with p. If the random number is less (greater) than p then the rule sets the spin to be up (down). The rule for each of the other configurations is determined in the same way, only using different random numbers, and the whole procedure is repeated for each site. Once the rules are set they do not change. In other words, the

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value of a spin at step $t+1$ is completely determined by the configuration of its neighbours at step t and the corresponding fixed rule. Note that for Kauffman automata p takes the same value for all random rule choices.

Ising cellular automata, or ICA, introduce temperature into cellular automata by incorporating the Boltzmann probability distribution of the Ising model in the rule selection [6–8]. In the Ising model the energy of a spin at site i is

$$E_i = -J\sigma_i \sum_j \sigma_j \tag{1}$$

in the absence of any external field. The probability that the spin at site i is up ($\sigma_i = +1$) is

$$p_i = e^{-E_i/kT}/(e^{-E_i/kT} + e^{E_i/kT}). \tag{2}$$

This probability is used to generate the rules of the ICA in the following way. A temperature is first specified and each of the five distinct energies for the 16 possible different neighbour configurations is determined. This specifies, through equation (2), a value of p for each configuration. A random number is chosen for a configuration and compared with the corresponding p. As before, if the random number is less (greater) than p the rule sets the spin to be up (down). The process is performed for all the configurations of each site.

The procedure followed by MacIsaac *et al* [6–8] uses a different random number for each of the 16 configurations. We propose a simpler and more efficient ICA for which the local rules depend only on the sum of the spins of the neighbours and not on their individual values. The ICA is therefore a totalistic cellular automaton [10]. The rules are determined by choosing a different random number for each different value $(4, 2, 0, -2, -4)$ of the energy and comparing it with the value of p given by equation (2). In this way the number of rules for each site is reduced to five.

Let us return briefly to the non-totalistic automaton. For the square lattice there are 16 possible different neighbour configurations. At each time step an algorithm determines, by means of logical operations, which of the neighbour configurations is present and whether the corresponding rule gives spin up (+1) or down (−1). Since, at most, only one of these logical expressions can be true, the result can be achieved by means of logical XORs. in fact, on the Cray Y-MP and NEC-SX3 it proves to be more efficient to add the 16 logical expressions [11]. When additions are combined with logical expressions, the Cray Y-MP employs the integer processor in parallel with the logical one, resulting in a net improvement in efficiency (20–25% for this particular problem). Using multispin coding the simultaneous update of 64 spins is achieved by means of a total of 51 logical operations and 4 additions. In the case of the totalistic ICA, an update requires only 22 logical operations and 4 additions.

Monte Carlo simulations on $L \times L$ square lattices were performed on both totalistic and non-totalistic ICA and the equilibrium magnetization M was found to depend strongly on the initial configuration. The point is illustrated by figure 1 for several temperatures near T_c for the totalistic ICA. The results represent 50 000 updates of the system, with averages based on measurements of M at every 1000 steps. It is not surprising, perhaps, that a deterministic automaton gives evidence of non-ergodicity. Clearly, the system cannot sample a sufficiently large region of phase space to reach true equilibrium.

We found that the introduction of a small degree of randomness in the form of a random mixing (actually a shift) of the automaton rules was sufficient to remove this

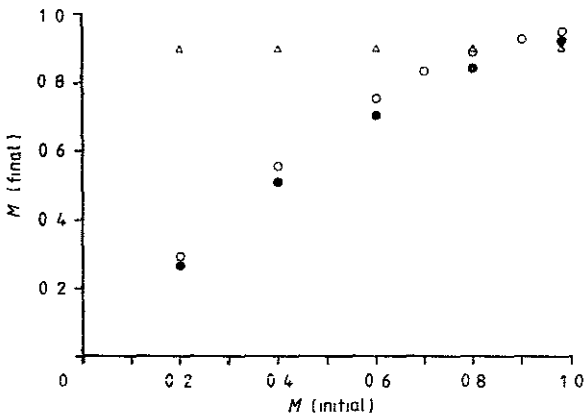

Figure 1. Final magnetization as a function of the magnetization of the initial configuration for the totalistic ICA on a lattice of size $L=256$ (●) $T=0.98T_c$, (○) $T=0.90T_c$, (△) $T=0.90T_c$, with random rule mixing. Averages are based on 50 values of M taken every 1000 MCs.

effect. In a first variant called the random bit-shifted totalistic ICA we introduce a single random number at each time step. By means of a circular bit-shift we simultaneously shift all the rules by the same random amount. Imagine a map of all the site rules superimposed on the lattice. The rule map then undergoes a random shift to the left over the lattice. The effect is to mix rules within groupings of 64 sites each. In a second variant which we call the fully randomized totalistic ICA we introduce a second random number at each time step for a simultaneous random shift of the automaton rules from row to row (i.e. along the second direction). The combined effect is to mix rules within groupings of $64L$ sites. Clearly, it would be possible to use a single random number to shift rules over the whole of the lattice. We did not extend the model in this logical way. Both variants of the model are much more efficient than the usual Metropolis Monte Carlo which requires a new random number for each site at each step.

Figure 2 compares the magnetization near T_c for the fully randomized totalistic ICA with the exact Ising model on a lattice of size $L=1024$. The agreement is very good, even very close to T_c which is well reproduced. On the other hand, in the case of the random bit-shifted ICA, we found considerable deviations within roughly 10% below T_c of the critical temperature suggestive of a lower critical temperature. It is interesting, however, that in the interval $(0.9\text{–}1.0)T_c$ the magnetization seems to relax very slowly to zero on a time scale of the order of 100 000 steps, which is several orders of magnitude greater than normally found for relaxation times (for the fully randomized ICA above T_c). Similar effects were observed for Q2R also [4]. The failure of the random bit-shifted version to reproduce the magnetization near T_c may indicate that it contains insufficient randomness. On the other hand, we know that if we go to the extreme of completely mixing all the rules at each time step on an infinite lattice we certainly have exactly the Ising model.

The case of Q2R automata has demonstrated that an agreement of the spontaneous magnetization with the Ising model behaviour is no assurance that other properties such as the magnetization fluctuations describe the correct behaviour [11]. While the apparent discrepancy in Q2R was resolved by Moukarzel and Parga [5] by redefining

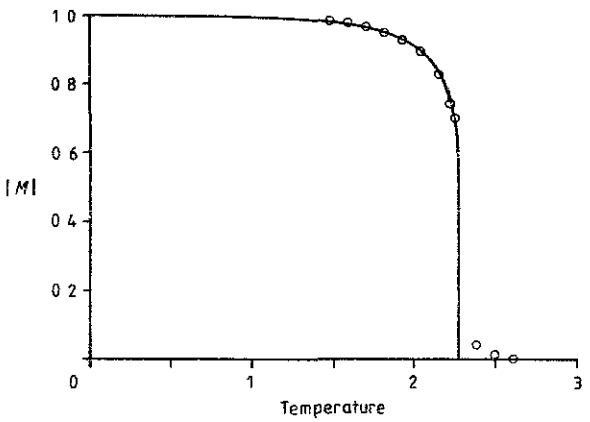

Figure 2. Equilibrium magnetization against temperature for the square lattice (——) exact Ising model, (○) ICA with random shift of automaton rules in both directions for lattice size $L = 1024$.

the quantities properly, the message that this example provides is clear. So we also measure the zero-field susceptibility χ. This is done in the usual way through fluctuations in the magnetization.

$$\chi = N\frac{\langle M^2\rangle - \langle M\rangle^2}{kT} \tag{3}$$

Our simulations on a lattice of size 1024 involve 110 000 total updates of the lattice. The first 10 000 iterations allow for thermalization of the system and M is measured at every subsequent 1000 steps. Results for χ near T_c for the fully randomized totalistic ICA are presented in figure 3 and compared with simulations on the Ising model. Data

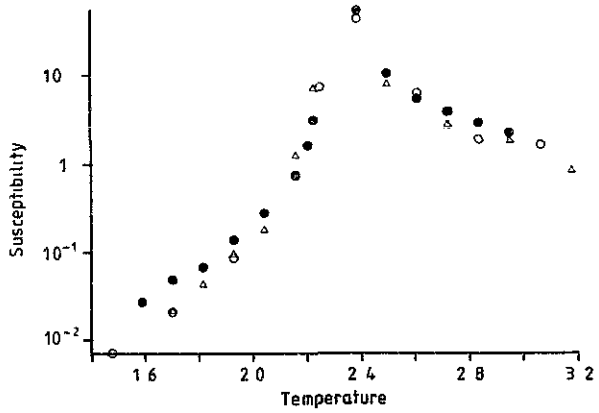

Figure 3. Zero-field susceptibility against T/T_c for ICA for lattice size $L = 1024$. Averages are based on 100 measurements of M taken every 1000 time steps after allowing for a equilibration times of 10 000 MCs (○), 1000 MCs (△). The full dots were obtained using the usual Metropolis algorithm. The statistical error bars are roughly three times the size of the symbols.

from an earlier run with a shorter thermalization time is also shown. It would appear that the susceptibility for the randomized totalistic ICA is in agreement with the Ising result within the errors of both calculations.

The basic algorithm using 22 logical operations and 4 additions to update the spins reaches a speed of 435 million updates per second on the Cray-YMP. The inclusion of two random rule shifts at each step reduces the speed to 235 million updates per second. By comparison, we find that the speed for the non-totalistic ICA (with no random shift) is 230 million updates per second, a result which is consistent with that achieved by Stauffer [12] on the Kauffman model. For comparison, for the usual Metropolis Monte Carlo vectorized multispin coding algorithms have reached speeds of 38 million updates per second (130 million updates per second if random numbers are re-used) [13]. Bhanot *et al* [14] achieved a speed of 98 million updates per second using a vectorized multilattice coding algorithm which have been improved in [15] and [16] by a factor up to 8. The speeds we have achieved on the totalistic ICA represent a method competitive with those benchmarks.

In any assessment of the speed of the model, it is important to consider not only the spin update speed but also the relaxation time near the critical temperature. Define the nonlinear relaxation time τ of the magnetization $M(t)$ for $T > T_c$ as

$$\tau = \int_0^\infty M(t)\,\mathrm{d}t. \tag{4}$$

Close to T_c one expects critical slowing down [17] according to

$$\tau \sim (T - T_c)^{-z} \tag{5}$$

where z is the nonlinear dynamical critical exponent. Figure 4 is a log-log plot of τ against $(T - T_c)/T_c$. The slope yields $z = 1.8$ (1). For the usual Metropolis Monte Carlo simulations on a two-dimensional Ising system a nonlinear dynamical critical exponent of $z = 2.04(4)$ has been found [18]. For Q2R automata $z = 2.1(2)$ [3]. This means that our cellular atomaton rule luckily seems to have weaker critical slowing down than the usual canonical Monte Carlo.

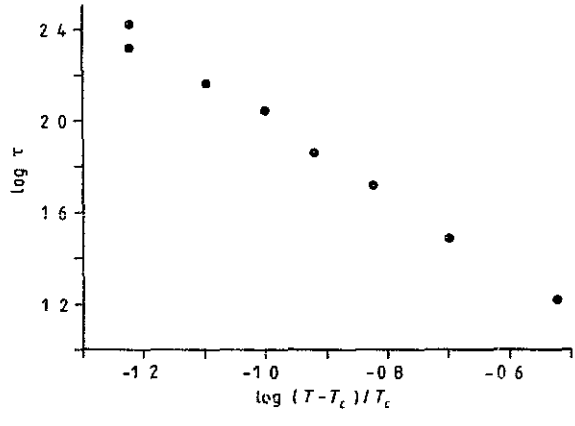

Figure 4. Log-log plot of nonlinear relaxation time τ against $(T - T_c)/T_c$ for totalistic ICA $L = 2048$

We have introduced a totalistic ICA which allows for fast simulation of the Ising model. We have found that this and similar ICA [6–8] do not lead to the correct magnetization unless some randomness is introduced into the model similar to effects reported for Q2R [19]. In our case, this took the form of a simultaneous random shift of the automaton rules over the lattice at each time step. No new automaton rules were chosen. Instead, the set of existing rules was randomly shifted along one or both directions at each time step by means of just one or two random numbers.

The fully randomized totalistic ICA was found to have the same thermodynamic behaviour as the Ising model, at least insofar as the magnetization and zero-field susceptibility are concerned. An examination of the energy and specific heat would provide additional support for the model. Our ICA is vectorized and multispin coded and reaches speeds of 235 million updates per second, comparable to the highest Metropolis Monte Carlo speeds that have been reported [13–16]. Some improvement on this speed is likely to be possible. The automaton also seems to have the advantage of weaker critical slowing down than has been found in Metropolis Monte Carlo simulations. We report a value $z = 1.8(1)$ for the nonlinear dynamical critical exponent. This is of course still much larger than the z found for cluster algorithms [20] which at the end might remain the most efficient way to simulate the Ising model close to the critical point.

Further investigation would be useful in the following areas. Our results for the random bit-shifted totalistic ICA suggest that some minimum randomness is necessary in order for the ICA to give the correct thermodynamic behaviour as the Ising model (within certain statistical error bars) The non-random ICA might also be examined for periodic cycles to determine whether it suffers significantly from a lack of ergodicity. We would like to emphasize that our models are completely generalizable and can easily be applied to Potts models and extended to include a field, to more neighbours, to higher dimensions and to different types of lattices. The fact of its vectorizability, its high speed and its generality offer attractive possibilities for simulations of Ising-type models

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