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DAMAGE SPREADING IN THE Q2R ISING MODEL

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We find evidence of metastability in the spreading of damage in the Q2R cellular automaton approximation for a 2D Ising system which is first equilibrated with a standard Metropolis simulation. A subsequent study of both single-site and whole-line damage spreading in Metropolis/Q2R systems as well as in pure Q2R systems shows a logarithmic dependence of the damage-spreading threshold on time, and saturation effects in single-site damage suggest a transition in the damage-spreading threshold at low initial energy values. Examination of the magnetization as a function of energy in pure Q2R shows extremely long relaxation times for $p < p_c$, which may bear some relation to the extremely slow convergence of the damage-spreading threshold.

1. Introduction

If two replicas of a model spin system are simulated simultaneously and if the two lattices differ initially at only one site, then the set of sites which differ in the two lattices during the later evolution is called the damage. Does this damage spread over the whole lattice, or does it remain localized? And how does the phenomenon depend on the initial "temperature" of the lattice?

These questions have been investigated in various systems, first by Kauffman in 1969 [1] and more recently by others interested in damage spreading in Ising magnets and related models [2]. One such model is the Q2R cellular automaton approximation of the two-dimensional Ising system, in which a lattice is updated by flipping spins if as many nearest neighbor spins are up as down [3]. For Q2R, Stanley et al. [2] found evidence of metastability in the sense that, in the ferromagnetic region (below the Curie point), the damage may remain roughly constant for hundreds or even thousands of time steps before suddenly growing. In the paramagnetic region, however, damage spreads immediately through the lattice.

But Q2R is a deterministic, reversible and nonergodic system, and because of this fact certain deviations from the Ising model behavior arise for short

simulation times. Moukarzel found [4] that these deviations vanish if the starting configuration of the Q2R model is produced by a standard Metropolis simulation of the Ising model [5]. If this Moukarzel trick is used before the damage is introduced, is the spreading of the damage different from what Stanley et al. observed?

To answer this question, we perform the Metropolis/Ising simulation in a simple, non-vectorized form. After sufficiently equilibrating the system via a standard Monte Carlo method, one site is damaged. Then we apply the much faster Q2R algorithm [3]. At a temperature about 5% below the Curie point, we observe a case where the damage remained at its initial value of unity for tens of thousands of iterations, until it finally spreads over hundreds of sites. The metastability observed by Stanley et al. exists even when the Moukarzel trick is employed.

We now reinvestigate damage spreading in Q2R, both with and without the Moukarzel trick, and address the question of the time dependence of damage spreading for both single-site damage and whole-line damage. Finally, we reexamine [5] Q2R equilibration via the relaxation of the magnetization.

2. Computation

Most of these calculations are performed on a Cray-YMP at the Jülich supercomputer center. In damage spreading, each time step consists of updating two lattice sites in a system of edge length L, and approximately one site is updated per nanosecond on one Cray processor for $L = 128$. For larger lattices, this speed increases to 1.77 sites per nanosecond. Calculations are also made on Boston University's Connection Machine, a SIMD computer with 32K parallel processors. Using a program written in C/Paris (details in the appendix), we achieve a speed of 0.8 sites per nanosecond, which translates to 1.6 sites per nanosecond on a full 64K machine. This is slower than the speed achieved using Lisp Microcode (4 sites per nanosecond, D. Rockmore, Thinking Machines Corporation [6]), but surprisingly fast considering no microcode is used. We use a variation of multispin coding (which is usually used for a single lattice only) to store the spin values of corresponding sites of independent lattices in a single variable field, so that each spin field has a length equal to the number of lattices to be simulated. With this multi*lattice* coding algorithm, logical operations involved in the updating of the spins are then performed on all lattices in a bitwise fashion, allowing an ensemble of many lattices to be simulated in a single run. For example, in some cases we simulate damage spreading in an ensemble of 600 $L = 256$ independently initialized lattices per run. It remains to be seen if programming in the Paris microcode CMIS speeds up the simulation appreciably.

3. Method

Our study of damage in pure Q2R (i.e. Q2R *without* the Moukarzel trick) consists of randomly initializing an $L \times L$ square lattice with an average concentration p of up spins, copying the lattice, damaging either the central spin or the center horizontal line of spins in one of the copies, and then applying Q2R dynamics to the two lattices simultaneously. While updating, we continuously check if the damage reaches the upper edge of the lattice in a fixed time τ. The damage spreading threshold is defined to be the concentration p_τ for which half of the lattices simulated have damage spreading to one particular edge (in this case, the upper edge) of the lattice in the given time. Damage spreading in Metropolis/Q2R (i.e. Q2R *with* the Moukarzel trick) is performed in a similar manner, but with the damage introduced after the lattice has already been equilibrated with the Metropolis algorithm.

In Q2R, the energy per spin, in units of the ferromagnetic coupling constant J, is related to the initial concentration p of up spins in the lattice through[#1]

$$\frac{E}{J} + 2 = 8p(1-p)\,. \tag{1}$$

Because the dynamics of Q2R is such that spins are flipped if and only if the flip conserves energy, the energy E is constant and equal to the initial energy of the lattice.

In Metropolis/Ising dynamics, a lattice is initialized according to a given temperature T, which at low temperatures is related exponentially to the energy through [7]

$$\frac{E}{J} + 2 \sim \mathrm{e}^{-8J/kT}\,. \tag{2}$$

In an Ising system it is the temperature, and not the energy, that is constant. But through the initial energy of the lattice, the threshold concentration in pure Q2R and the threshold temperature in Metropolis/Q2R can be related using eqs. (1) and (2).

4. Results

4.1. Pure Q2R

In the pure Q2R case with an entire line initially damaged, we vary the number τ of iterations, and find that

[#1] Each broken bond contributes $2J$ to the thermal energy, and $2p(1-p)$ is the probability to break a bond, refs. [7, 8].

$$p_\tau \sim \frac{1}{\log \tau} . \tag{3}$$

That is, the damage-spreading threshold concentration decreases in a roughly logarithmic fashion with increasing observation time τ: For example, the values of p_τ for $L = 128$ are roughly 0.077, 0.064, 0.054, 0.044, 0.037 and 0.03 for $\tau = 10^3$, 10^4, 10^5, 10^6, 10^7 and 10^8, respectively (corresponding to (see eq. (1)) energies per site between $-1.43J$ and $-1.77J$). These values are obtained from a simulation of between 10 and 100 lattices (10 for the longest times).

For 10^9 time steps, we decrease the concentration for one lattice until the damage no longer spreads: this occurs at p_τ between 0.022 and 0.024. Since there is as yet no evidence of saturation, it is conceivable that p_τ goes to zero logarithmically as τ approaches infinity.

The damage-spreading thresholds are larger by about 0.01 if initially only one site is damaged. For example, for an ensemble of 3000 128×128 lattices (5 runs, 600 independent lattices per run), p_τ is found to be 0.085, 0.071 and 0.061 for $\tau = 10^3$, 10^4 and 10^5, respectively. However, for very long times saturation seems to set in, with p_τ remaining at about 0.054 for $\tau = 10^6$, 10^7 and 10^8.

That the two cases produce similar time dependence for at least short and intermediate times, with lower threshold values for the case of line damage, can perhaps be understood by examining the metastability of single-site damage. We see, as did Stanley et al., that for a given initial lattice energy, the time it takes for single-site damage to begin spreading can be anywhere from one to millions of time steps. The reason for this is that a lattice with a given energy (i.e. a given initial concentration of up spins) can be initialized in many different configurations. If a given configuration has a "good" mix of up and down spins near the damaged spin, the damage may start spreading immediately. It then may stay constant for awhile before it can spread again, or the configuration may be such that the damage can spread steadily through the lattice. On the other hand, if the initial configuration of spins is such that all the spins in the vicinity of the damaged spin point in the same direction as the damaged spin, then it may take quite some time for the damage to start propagating through the system. And again, once the damage begins to spread, there is no guarantee at low concentrations of spins below p_c that the damage will spread unhindered through the system.

However, one could imagine that if two spins, rather than one, were damaged initially, the probability that the damage could spread easily is larger, because the change that the spin configuration is "right" for information to propagate is better. Indeed, if an entire line of spins is damaged, one almost ensures that the damage will begin to propagate immediately, and continue to propagate, from at least one point on the line. Stated another way, the

"damage clouds" produced by each site on the line cooperate to encourage the propagation of the damage through the system. This cooperation means that a lower initial concentration of up spins is needed for damage spreading if a whole line, as opposed to one site, is initially damaged. Hence for a given time τ, we expect that the damage-spreading threshold will be lower for line damage than for single-site damage. And the cooperation between damage clouds masks the metastability of single-site damage in such a way that the time dependence of the damage spreading is the same.

Extrapolation to a very small or zero threshold concentration for whole-line damage spreading corresponds to the limit of infinite observation time τ at fixed large system size. In the opposite order of limits, size L going to infinity at fixed large τ, damage will never spread over a distance $L/2$. Actually, we find that, at least for the case of whole-line damage, τ seems to scale like L. If these threshold concentrations are plotted as a function of $\log(L/\tau)$, one scaling curve for different system sizes results ($L = 128$, 256, 384, 512, 640 and 1152). For single-site damage, on the other hand, if L and τ are increased such that their ratio remains constant, a concentration slightly less than the p_τ found that $L = 128$ is needed for damage to reach the boundary of only 50% of the lattices. For each lattice size and corresponding τ an appropriate p_τ can be found. For example, for $L = 128$ and $\tau = 316$, the threshold concentration is $p_\tau = 0.097$. If L is increased to 3840, and we increase τ according to $\tau = 316 \times L/128$, we find a threshold concentration of $p_\tau = 0.085$. This implies that the single-site damage spreading threshold decreases with increasing system size.

We also find that the fraction of samples with damage touching the boundary increases from zero to one over an interval centered about the listed values of p_τ. The size of this interval decreases as L is increased from 128 to 3840, suggesting an increasing sharpness in the threshold with increasing system size.

4.2. *Metropolis/Q2R*

Results similar to the pure Q2R results are obtained by combining Metropolis initialization with Q2R damage spreading. For an entire line damaged initially, we find the threshold temperatures, T/T_c in units of the Curie temperature T_c to be 0.99, 0.965, 0.94 and 0.92 for $\tau = 10^3$, 10^4, 10^5 and 10^6, respectively. The lowest threshold temperature corresponds to an energy E of about $-1.68J$ per spin. From eq. (1), this energy implies a threshold concentration of about 0.042 in the pure Q2R case, roughly compatible with the above results. Since the energy difference to the ground state in this combined Ising–Q2R system varies exponentially with J/T (eq. (2)), which implies

$$T \sim \frac{1}{\log E}\,, \tag{4}$$

then from eq. (3), which gives a logarithmic dependence of p_τ on τ, and eq. (1), which gives a parabolic dependence of E on p, it follows that the damage-spreading threshold *temperature* varies as

$$T \sim \frac{1}{\log(\log \tau)} \tag{5}$$

at low temperatures.

In analogy to what we see for the case of pure Q2R, the damage-spreading threshold temperature logarithmically approaches zero for infinitely long observation times. For practical applications, however, the threshold temperatures for long times will be much closer to the Curie temperature than to the possible asymptotic limit of zero.

If instead only a single site is damaged initially, the effective spreading temperature first decreases logarithmically with increasing observation time, and then saturates: $T/T_c = 0.98$, 0.96, 0.94, 0.92 and 0.92 at $\tau = 10^4$, 10^5, 10^6, 10^7 and 10^8. Again, these results show the same energy dependence on time as we see for the pure Q2R case.

Our results in terms of the energy dependence on observation time for all four cases are depicted in fig. 1. Note that in the pure Q2R simulation, damage

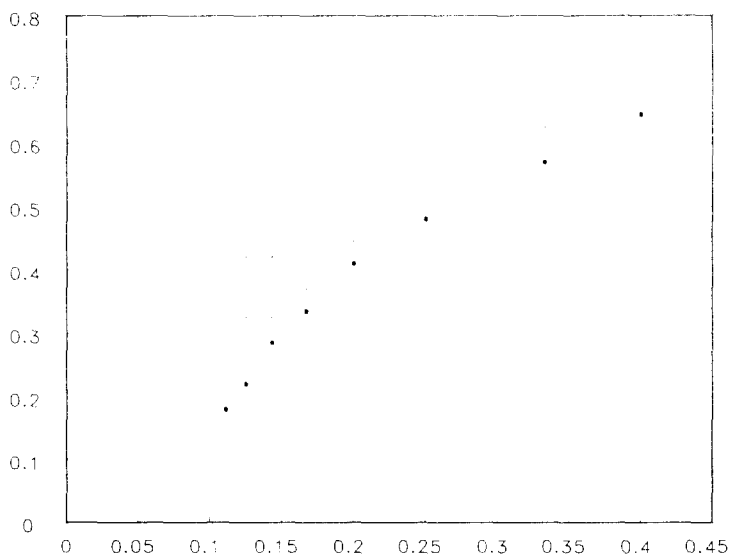

Fig. 1. Plot of thermal energy $E/J + 2$ versus $1/\log_{10}\tau$ in 128×128 square lattice. *Lower data*: Initial damage is a lattice line (● for pure Q2R, ○ for Metropolis/Q2R). *Upper data*: Initial damage is one site (+ for pure Q2R, × for Metropolis/Q2R). Zero temperature ($p = 0$) corresponds to $E/J = -2$, the Curie point ($p = 0.08$) to $E/J = -\sqrt{2}$. Later simulations for $\tau = 10^7$ and 10^8 for the circles gave relative threshold temperatures 0.90 and 0.86, close to the corresponding dots, confirming the downward trend.

was introduced at the beginning of the simulation, i.e. *before* equilibration of the system, while in the Moukarzel combination the system is equilibrated and *then* damage is introduced. From our results, we see that this distinction makes little difference in the general form of the energy dependence on time. Because of this, one might presume that there would be little or no qualitative difference between damage spreading in a nonequilibrated system and damage spreading in a system equilibrated first with Q2R. To confirm this, we ran damage spreading on a 128×128 lattice with $p_\tau = 0.065$ after 0, 10^4, 10^5 and 10^6 time steps of equilibration with no damage. Out of 100 lattices, 50, 54, 72 and 77 lattices, respectively, had damage spreading to the upper edge after 31 623 time steps. This implies that the threshold concentration, defined as the concentration at which 50% of the lattices simulated have damage spreading to the upper edge in a fixed time τ, decreases as the amount of equilibration performed on the lattice *before* introducing damage increases. We therefore expect that the threshold values for pure Q2R will approach the threshold values for Metropolis/Q2R when the damage is introduced in pure Q2R *after* t iterations, with t going to infinity.

4.3. Relaxation in Q2R

We also reconsider the magnetization M as a function of energy E in the pure Q2R model. Herrmann [3] had found it to agree numerically with the exact solution of the two-dimensional Ising model. However, he looked at non-random initial conditions, whereas we initialize the spins randomly with an average concentration p of up spins. As a result, for all values of the initial concentration below the critical point ($p_c = 0.08$), at moderate numbers of iterations (10^4 time steps for $L = 6528$) our magnetization M is slightly higher than the exact Ising solution, close to the upper limits of Herrmann's error bars. Only for very long simulations does it settle on the exact value. For example, at $p = 0.05$ ($E/J = -1.62$), M is about 0.90 at time $t = 0$, near 0.89 for t near 10^4, and does not decay fully to the exact value of $M = 0.84$ until after nearly 10^7 iterations ($L = 1024$). It seems likely that this extremely slow relaxation to equilibrium and the extremely slow convergence of the damage-spreading threshold are related.

Furthermore, we find that closer to the Curie point, at $p = 0.06$ and 0.065, the relaxation to equilibrium is *faster* than for lower values of p, contrary to the phenomenon of critical slowing down; see also fig. 5 of Zabolitzky and Herrmann [5]. For example, at $p = 0.065$, the time necessary for the magnetization to fully relax to its equilibrium value of 0.7504 is "only" about 180 000 time steps, as compared with 10^7 time steps needed for equilibration at $p = 0.05$.

This slow relaxation may also explain the deviations observed by Lang and Stauffer [8] in the nearest-neighbor correlations, which were removed by the Moukarzel trick. With millions of iterations ($L = 640$) at $p = 0.05$ and 0.065, these deviations nearly vanish even without the Moukarzel trick.

5. Summary

In conclusion, we find that the damage-spreading threshold for a Q2R cellular automaton decreases logarithmically towards zero with observation time. That is, the average time it takes for damage to spread to the edge of the system increases exponentially as the initial energy of the lattice decreases. We find that this time dependence holds whether or not Metropolis equilibration is performed before the damage is introduced, and in fact holds whether or not the system has been equilibrated first at all. The actual numbers are different: the thresholds of Metropolis/Q2R are lower than for pure Q2R with no initial equilibration, but in the limit that the amount of time for which the system is first equilibrated (with Q2R) goes to infinity, the two threshold values become close.

We also find that the threshold energies for line damage and the threshold energies for single-site damage both have the same general time dependence for short and intermediate times, but for more than a million iterations saturation sets in for the case of single-site damage. An increase in the threshold is expected for single-site damage, since there metastability effects are important, and a higher concentration of up spins is needed for the damage to spread to the edge in the same amount of time. This we confirm; however, the observed saturation in p_τ for single-site damage suggests a genuine transition not coincident with the Curie point, reminiscent of the cluster-period transition found by Herrmann et al. [9]. This transition, which occurred at $p = 0.033$ ($E = -1.75$) for a 64×64 square lattice, denoted the minimum initial lattice concentration for which an infinite-period cluster spanned the system. Further studies of this cluster transtion for larger lattices and similar initialization procedures may show it to be identical to the single-site damage-spreading transition, or even that it goes to zero as does the damage-spreading threshold for line damage.

Lastly, we find that the relaxation time to equilibrium in Q2R is enormous for concentrations lower than the critical concentration $p_c = 0.08$. Moreover, it seems that the equilibration time *increases* as the initial lattice concentration *decreases*. The implications of these effects will be studied in detail later.

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Appendix

C/Paris algorithm for initializing and spin updating on the Connection Machine

As described in section 2, the simulations on the CM at Boston University are carried out for an ensemble of lattices using bitwise logical operations for the updates. A spin field at each lattice point (j, k) is created with a bitlength L such that the ith bit of this field contains the value of the spin in the position (j, k) on the ith lattice in the ensemble.

Of course, in order for this method to be useful each lattice must be initialized independently, with the same average concentration p of up spins. This is done by initializing each bit of the spin field separately: by throwing a random number for each spin and comparing it to p, the probability for the spin to be up (i.e. concentration). Thus, the set of values (0 or 1) of each bit of the spin fields corresponds to a different initialization of the lattice, with the same p. The relevant part of the C/Paris code is shown below:

```
for(i = 0; i < bitlength; + +i) (
-CMI-u-fast-rng-1l(random, 14, 10000);      Generates a random number in
                                                          [0,10000]
CM-u-le-1L (cmprob, random, 14);           Compares random number with p
CM-logand-context-with-test();             The result of the 'logand' of the
                                           above test with the 'context' flag
                                           indicates whether the following steps
                                           should be executed for a lattice point
CM-set-bit (spin + i);                     Sets the ith bit of spin to 1
CM-set-context();                          All processors are set active again
```

Here 'bitlength' is the length of the spin field. In the CM, each lattice point resides on a virtual processor, and a controllable 'context' flag in each processor dictates whether the processor should execute a particular command.

The Q2R updating rule is usually implemented [3, 5] as follows:

$$S(t + 1) = (S(t).XOR.(A.IOR.B))$$

where
A = (I1.XOR.I2).AND.(I3.XOR.I4)
B = (I1.XOR.I3).AND.(I2.XOR.I4)

I1, I2, I3 and I4 being the nearest neighbor spins at time t. But we can use the information already evaluated in A to reduce the number of operations for getting the rest of the complete logical expression as follows: The only configurations of nearest neighbor spins for which A does not itself give the correct flag are (0 0 0 0) and (1 1 1 1); that is, all spins down or all spins up. In both cases, XOR(I1, I2) and XOR(I1, I3) are going each to be equal to FALSE, while for all the other cases for which A is TRUE, one of the two XOR's will be TRUE. Hence, we an express the Q2R rule as

$S(t+1) = (S(t).XOR.(A.AND.B))$
where
A = ((I1.XOR.I2).EQV.(I3.XOR.I4))
B = ((I2.XOR.I3).IOR.(I1.XOR.I2))

Thus, with our method the updating can be achieved using only 7 operations instead of 8 as in the method shown earlier. Further, since these operations are bitwise, each bit of the spin field is updated independently of the rest of the bits and hence we can simulate a large number of independent lattices in a single run. The code for the updating is shown below. The 'get-from-news' operations get the values of the spins from neighboring processors in the news array, which correspond to neighboring lattice points (news = north-east-west-south):

```
CM-get-from-news-1L(I1, spin, 1, CM-downward, bitlength);          north
CM-get-from-news-1L(I2, spin, 0, CM-downward, bitlength);          west
CM-get-from-news-1L(I3, spin, 1, CM-upward, bitlength);            south
CM-get-from-news-1L(I4, spin, 0, CM-upward, bitlength);            east
CM-logxor-3-1L(I1,I1,I2,bitlength);      I1 ← xor(neighborspin1,neighborspin2)
CM-logxor-3-1L(I4,I3,I4,bitlength);      I4 ← xor(neighborspin3,neighborspin4)
CM-logeqv-3-1L(I4,I1,I4,bitlength);        I4 ← eqv(xor(1,2),xor(3,4)); flag A
CM-logxor-3-1L(I3,I2,I3,bitlength);      I3 ← xor(neighborspin2,neighborspin3)
CM-logior-3-1L(I1,I1,I3,bitlength);        I1 ← logior(xor(1,2),xor(2,3));flag B
CM-logand-3-1L(I1,I1,I4,bitlength);                          I1 ← (A.AND.B)
CM-logxor-3-1L(spin, spin, I1, bitlength);                   flips spin appropriately
```

Note added in proof

The speed on the Connection Machine was doubled when we reformulated

the logical operations, replacing for example **CM-logand-3-1L** by **CM-logand-2-1L** at the end of the appendix.

References

[1] S.A. Kauffman, J. Theor. Biol. 22 (1969) 437.
[2] H.E. Stanley, D. Stauffer, J. Kertesz and H.J. Herrmann, Phys. Rev. Lett. 59 (1987) 2326.
U.M.S. Costa, J. Phys. A: Math. Gen. 20 (1987) L583.
B. Derrida and G. Weisbuch, Europhys. Lett. 4 (1987) 657.
A. Coniglio, L. de Arcangelis, H.J. Herrmann and N. Jan, Europhys. Lett. 8 (1989) 315.
G. Le Caer, J. Phys. A 22 (1989) L647.
H.R. da Cruz, U.M.S. Costa and E.M.F. Curado, J. Phys. A 22 (1989) L651.
A.M. Mariz and H.J. Herrmann, preprints.
[3] Y. Pomeau, J. Phys. A: Math. Gen. 17 (1984) L415.
G.Y. Vichniac, Physica D 10 (1984) 96.
H.J. Herrmann, J. Stat. Phys. 45 (1986) 145.
[4] C. Moukarzel, J. Phys. A 22 (1989) 4487.
[5] J. Zabolitzky and H.J. Herrmann, J. Comput. Phys. 76 (1988) 426.
[6] As communicated by B. Boghosian.
[7] C. Domb, Adv. Phys. 9 (1960) 149.
[8] W.M. Lang and D. Stauffer, J. Phys. A: Math. Gen. 20 (1987) 5413.
[9] H.J. Herrmann, H.O. Carmesin and D. Stauffer, J. Phys. A: Math. Gen. 20 (1987) 4939.