Parallel processing: the Ising model and Monte Carlo dynamics

J. Phys. A: Math. Gen. 18 (1985) 1781-1794. Printed in Great Britain

Parallel processing: the Ising model and Monte Carlo dynamics

J K Williams[†]

Department of Physics, University of Edinburgh, James Clerk Maxwell Building, Kings Buildings, Mayfield Road, Edinburgh EH9 3JZ, UK

Received 4 October 1984

Abstract. This paper investigates the dynamics of Monte Carlo simulations of the kinetic Ising model involving multi-spin-flip updating schemes as opposed to the conventional random single-spin-flip updating schemes normally used.

1. Introduction

In the field of critical phenomena there are few models for which exact solutions may be found; in most cases our understanding rests on insights gained from various approximate methods such as renormalisation group methods, series expansions and Monte Carlo computer simulations. For many models Monte Carlo methods provide the most useful information on their behaviour, particularly when the model is supposed to simulate a realistic physical system. The determination of the critical properties of these models, however, makes huge demands on computer resources—as Binder (1979) has pointed out 'Good Monte Carlo work obviously is not cheap'.

Over the past decade the ever-increasing demand for cost-effective, high-performance computer facilities has been met by major changes in computer hardware, most significantly through the introduction of parallel architectures (Hockney and Jesshope 1981). Two main trends can be discerned, exemplified by the 'pipelined' processor and the 'array' processor (typical examples being the Cray 1 and the ICL DAP respectively); both have been designed to try to maximise the concurrent activities within the computer.

These improvements in computer performance are making a great impact on the study of critical phenomena by Monte Carlo methods. In order to take full advantage of these developments it is clearly essential that the updating schemes employed in the Monte Carlo simulations are tailored ('parallelised') to exploit the parallel architecture of the machine used; in the case of an array processor it is important that the calculation is effectively partitioned over all the processing elements. Several authors, see for instance Zorn *et al* (1981) and Pawley *et al* (1984), have used 'parallel' updating schemes to study static equilibrium properties of the Ising model. In these updating schemes conventional single-spin-flip updating has been replaced by some type of multi-spin-flip updating. So far the dynamical aspects of these parallel updating schemes have been ignored. It is not clear *a priori* that multi-spin-flip and single-spin-flip realisations of the dynamics of a given model lie in the same dynamical universality

[†] Present address: Department of Mineral Resources Engineering, Imperial College of Science and Technology, Prince Consort Road, London SW7 2BP, UK.

class. The principal objective of the work described in this paper is to investigate the dynamical behaviour of multi-spin-flip updating schemes, focusing on simulations of the kinetic Ising model.

More specifically, we will begin in § 2 by reviewing the standard single-spin-flip Monte Carlo method (Binder 1979). We will then discuss very briefiy the multi-spin-coding technique, which has been used to reduce both the memory space requirements and the execution time of simulations on serial computers (Zorn *et al* 1981). The basic idea of multi-spin-coding, where several spins are 'updated' simultaneously, can be readily extended for implementation on a parallel processor; this leads us on to the concept of 'parallel updating' and we present results of a test simulation based on this approach.

In § 3 we turn to dynamics, where first we review the two main Monte Carlo approaches, 'event-by-event' or 'timestep-by-timestep' simulations, and then we show that parallel updating is tailored to the 'timestep-by-timestep' approach.

Parallel updating has some interesting consequences for dynamics and this is illustrated in § 4. We compare simulations on the one-dimensional kinetic Ising model with Glauber's exact solution for a random single-spin-flip dynamics (Glauber 1963). For simulations using 'Glauber flipping probabilities' we find good agreement with the exact results when an overall time rescaling is taken into account. However, when 'Metropolis flipping probabilities' are used we observe a breakdown of dynamic universality; this is not altogether unexpected in one dimension since several dynamic universality classes have previously been found corresponding to special choices of single-spin-flip dynamics (Cordery *et al* 1981). Both sets of results can be understood in terms of the motion of domain boundaries. We have also looked at other choices of flipping probabilities in the one-dimensional model and again the results can be understood in terms of domain boundary motion. We also indicate what happens in the case of the two-dimensional kinetic Ising model, where we have studied various time-delayed correlation functions at the critical point. The critical dynamics of this model are discussed in more detail in a separate paper (Williams 1985). Although we find a time rescaling with respect to the single-spin-flip dynamics the universal dynamical properties remain intact.

Finally, in § 5 we summarise our results and discuss remaining problems and future lines of development.

2. Review of the Monte Carlo method and an introduction to parallel updating

The theoretical basis for the application of Monte Carlo methods to the study of the Ising model has been discussed in the literature many times (e.g. Binder 1979). Nevertheless it will be useful for later purposes to briefly review the standard single-spin-flip method. We will consider a lattice of N sites, where an Ising spin, σ_i, is located at each site i; the spin coordinate, σ_i, assumes the values ±1. A configuration is completely described by specifying the state of all the spins $\{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ and is denoted by $\{\sigma\}$. For simplicity we will assume that the energy of this set of spins is due to a nearest-neighbour interaction only, so the Hamiltonian for the system, including the inverse temperature factor $(-\beta)$, is

$$\mathscr{H}(\{\sigma\}) = K \sum_{\langle ij\rangle} \sigma_i\sigma_j \tag{2.1}$$

where the summation extends over all nearest-neighbour pairs. The equilibrium probability distribution function can then be written as

$$P_{\mathrm{eq}}(\{\sigma\}) = Z^{-1}\exp[\mathcal{H}(\{\sigma\})] \tag{2.2}$$

where Z is the partition function,

$$Z = \sum_{\{\sigma\}} \exp[\mathcal{H}(\{\sigma\})]. \tag{2.3}$$

Correlation functions are calculated in the usual way by averaging over this equilibrium distribution,

$$\langle S\rangle = \sum_{\{\sigma\}} S(\{\sigma\})P_{\mathrm{eq}}(\{\sigma\}) \tag{2.4}$$

where S denotes the relevant combination of the σ_i's for the correlation function of interest.

The standard Monte Carlo method is used to generate a sequence of configurations with the probability distribution of (2.2): then the Monte Carlo estimate $\bar{S}$ for the quantity $\langle S\rangle$ simply reduces to an arithmetic average

$$\bar{S} = \frac{1}{M}\sum_{\nu=1}^{M} S(\{\sigma\}_\nu) \tag{2.5}$$

where M is the total number of configurations generated in the sequence. The realisation of this scheme is made possible by the use of a Markov process to generate the M configurations in (2.5). This process is constructed so that the probability of the occurrence of the configuration $\{\sigma\}$, $P(\{\sigma\})$, tends towards $P_{\mathrm{eq}}(\{\sigma\})$ as M tends towards infinity.

The evolution of the sequence of configurations can be thought of as a 'discrete time' process; the probability of the occurrence of the configuration $\{\sigma\}$ at time t is denoted by $P(\{\sigma\}; t)$ and the evolution of the system is described by the following master equation,

$$\begin{aligned} P(\{\sigma\}; t+\Delta t) = P(\{\sigma\}; t) &+ \sum_{\{\sigma\}'} P(\{\sigma\}'; t)\, W(\{\sigma\}' \to \{\sigma\}) \\ &- \sum_{\{\sigma\}'} P(\{\sigma\}; t)\, W(\{\sigma\} \to \{\sigma\}') \end{aligned} \tag{2.6}$$

where $W(\{\sigma\} \to \{\sigma\}')$ is the conditional probability of finding the system with configuration $\{\sigma\}'$ at time $t+\Delta t$ given that it had the configuration $\{\sigma\}$ at time t. If the W's are chosen to satisfy detailed balance

$$P_{\mathrm{eq}}(\{\sigma\})\, W(\{\sigma\} \to \{\sigma\}') = P_{\mathrm{eq}}(\{\sigma\}')\, W(\{\sigma\}' \to \{\sigma\}) \tag{2.7}$$

and if the following ergodic condition is fulfilled, namely, that any configuration can be reached from any other configuration in a finite number of steps with non-vanishing probability, then the evolution of $P(\{\sigma\}; t)$ towards $P_{\mathrm{eq}}(\{\sigma\})$ is assured, see for instance Binder (1979).

The detailed balance condition does not determine $W(\{\sigma\} \to \{\sigma\}')$ uniquely. W is usually restricted to a single-spin-flip, that is $W(\{\sigma\} \to \{\sigma\}') = 0$ unless $\{\sigma\}$ and $\{\sigma\}'$ differ by at most a single spin coordinate. For this special case let $\{\sigma\}_i$ denote a configuration differing from $\{\sigma\}$ by flipping over the ith spin, and let $\omega_i(\{\sigma\})$ denote $W(\{\sigma\}\rightarrow\{\sigma\}')$. The following choices of $\omega_i(\{\sigma\})$ have been frequently used

$$\begin{aligned}&\omega_i(\{\sigma\})=\tfrac{1}{2}[1-\sigma_i\tanh(E_i)] &&\text{Glauber}\\ &\omega_i(\{\sigma\})=\min\{1,\exp[-2\sigma_iE_i]\} &&\text{Metropolis}\end{aligned}\qquad(2.8)$$

where $E_i=K\Sigma\sigma_{(i)}$ and (i) denotes nearest neighbours of i.

In a Monte Carlo simulation we choose an initial spin configuration and then select an active site, j, for a spin-flip trial; this selection may be made randomly or by proceeding through the lattice in a regular fashion. Once j has been selected we calculate $\omega_j(\{\sigma\})$ and then generate a pseudo-random number, r, uniformly distributed in the interval from 0 to 1. If $\omega_j>r$ the active spin is flipped, otherwise it is left alone, and the spin-flip trial is completed. The process is then repeated. We adopt the convention that N spin-flip trials constitutes one Monte Carlo step per spin (MCS/spin) or one lattice update. After allowing the system 'time' to equilibrate, correlation functions can be estimated according to (2.5).

An important limitation on the scope of these simulations is the availability of memory space and computer time. One technique which has been used to reduce these burdens in a serial computation is multi-spin-coding (MSC) (Zorn *et al* 1981). It has long been recognised that it is wasteful to represent the state of an Ising spin by a whole computer word, and the basic idea of MSC is that information on the state of several spins can be packed into each computer word used to represent a spin configuration. This packing is done in such a way that it allows operations involving these spins to be processed simultaneously. To be more specific, we note that a spin-flip trial consists of two stages: the evaluation of $\omega_j(\{\sigma\})$ for the active spin j and then the decision on whether to flip σ_j or not. The first stage can be handled efficiently by MSC by exploiting the fact that the $\omega_j(\{\sigma\})$ only depend on the states of the nearest neighbours of j; this allows us to consider a set of mutually non-interacting active sites simultaneously. Suppose n such spins are coded in a single word $S(I,J)$ and that their neighbours are coded in $S(I-1,J)$, $S(I+1,J)$, $S(I,J-1)$ and $S(I,J+1)$ in such a way that neighbouring spins occupy the same bit positions in their respective words. Now let all n sites in $S(I,J)$ be considered to be active; it is then possible, by using logical operations on $S(I,J)$ and its neighbouring words, to evaluate the σ_j's for all n active sites simultaneously. The decision stage of the spin-flip trials then has to be conducted sequentially. Detailed balance is preserved since any subsequent readjustments of the active spins will not affect the σ_j's of the remaining active sites being considered; the particular choice of active sites stored in the 'active word' guarantees the independence of the spin flip trials. This idea of conducting several independent spin-flip trials concurrently is ideally suited to the use of a parallel processor and leads us on to the idea of parallel updating.

The principal feature of parallel updating is that a whole set of independent spin-flip trials take place simultaneously through the use of a parallel processor; both stages of the spin-flip trial can be calculated at a set of independent active sites, where each active site is allocated a single processing element. The detailed implementation of this scheme will, of course, depend on the particular architecture of the computer being used; nevertheless it is probably useful to briefly outline the procedure we have followed. Our simulations have been performed on an ICL Distributed Array Processor (DAP); modifications for adapting the basic scheme to suit other parallel processors should be fairly trivial.

For simplicity, we will assume that our array processor has N processing elements and that the lattice we wish to simulate also has N sites; we can then allocate each site of the lattice to an individual processing element. The parallel updating procedure is as follows: first we generate N random numbers r_j, at each site j, then we calculate the ω_j's for all the active sites which we take to be an entire active sublattice then we decide which of these active spins are to be flipped according to whether $r_j < \omega_j$ or not, and finally we repeat the second and third stages for the other sublattice to complete one lattice update. Each parallel update is equivalent to N single spin-flip trials where the active spins are chosen in such a way that all the spins on one sublattice are considered once before all the spins on the other sublattice are considered. This has some interesting consequences for the dynamic interpretation of the Monte Carlo process, but before we consider that aspect we will present results of a simulation of some static properties, based on the above procedure.

As a test of the method we compared simulations on a 4×4 square lattice (with periodic boundary conditions) with the values obtained from an exact calculation. At each temperature considered 256 independent samples were simulated. Each sample started perfectly ordered and the simulations ran for 520 000 MCS/spin, dropping 20 000 MCS/spin for equilibration. Data were collected every 5 MCS/spin (i.e. 100 000 observations per sample), and the two quantities monitored were $\langle|M|\rangle = \langle 1/N|\Sigma\sigma_i|\rangle$ and $\langle\sigma_i\sigma_j\rangle$ where i and j were nearest neighbours. Table 1 shows the results for simulations using Glauber flipping probabilities, see (2.8). The numbers in parentheses indicate the statistical uncertainty in the last digits as estimated by calculating the standard deviation over the data from the 256 samples.

The good agreement between the simulated and exact results suggest that the parallel updating procedure works effectively for the equilibrium static properties (cf the comparable table in Landau 1976). We also note that the procedure is extremely efficient computationally, this particular simulation evaluating more than 2500 000 spin-flip trials every second.

Table 1. Comparison of simulated and exact results for a 4×4 Ising model with periodic boundary conditions using parallel updating.

K^{-1}	$\langle M\rangle_{\text{exact}}$	$\langle M\rangle_{\text{sim}}$	$\langle\sigma_i\sigma_j\rangle_{\text{exact}}$	$\langle\sigma_i\sigma_j\rangle_{\text{sim}}$
1.087	0.998 579	0.998 582 (3)	0.997 242	0.997 249 (5)
1.449	0.988 980	0.988 993 (9)	0.980 053	0.980 075 (15)
1.811	0.954 687	0.954 714 (22)	0.926 983	0.927 031 (29)
2.173	0.873 596	0.873 614 (45)	0.819 400	0.819 413 (50)
2.536	0.751 975	0.752 050 (55)	0.674 981	0.675 034 (60)
2.898	0.631 022	0.631 115 (62)	0.540 679	0.540 761 (65)
3.260	0.536 103	0.536 152 (58)	0.438 783	0.438 841 (55)
3.622	0.468 119	0.468 217 (59)	0.366 425	0.366 540 (52)

3. Dynamics and the Monte Carlo method

The Ising model has no intrinsic dynamics, but a stochastic dynamics may be introduced which can be interpreted in terms of a coupling of the spins to an infinite heat bath which induces random spin flips in the system (Glauber 1963). The simplest model is the single spin-flip kinetic Ising model which, using the notation of § 2, is described by the following master equation

$$(\mathrm{d}/\mathrm{d}t)P(\{\sigma\};t)=-\sum_i \omega_i(\{\sigma\})P(\{\sigma\};t)+\sum_i \omega_i(\{\sigma\}_i)P(\{\sigma\}_i;t) \tag{3.1}$$

where the choice of the $\omega_i(\{\sigma\})$ is governed by the same criteria as before.

The dynamical evolution of this model may be simulated by Monte Carlo methods, see for instance Binder (1979) and Ma (1976). The theoretical basis for these methods results from the Markovian character of the dynamics. It can be demonstrated that for any Markov process the waiting time is distributed exponentially. In the present context, given a configuration at time t, the probability that no spin flip occurs during the subsequent interval t' is

$$P(T(\{\sigma\})>t')=\exp(-\Omega(\{\sigma\})t') \tag{3.2}$$

where $T(\{\sigma\})$ is the waiting time in the current configuration and $\Omega(\{\sigma\})$ is given by

$$\Omega(\{\sigma\})=\sum_i \omega_i(\{\sigma\}). \tag{3.3}$$

The probability that nothing happens for t' and then one spin flips during the subsequent interval $\mathrm{d}t'$ is given by

$$p(t')\,\mathrm{d}t'=\Omega(\{\sigma\})\exp(-\Omega(\{\sigma\})t')\,\mathrm{d}t' \tag{3.4}$$

and the probability that the spin which flips is σ_i is

$$\omega_i(\{\sigma\})/\Omega(\{\sigma\}) \tag{3.5}$$

combining these two results, we see that the probability that the earliest flip occurs between t' and $t'+\mathrm{d}t'$ and involves the spin at site i is given by

$$P_i(t')\,\mathrm{d}t'=\omega_i(\{\sigma\})\exp[-\Omega(\{\sigma\})t']\,\mathrm{d}t'. \tag{3.6}$$

We now outline the two main schemes for simulating this dynamic behaviour: the first scheme is an 'event-by-event' simulation, as used by Ma (1976), Yalabik and Gunton (1979) and others, which is a faithful realisation of the above continuous time process; the second scheme is a 'timestep-by-timestep' simulation, essentially a discrete time interpretation of the standard Monte Carlo method already discussed in § 2.

The first scheme, due to Ma (1976), may be summarised as follows. Two pseudo-random numbers are generated to determine both the time t' and which spin, σ_i, to flip according to (3.4) and (3.5) respectively. In practice two uniformly distributed random numbers $0<x$, $y<1$ are generated and t' is given by

$$t'=-(\log x)/\Omega. \tag{3.7}$$

To determine i, the interval (0, 1) is divided into N portions of length given by (3.5), where N is the total number of spins; the random number y falls into one of the portions, i, and the spin σ_i is flipped. The whole procedure is then repeated.

The second scheme is the standard single-spin-flip Monte Carlo method, discussed in § 2, with the choice of active sites made randomly. This is the discrete time analogue of the first scheme, the master equation (3.1) being approximated by (2.6) (with the W's replaced by ω_i's). For the values of N which are of interest, the time increment Δt is short compared with any relevant physical time scale and in the thermodynamic limit the approximation becomes exact (see Binder 1979).

In the first scheme a spin is flipped at every elementary step so we call this an 'event-by-event' approach; in the second scheme each elementary step consists of a spin-flip trial which take place at discrete intervals in time so we call this a 'timestep-by-timestep' approach. The correspondence between time and the number of configurations generated is different in the two schemes. In order to identify the units of time used let us calculate the mean time, τ, until the next spin flip in both schemes. In the first scheme τ is given by

$$\tau = \int_0^\infty \Omega \exp[-\Omega t] t \, \mathrm{d}t$$
$$= 1/\Omega. \tag{3.8}$$

In the second scheme let P_k be the probability that the next event will take place at step k. For $k = 1$ we have

$$P_1 = \sum_i \omega_i / N = \Omega / N$$

so

$$P_k = (1 - \Omega/N)^{k-1} \Omega/N$$

and τ is given by

$$\tau = \sum_k kP_k = N/\Omega \qquad \text{in steps}$$
$$= 1/\Omega \qquad \text{in MCS/spin.} \tag{3.9}$$

By identification, one unit of time in scheme 1 is equivalent to one MCS/spin in scheme 2. We now turn to the merits of both schemes from the computational point of view.

In the first scheme knowledge of Ω and of all the ω's is required. For the selection of i we can use cumulated variables C_{i}, defined by $C_i = \Sigma\omega_j$ ($C_N = \Omega$), to divide up the interval (0, 1). After the spin flip has occurred we do not have to recalculate all the C's, but only those at site i and its nearest neighbours and we have to shift those C_j's with 'higher' index j than the modified C's by fixed amounts that are easily determined. The most time consuming steps are updating the C's and selecting the site i. Much of this computation and book-keeping is avoided in the other scheme, where knowledge of Ω is not required and ω_i need only be calculated when the site i is selected. However, computing time is wasted on unsuccessful spin-flip trials; at high temperatures most trials are successful but at low temperatures most are not. There is a trade-off between the extra computational requirements of the first scheme and the physical inefficiency of the second scheme, which favours the first scheme as the temperature is lowered. Recent simulations of dynamic critical phenomena have tended to employ the first scheme, Ma (1976), Yalabik and Gunton (1979), and Takano (1982) for instance. Several parts of the computation can be processed efficiently using parallel processing, the updating of the C's for instance, but the restriction to single spin flips does not make the best use of an array processor. In order to fully exploit the architecture of an array processor we have to abandon the constraint of single spin flips and use parallel updating; this dictates a timestep-by-timestep approach, with many trials occurring within a timestep.

The dynamic interpretation of parallel updating is similar to that of the standard Monte Carlo method. The timestep, Δt, is no longer short compared with the shortest physical time scale, and we expect the short time behaviour to be different from that governed by (3.1). After one MCS/spin, N spin-flip trials, in the standard method some spins will have been considered more than once and others not at all, whereas in parallel updating all the spins will have been given the opportunity to flip in one MCS/spin; furthermore the sequential order in which the spins are sampled in parallel updating also has dynamic consequences. Although there are dynamical differences between the two methods we expect, on the grounds of universality, that the interesting long time dynamical critical behaviour will be correctly captured by parallel updating. Evidence to support this claim will be given in § 4.

4. Results: one and two-dimensional kinetic Ising models

An exact solution of (3.1) has been given by Glauber (1963) for the case of a one-dimensional Ising chain, with flipping probabilities given by

$$\omega_i(\{\sigma\}) = \tfrac{1}{2}(1 - \tfrac{1}{2}\gamma\sigma_i[\sigma_{i-1} + \sigma_{i+1}]) \tag{4.1}$$

with

$$\gamma = \tanh 2K.$$

A comparison of simulated results with the exact results provides a good test of the dynamic interpretation of the parallel updating technique. The exact results we require are given by

$$M(t) \equiv \sum_j \langle\sigma_j(t)\rangle = \exp[-(1-\gamma)t] \sum_j \langle\sigma_j(0)\rangle \tag{4.2}$$

$$\langle\sigma_j(t)\sigma_k(t+t')\rangle_{\mathrm{eq}} = \exp(-t') \sum_{m=-\infty}^{\infty} \eta^{|j-k+m|} I_{\mathrm{m}}(\gamma t') \tag{4.3}$$

where $I_{\mathrm{m}}(x)$ is a modified Bessel function and $\eta = \tanh K$. From (4.3) we obtain the autocorrelation function,

$$\Gamma(t) \equiv \langle\sigma_i(0)\sigma_i(t)\rangle_{\mathrm{eq}} = \exp(-t) \sum_{m=-\infty}^{\infty} \eta^{|m|} I_{\mathrm{m}}(\gamma t) \tag{4.4}$$

when (a) $\gamma t \gg 1$ and (b) both $\gamma t \gg 1$ and $1 - \eta \ll 1$ we have

$$\Gamma(t) \sim (1+\eta)/2\eta^{1/2}(1 - \mathrm{erf}[(1-\eta)^2\gamma t/2\eta]^{1/2}) \tag{4.4a}$$

$$\Gamma(t) \sim 1 - \mathrm{erf}[t/2\xi^2]^{1/2} \tag{4.4b}$$

where

$$\xi = -1/\log(\tanh K) \tag{4.5}$$

is the correlation length.

In order to investigate the dynamics of the parallel (or sublattice) updating technique we have performed simulations on 1D Ising chains containing 4096 sites connected in a ring. Where appropriate we have taken advantage of our knowledge of the static behaviour to set up initial configurations that are typical of equilibrium. Figures 1 and 2 and tables 2 and 3 give the results for the simulations using Glauber flipping probabilities. Two values of the coupling, K, were chosen to yield correlation lengths of 10 and 20 lattice spacings (as given by (4.5)). The numbers in parentheses indicate the statistical uncertainty in the last digit as estimated by calculating the standard deviation of the data from 1000 independent runs. As one can see from the data we find good agreement with the exact results (except at short times) when an overall time rescaling by a factor of 2 is taken into account.

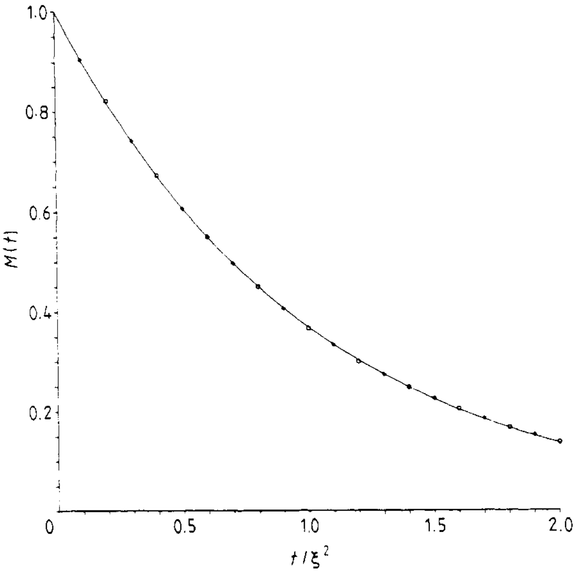

Figure 1. A plot of the magnetisation decay in the 1D Glauber model simulated by sublattice updating. ◆, Correlation length = 20; ○, corelation length = 10; curve gives exact results for a single-spin-flip realisation up to a time rescaling.

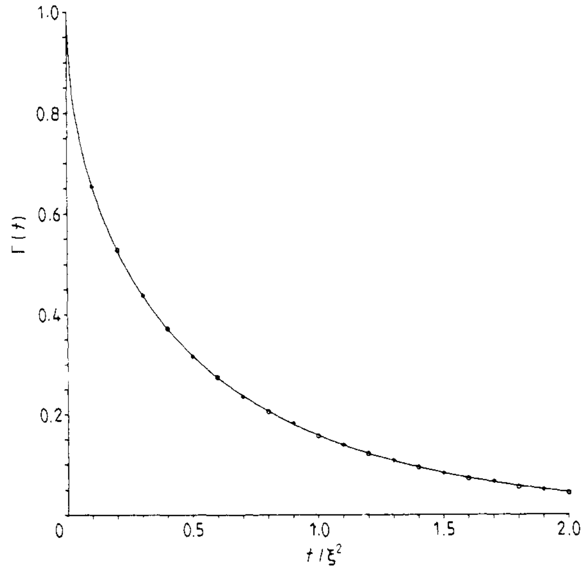

Figure 2. A plot of the autocorrelation function in the 1D Glauber model simulated by sublattice updating. ◆, Correlation length = 20; ○, correlation length = 10; curve gives exact results for a single-spin-flip realisation up to a time rescaling.

The critical (low temperature; $\xi \to \infty$) dynamics of the random single spin-flip 1D Glauber model can be understood in terms of the motion of domain boundaries as discussed by Cordery, Sarker and Tobochnik (1981), hereafter referred to as CST. A spin sitting at a domain boundary has one neighbour up and the other down and has

Table 2. Comparison of simulated and exact results for the magnetisation decay in the 1D Glauber model.

t/ξ^2	M_{exact}	t_{sim}/ξ^2	$M_{\text{sim}}(t/\xi^2)$ $(\xi = 10)$	$M_{\text{sim}}(t/\xi^2)$ $(\xi = 20)$
0	1.000	0	1.000	1.000
0.4	0.819	0.2	0.822 (1)	0.818 (1)
0.8	0.671	0.4	0.672 (1)	0.669 (2)
1.2	0.549	0.6	0.549 (2)	0.548 (2)
1.6	0.450	0.8	0.449 (2)	0.448 (2)
2.0	0.368	1.0	0.365 (2)	0.366 (3)
2.4	0.302	1.2	0.298 (2)	0.301 (3)
2.8	0.247	1.4	0.247 (2)	0.245 (3)
3.2	0.202	1.6	0.204 (2)	0.205 (2)
3.6	0.166	1.8	0.166 (2)	0.166 (3)
4.0	0.136	2.0	0.136 (2)	0.138 (3)

Table 3. Comparison of simulated and exact results for the autocorrelation function in the 1D Glauber model.

t/ξ^2	$\Gamma(t/\xi^2)$ (4.4*b*)	t_{sim}/ξ^2	$\Gamma_{\text{sim}}(t/\xi^2)$ $(\xi = 10)$	$\Gamma_{\text{sim}}(t/\xi^2)$ $(\xi = 20)$
0	1.000	0	1.000	1.000
0.4	0.527	0.2	0.529 (1)	0.527 (1)
0.8	0.371	0.4	0.372 (1)	0.371 (2)
1.2	0.273	0.6	0.274 (1)	0.271 (2)
1.6	0.206	0.8	0.205 (1)	0.206 (2)
2.0	0.157	1.0	0.156 (2)	0.158 (2)
2.4	0.121	1.2	0.121 (2)	0.122 (2)
2.8	0.094	1.4	0.094 (2)	0.096 (2)
3.2	0.074	1.6	0.073 (2)	0.075 (2)
3.6	0.058	1.8	0.056 (2)	0.056 (2)
4.0	0.045	2.0	0.044 (2)	0.046 (2)

a constant flip rate $\frac{1}{2}$, whereas a spin sitting inside a domain is aligned with both of its neighbours and has a flip rate $1/2(1-\gamma)$ which is proportional to ξ^{-2} at low temperatures. So, as CST argue, the dominant way for correlations to decay is by the random motion of the domain boundaries (the motion is random since spins on either side of the domain boundary are equally likely to be selected for spin-flip trials). Simple random walk arguments show that the time taken for an average domain of length 2ξ to be destroyed is proportional to ξ^2 yielding a dynamical critical exponent $z = 2$ as found by Glauber.

The time rescaling for the sublattice updating results can be understood quantitatively in terms of correlations between the steps of the domain boundary random walk, arising from the regular order in which the spins are sampled. To see how these correlations arise we will consider the behaviour of a single domain boundary. Suppose the site immediately to the left of the boundary is active and the resulting spin-flip trial leads to a successful spin flip then the domain boundary moves one step to the left. Since even and odd sites are alternatively active the domain boundary again finds the site immediately to the left of the boundary active and the spin-flip trial leads with equal probability to either the boundary again moving one step to the left or not moving at all. If the boundary does move to the left then on the next step it will again have equal probability of continuing to the left or of not moving at all. On the other hand if the boundary does not move then on the next step it will have equal probability of either moving to the right or of not moving at all. In general if the boundary does not move for an even number (including zero) of steps it will, on the next trial with equal probability, either not move or move on in the same direction as it previously moved; if it does not move for an odd number of steps it will, on the next trial with equal probability, either not move or move in the opposite direction to its previous move. Let us call this a type A walk. The random walk behaviour of the domain boundary when random single spin-flip updating is used corresponds to a walk with probabilities of $\frac{1}{2}$ for not moving, of $\frac{1}{4}$ for moving to the left, and of $\frac{1}{4}$ for moving to the right. Let us call this a type B walk. Let $d(n)$ denote the distance travelled by the boundary after n steps; then for the two processes described above it is easy to show that

$$\langle d^2(n)\rangle_{\mathrm{A}} = n - \tfrac{1}{2}, \qquad \langle d^2(n)\rangle_{\mathrm{B}} = \tfrac{1}{2}n. \tag{4.6}$$

For large n the two types of walk differ essentially by a time rescaling (time corresponding to n) and following the arguments of CST this accounts for the observed time rescaling necessary to match the simulation results on to the Glauber results.

Table 4 shows the results for simulations using sublattice updating with Metropolis flipping probabilities

$$\omega_i(\{\sigma\}) = \min\{1, \exp(-2K\sigma_i[\sigma_{i-1} + \sigma_{i+1}])\}. \tag{4.7}$$

Two values of the coupling, K, were chosen to yield correlation lengths of 40 and 80 lattice spacings, again results are taken from 1000 independent runs. The data show that time is scaled by ξ and not ξ^2, yielding a dynamical critical exponent $z = 1$. We see that Metropolis sublattice updating realises a different dynamic universality class, although random single-spin-flip Metropolis updating realises the same dynamic universality class as Glauber updating. This result is easily understood in terms of domain boundary motion and the regular order in which the spins are sampled. We see from (4.7) that when a spin sitting at a domain boundary is selected the spin-flip trial automatically leads to a flip; this coupled with the alternating activity of the even and odd sites leads to propagation rather than diffusion of the domain boundaries, and

Table 4. Metropolis simulation of the autocorrelation function in the 1D kinetic Ising model.

t	$\Gamma(t)$ $(\xi = 40)$	t	$\Gamma(t)$ $(\xi = 80)$
0	1.000	0	1.000
5	0.764 (1)	10	0.764 (1)
10	0.560 (2)	20	0.559 (2)
15	0.388 (2)	30	0.387 (3)
20	0.250 (3)	40	0.247 (4)
25	0.141 (3)	50	0.138 (4)
30	0.059 (3)	60	0.058 (4)
35	0.001 (3)	70	0.000 (4)
40	−0.036 (3)	80	−0.036 (4)

hence a decay time proportional to ξ. This simple example illustrates the need to ensure that the update procedure captures the essential physics correctly.

We have also considered another model where domain boundary creation and annihilation processes have been totally suppressed,

$$\omega_i(\{\sigma\}) = \tfrac{1}{4}(1 - \sigma_{i-1}\sigma_{i+1}) \qquad (4.8)$$

in this model the number of boundaries is conserved. In the simulations we set up initial configurations typical of equilibrium with correlation lengths of 10 and 20 lattice spacings. The results taken from 1000 independent runs are shown in figure 3 and table 5. Harris (1982) has shown that the asymptotic long time behaviour of the

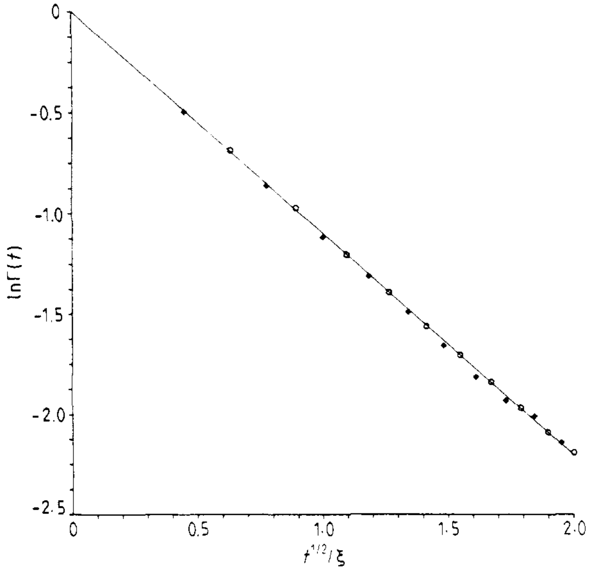

Figure 3. A plot of the autocorrelation function in the 1D domain boundary diffusion model simulated by sublattice updating. ◆, Correlation length = 20; ○, correlation length = 10; line gives exact results for a single-spin-flip realisation up to a time rescaling.

Table 5. Simulation of a domain wall diffusion model.

t/ξ^2	$\Gamma_{\rm sim}(t/\xi^2)$ $(\xi = 10)$	$\Gamma_{\rm sim}(t/\xi^2)$ $(\xi = 20)$
0	1.000	1.000
0.4	0.502 (1)	0.494 (1)
0.8	0.378 (1)	0.370 (2)
1.2	0.300 (2)	0.295 (2)
1.6	0.249 (2)	0.247 (2)
2.0	0.210 (2)	0.207 (2)
2.4	0.182 (2)	0.178 (2)
2.8	0.159 (2)	0.156 (2)
3.2	0.140 (2)	0.135 (2)
3.6	0.124 (2)	0.118 (2)
4.0	0.112 (2)	0.111 (2)

autocorrelation function is given by

$$\Gamma(t) \sim \exp(-[2t/\pi\xi^2]^{1/2}). \tag{4.9}$$

The simulation results as shown in figure 3 are in agreement with (4.9) up to a time rescaling which is again accounted for by the regular order in which the spins are sampled.

It is encouraging to note that for both the Glauber model and the domain boundary diffusion model the sublattice updating scheme yields not only the correct dynamical exponent but also the correct scaling forms of the autocorrelation functions as derived from random single-spin-flip dynamics. In other words the regular multi-spin-flip and random single-spin-flip schemes lie in the same dynamic universality class provided the essential character of the dynamics is respected.

We have also used sublattice updating in a study of the dynamical critical behaviour of the 2D kinetic Ising model (Williams 1985). Using both Glauber and Metropolis schemes we looked at the long time behaviour of various time-delayed correlation functions and found evidence for universal behaviour obtaining the same value for the dynamical exponent from both schemes. The long time behaviour of this model is controlled by the slow relaxation of the magnetisation and this is captured by both updating schemes. There is, however, an overall time rescaling of the correlation functions between the two schemes that does not appear to be trivially related to the microscopic flip rates. Apart from this detail the 2D simulations are understood and yield the same critical behaviour as would be obtained from random single-spin-flip schemes up to an overall time rescaling.

5. Concluding remarks

In the preceding sections we discussed multi-spin coding and introduced the idea of parallel updating. We then went on to discuss the two main Monte Carlo approaches to dynamics, namely, 'event-by-event' and 'timestep-by-timestep' simulations. Parallel updating can be interpreted dynamically as a 'timestep-by-timestep' method with random spin sampling replaced by alternate sublattice sampling. We have shown that provided the update scheme reflects the essential character of the microscopic dynamics then the universal dynamical behaviour is obtained. In particular, in 1D the choice of Metropolis flip rates in conjunction with the regular spin sampling imposed by parallel updating removes the element of randomness in the motion of domain boundaries leading to anomalous behaviour, whereas the choice of Glauber flip rates and parallel updating maintains the randomness of the domain boundary motion yielding results consistent, up to a time rescaling, with exact results for the original random single-spin-flip version of the model.

A general feature of parallel or sublattice updating is that an overall time rescaling occurs with respect to random single-spin-flip dynamics which appears always to reduce the relaxation times. This arises from the regular order in which the spins are sampled, and a more detailed explanation was given in the previous section for the 1D Glauber model. A detailed understanding of the 2D dynamics is still needed, but this will probably require a dynamical droplet picture extending the static droplet picture of Bruce and Wallace (1983).

Although the recent trend in simulation work on dynamical critical phenomena has been to adopt 'event-by-event' methods we would point out that 'timestep-by-timestep' methods in conjunction with parallel updating (implemented by either parallel processing or multi-spin coding on serial machines) offer two advantages. The first is much improved computational efficiency; the second is the above mentioned time rescaling both of which increase the effective speed of the simulation, a crucial factor when attempting to probe the large length and time scales essential for studying dynamical critical phenomena.

The parallel updating approach has been used in a Monte Carlo renormalisation group study of the dynamical critical behaviour of the 2D kinetic Ising model (Williams 1985). It would be of interest to use this approach to study models in other dynamical universality classes, particularly where very slow relaxational behaviour is involved where again the computational efficiency would be advantageous.

Acknowledgments

I would like to thank C K Harris, G S Pawley, D J Wallace and, in particular, A D Bruce for helpful discussions and the SERC and ERCC for providing computer time on an ICL Distributed Array Processor. I would also like to thank the SERC for financial support whilst this work was carried out.

References

Binder K 1979 in *Statistical Physics* ed K Binder (*Topics in Current Physics*) (Berlin: Springer)
Bruce A D and Wallace D J 1983 *J. Phys. A: Math. Gen.* **16** 1721
Cordery R, Sarker S and Tobochnik J 1981 *Phys. Rev.* B **24** 5402
Glauber R J 1963 *J. Math. Phys.* **4** 294
Harris C K 1982 Unpublished
Hockney R W and Jesshope C R 1981 in *Parallel computers* (Bristol: Adam Hilger)
Landau D P 1976 *Phys. Rev.* B **13** 2997
Ma S K 1976 *Phys. Rev. Lett.* **37** 461
Pawley G S, Swendsen R H, Wallace D J and Wilson K G 1984 *Phys. Rev.* B **29** 4030
Takano H 1982 *Prog. Theor. Phys.* **68** 493
Williams J K 1985 *J. Phys. A: Math. Gen.* **18** 49
Yalabik M C and Gunton J D 1979 *Prog. Theor. Phys.* **62** 1573
Zorn R, Herrmann H J and Rebbi C 1981 *Comp. Phys. Commun.* **23** 337