Algorithms for Faster and Larger Dynamic Metropolis Simulations

M.A. Novotny*, Alice K. Kolakowska* and G. Korniss†

* Dept. of Physics and Astronomy, ERC Center for Computational Sciences, P.O. Box 5167, Mississippi State University, Mississippi State, MS 39759-5167
† Dept. of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, 110 8th Street, Troy, NY 12180-3580

Abstract. In dynamic Monte Carlo simulations, using for example the Metropolis dynamic, it is often required to simulate for long times and to simulate large systems. We present an overview of advanced algorithms to simulate for longer times and to simulate larger systems. The longer-time algorithm focused on is the Monte Carlo with Absorbing Markov Chains (MCAMC) algorithm. It is applied to metastability of an Ising model on a small-world network. Simulations of larger systems often require the use of non-trivial parallelization. Non-trivial parallelization of dynamic Monte Carlo is shown to allow scalable algorithms, and the theoretical efficiency of such algorithms are described.

INTRODUCTION

Dynamic Monte Carlo is used when dynamic information about a particular system is required. For example, for spin-1/2 lattice systems, starting from a quantum Hamiltonian coupled to a heat bath, the underlying dynamic for the Ising model can be derived as: 1) randomly and uniformly choose one spin; 2) decide whether or not to flip the spin based on a spin-flip probability \( p \). The functional form for \( p \) may for instance be Metropolis [1], Glauber (derivable from coupling the quantum system to a fermionic heat bath [2]), or a form obtained from coupling the quantum system to a bosonic heat bath [3]. Since the simulated dynamic is defined by the underlying physical system, it should not be altered. While remaining faithful to the dynamic, algorithms that allow for long-time simulations and non-trivial parallelization are still possible. Some of these algorithms will be presented (for a review see [4]).

In this article we review the use of the Monte Carlo with Absorbing Markov Chains (MCAMC) method and apply the method to an Ising ferromagnet on a small-world network. We also describe the use of ideas from non-equilibrium surface science to study the theoretical scalability of non-trivial parallelization applied to parallel discrete event simulations (PDES), such as the dynamic Monte Carlo method.
### TABLE 1. The spin arrangements for the first 7 of 12 spin classes used in the MCAMC calculations. The energies associated with these spin configurations enter the spin flip probabilities, $p_i$.

| Spin Orientation | Number of nn spins | Small-world spin | Flip Probability |
|------------------|--------------------|------------------|-----------------|
| $\uparrow$      | 2                  | $\uparrow$       | $p_1$           |
| $\uparrow$      | 1                  | $\uparrow$       | $p_2$           |
| $\uparrow$      | 0                  | $\uparrow$       | $p_3$           |
| $\uparrow$      | 2                  | $\downarrow$     | $p_4$           |
| $\uparrow$      | 1                  | $\downarrow$     | $p_5$           |
| $\uparrow$      | 0                  | $\downarrow$     | $p_6$           |
| $\downarrow$    | 2                  | $\uparrow$       | $p_7$           |

### FASTER DYNAMIC METROPOLIS SIMULATIONS

In dynamic Monte Carlo simulations, the dynamic is given by the underlying physical system, so it cannot be changed. Consequently, many of the well-known algorithms, such as loop algorithms, cluster algorithms, and multicanonical algorithms cannot be used since they are not faithful to the dynamic. Furthermore, one Monte Carlo step per spin (MCSS) corresponds to an underlying microscopic time [3], which often is much shorter than the time scale needed for the simulation. For example, in simulating ferromagnets a Monte Carlo step is approximately an inverse phonon frequency [2, 3], about $10^{-13}$ seconds. The lifetime of a metastable state desired for device time scales is years for magnetic recording. In modeling paleomagnetism, the time scales of the metastable state are millions of years. To simulate over such disparate time scales requires faster-than-real-time algorithms.

Whenever the rejection rate is high, event-driven rejection-free methods are useful. These include the $n$-fold way [5] and its generalization to the MCAMC method [6]. A rejection-free algorithm for continuous spin systems has recently been published [7]. An alternative algorithm for first-passage times is the projective dynamics method [8]. These algorithms can often accelerate simulations by many orders of magnitude.

Here we apply the MCAMC method to study metastability of the Ising model on a small-world network. The Hamiltonian is

$$\mathcal{H} = -J_1 \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - J_2 \sum_{i=1}^{N} \sigma_i \sigma_{sw(i)} - H \sum_{i=1}^{N} \sigma_i.$$  \hspace{1cm} (1)

Here $\sigma_i = \pm 1$, $J_1$ is the ferromagnetic interaction along the chain, $J_2$ is a ferromagnetic interaction for the small-world connections (see below), and $H$ is the applied external field. We use periodic boundary conditions for the $N$ Ising spins. Each Ising spin has one small-world connection. It is obtained by starting with the first spin, and randomly connecting it to any of the other $N-1$ spins. If the next spin is not yet connected with a small-world connection, one of the remaining unconnected spins is randomly connected to it. These connections are quenched, and do not change in a particular simulation. Many quenched random small-world bond configurations are needed to determine the effect of the randomness.
The applied Monte Carlo dynamic is: 1) one of the $N$ spins is chosen at random, 2) a uniform deviate $r$ on $(0,1]$ is chosen, and 3) the chosen spin is flipped if the Glauber flip probability \( r \leq \exp(-E_{\text{new}}/T)/[\exp(-E_{\text{new}}/T) + \exp(-E_{\text{old}}/T)] \). Here Boltzman’s constant has been set to unity, $E_{\text{old}}$ is the energy of the current spin configuration, and $E_{\text{new}}$ is the energy of the spin configuration with the chosen spin flipped. We start with all spins $\sigma = +1$, apply a field $H < 0$, and measure the lifetime $\tau$ until the magnetization is first equal to zero. Using the same quenched random small-world bonds, we average over many such escapes to obtain the average lifetime $\langle \tau \rangle$ measured in MCSS.

To measure a metastable lifetime, one needs to be below the critical temperature, $T_c$. We estimate $T_c$ using the Binder fourth-order cumulant of the order parameter [9]. Similar equilibrium studies of small-world Ising ferromagnets have recently been performed [10]. The crossings of this cumulant provide a straightforward way of estimating $T_c$ (Fig. 1(a)). The average lifetime for $T < T_c$ grows exponentially in $T^{-1}$ (Fig. 1(b)). This necessitates the use of faster-than-real-time algorithms.

One way of accelerating the computations is to use a rejection-free algorithm. This includes the $n$-fold way algorithm [5] in continuous time, but it also has a counterpart in discrete time [4, 6]. When all spins are $+1$, then the probability of flipping a single spin in one step is $p_1$ and the average time required before a spin flips is $p_1^{-1}$. Therefore, for small $p_1$, computations can be accelerated by asking how long it takes to change from the state of all spins up to the state with one overturned spin. This is an example of the $s = 1$ MCAMC algorithm ($s = 1$ transient state, the current state). Whenever the spins are all $+1$, the time increment $m = \lfloor \ln(r_1)/\ln(1 - p_1) \rfloor + 1$ is added, and a randomly chosen spin is flipped. Here $r_1$ is a uniformly distributed random number on $(0,1]$, $\lfloor \cdot \rfloor$ is the integer part, and all spins are equivalent, so we can randomly pick one to flip (in the language of the $n$-fold way algorithm, all spins are in the same spin class).

At low temperatures and small fields the $s = 1$ MCAMC algorithm still does not give the best performance. However, the performance can be improved by adding additional
states to the transient subspace. For example, for \( s = 2 \) in this model, the transient part of the absorbing Markov chain is

\[
T = \begin{pmatrix} 1 - x - (p_7/N) & p_7/N \\ p_1 & 1 - p_1 \end{pmatrix}.
\]  

Here \( x \) is defined below. Then, whenever all spins are \(+1\), the time increment \( m \) that is added to \( \tau \), corresponding to exiting to a state with two overturned spins, is given using a uniform random deviate \( r_1 \) in \((0, 1]\) by the solution of

\[
\vec{v}_1^T T^m \vec{e} < r_1 \leq \vec{v}_1^T T^{m-1} \vec{e}
\]

where \( \vec{e}^T = (1, 1) \) and the initial vector is \( \vec{v}_1^T = (0, 1) \).

Once the time increment \( m \) to exit the transient subspace is obtained, the next spin configuration must be found, i.e. a configuration with two overturned spins. Let \( N_2 \) be the number of small-world bonds that connect nearest-neighbor (nn) spins. Let \( x = x_1 + x_2 \) with

\[
\begin{align*}
x_1 &= \frac{N - N_2}{N^2} [2p_2 + p_4 + (N - 4)p_1] = \frac{N - N_2}{N^2} y_1 \\
x_2 &= \frac{N_2}{N^2} [p_5 + p_2 + (N - 3)p_1] = \frac{N_2}{N^2} y_2.
\end{align*}
\]

Then the new spin configuration is chosen, using uniformly distributed random numbers \( r_i \) for \( i = 2, \cdots, 6 \).

If \( r_2 x > x_1 \), one of the spin pairs with small-world bonds longer than nn is randomly chosen using \( r_3 \), one of these two spins is chosen with \( r_4 \) and is flipped. If \( r_5 y_1 < 2p_2 \), using \( r_6 \) one of the two nn spins along the chain is chosen and flipped. If \( 2p_2 < r_5 y_1 \leq 2p_2 + (N - 4)p_1 \), the spin connected to the flipped spin by the small-world bond is flipped. If neither of the two conditions above involving \( r_5 \) is satisfied, then \( r_6 \) is used to choose one of the other \( N - 4 \) spins (except the flipped spin or the 3 spins it is connected to), and the chosen spin is flipped.

If \( r_2 x \leq x_1 \) a similar procedure is used for spins belonging to the \( N_2 \) doubly-connected bonds.

The MCAMC algorithms do not change the dynamics, but rather only implements the dynamics in a fashion that enables simulations to longer lifetimes. Results for the average lifetime obtained from \( 10^3 \) escapes for one realization of the quenched small-world bonds are shown in Fig. 1(b).
virtual time horizon in the Kardar-Parisi-Zhang (KPZ) universality class \cite{13}. Provided that this is the case, then all short-ranged asynchronous parallel DES simulations can be made to be perfectly scalable. This is because, as the number of processing elements (PEs) goes to infinity, the utilization stays finite \cite{12}, and the measurement portion of the algorithm can be bounded \cite{14}. A brief review is presented here.

The stochastic nature of the Metropolis dynamic makes it difficult to utilize a parallel computing environment to the fullest extent because \textit{a priori} there is no global clock to synchronize physical processes in a system with asynchronous dynamics. However, the system is not inherently serial.

The methodology for PDES simulations works in all dimensions, but for simplicity we consider parallelization of dynamic Monte Carlo for a one-dimensional Ising model. In non-trivial parallelization, the spin system is spatially distributed among \( L \) processing elements, i.e., physical processes and interactions between physical subsystems are mapped to logical processes and logical dependences between PEs (Fig. 2). In our model of PDES performance for the spin system with \( n \) interactions, we consider an ideal system of \( L \) identical PEs, arranged on a ring, where communications between PEs take place instantaneously. Each PE manages the state of the assigned subsystem of \( N \) spins, and has its own time (called the local virtual time, LVT). The LVT progresses on each PE during the simulation. The asynchronous nature of physical dynamics implies an asynchronous system of logical processes. Logical processes execute concurrently and exchange time-stamped messages to perform state updates of the entire physical system being simulated. A sufficient condition for preserving causality in simulations requires that each logical process works out the received messages from other logical processes in non-decreasing time-stamp order \cite{15, 16}. PDES are classified in two categories: optimistic \cite{15} and conservative \cite{17, 18, 19}. In conservative PDES, an algorithm does not allow a logical process to advance its LVT (i.e., to proceed with computations) until it is certain that no causality violation can occur. In optimistic PDES, an algorithm allows a logical process to advance its LVT regardless of the possibility of a causality error. The optimistic scenario detects causality errors and provides a recovery procedure to detect and fix such errors. Several aspects of a PDES algorithm should be considered in efficiency studies, including: the synchronization procedures; the average utilization \( \langle u \rangle \) of the parallel environment as measured by the mean fraction of working PEs between update attempts; the memory requirements per PE; and the scalability as measured by evaluating the performance when \( L \) is increased.

In our study the main concept is the virtual time horizon (VTH), defined as the set of the LVTs for all logical processes. We model the growth of the VTH as a deposition process of Poisson random time increments on a one-dimensional lattice of \( L \) processors. The growth rule of the VTH is defined by the PDES algorithm. The width of the VTH provides a measure of the desynchronization in the system of PEs and is related to the memory requirements for parallel simulations \cite{14, 20, 21}. Here the principle is: the larger the width, the larger the memory required per PE. The asymptotic scalability of an algorithm can be assessed by applying coarse-grained methods to the VTH \cite{12}. Computational speed-up (as measured by comparing the performance of the parallel with sequential simulations) can be derived from the microscopic structure of the VTH \cite{22}.

In modeling a conservative PDES, at each update attempt \( t \), on each PE the simulation
algorithm randomly selects one of the \( N \) spin sites. If the selected site is an interior site, the update happens and the simulated LVT is incremented for the next update attempt: 
\[
\tau(t+1) = \tau(t) + \eta,
\]
where \( \eta \) is a random time increment that is sampled from the Poisson distribution with unit mean. If the selected site is a border site, the PE must wait until the LVT of its neighbor(s) is not less than its own LVT, at which time the waiting PE makes the update and proceeds. For \( N = 1 \) the LVT of both neighboring PEs are considered, while for \( N > 1 \) only the corresponding neighboring PE’s LVT is considered.

In the most unfavorable case of conservative parallelization \( N = 1 \). For such a closed spin chain the mean utilization \( \langle u(L; N = 1) \rangle \) of the parallel processing environment is simply the mean density of local minima in the conservative VTH during the steady state. Analyzing the microscopic structure of the VTH at saturation, it is possible to derive approximate analytical formulas for \( \langle u(L; N) \rangle \) and the higher moments of \( u(L; N) \) (Fig. 3(a)). For example,
\[
\begin{align*}
\langle u(L; 1) \rangle &= (L+1)/4L, \quad L \geq 3 \\
\langle u(L; 2) \rangle &= (3L+1)/8L, \quad L \geq 3.
\end{align*}
\]

Note that as \( L \to \infty \), the utilization is about 1/4 for \( N = 1 \) and about 3/8 for \( N = 2 \). For large \( N \), the asymptotic utilization can be near the theoretical limit of unity.

The conservative PDES utilization depends on \( N \), as well as on the number \( N_b \) of effective border lattice sites per PE (here \( N_b = 2 \)), and on the communication topology. Our earlier large-scale simulations \[21\] show that the worst-case \( (N = 1) \) conservative scenario for a spin chain can be greatly improved when \( N \) is increased while retaining the ring communication topology with \( N_b = 2 \) (Fig. 3(b)). Thus, to take the best advantage of conservative parallelization one should use many PEs with many spins per PE [see

\textbf{FIGURE 2.} The mapping of short-ranged physical processes to logical processes. The nn physical interactions (two-sided arrows in the left part) on a lattice with periodic boundary conditions are mapped to the ring communication topology of logical processes (two-sided arrows in the right part). Each PE carries \( N \) lattice sites, but communications take place only for border sites.
FIGURE 3. (a) The steady-state mean utilization vs the system size in conservative PDES for a spin chain with \( N = 1 \). Analytical result (solid curve); infinite-\( L \) limit (dashed line); and simulation data (symbols). (b) The time evolution of the mean utilization in conservative PDES for spin chains when each PE carries \( N \) spin sites, two of which are the effective border sites. Observe that the utilization grows with \( N \).

In this case, preliminary analysis of the width of the VTH shows it scales as:

\[
\langle w(t) \rangle \sim \begin{cases} 
  t^{\beta_1}, & t \ll t_1 \\
  t^{\beta_2}, & t_1 \ll t \ll t_2 \\
  L^{\alpha} \sqrt{N}, & t \gg t_2
\end{cases}
\]  

(7)

where \( \alpha = 1/2 \) and the cross-over times are: \( t_1 \sim N \) independent of \( L \); \( t_2 \sim NL^z \). Here \( z = \alpha/\beta_2 \) is the dynamic exponent, and the growth exponents are \( \beta_1 \approx 1/2 \) (corresponding to random deposition) and \( \beta_2 \approx 1/3 \) (corresponding to the KPZ universality class) \[13\]. The scaling exponent \( \alpha = 1/2 \) of the VTH width at saturation (for \( t \gg t_2 \)) implies that the memory requirement for the state savings grows as a power law, i.e., \( \sqrt{LN} \). Recent applications of the conservative algorithm to modeling magnetization switching \[11\] and a dynamic phase transition in highly anisotropic thin-film ferromagnets \[23, 24\] indicate that conservative parallelization can be very efficient in simulating spin dynamics with short-range interactions.

**DISCUSSION AND CONCLUSIONS**

This brief paper has described how to make dynamic Monte Carlo simulations faster and larger. The algorithms described do not change the dynamics in any fashion, but rather implement the dynamics on the computers using advanced techniques.

To accelerate the simulations, faster-than-real-time algorithms may be implemented. These include the \( n \)-fold way algorithm \[3\] and its extension, the Monte Carlo with Absorbing Markov Chain (MCAMC) algorithm \[4, 6\], as well as the projective dynamics
method [8]. We outlined $s = 1$ and $s = 2$ MCAMC methods, as applied to magnetic field-reversal in a ferromagnetic Ising model on a small-world network.

To make the simulations larger, non-trivial parallelization is required. We briefly described how ideas from non-equilibrium surface science can be used to understand such simulations. In particular, all short-ranged conservative PDES should have a virtual time horizon governed by the KPZ universality class. In this case, all short-ranged PDES (such as dynamic Monte Carlo) can be made scalable using a conservative PDES approach. Conservative PDES references include [4, 17, 11, 12, 14]. The alternative implementation, optimistic PDES simulations [15, 16] for dynamic Monte Carlo simulations, have shown some of the difficulties with scalability [25].

ACKNOWLEDGMENTS

Supported in part by NSF grants DMR-0113049 and DMR-0120310.

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