Fast Simulation of Facilitated Spin Models

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Abstract. We show how to apply the absorbing Markov chain Monte Carlo algorithm of Novotny to simulate kinetically constrained models of glasses. In detail we consider the East model in one dimension. We investigate how to maximize the efficiency of the algorithms, and show that simulation times can be improved on standard continuous time Monte Carlo by several orders of magnitude. We discuss how the method can be applied to other kinetically constrained models with specific focus on the 2-spin facilitated FA model.

1. Introduction

One of the key features common to all glassy systems is a remarkable slow down in dynamical behaviour as temperature $T$ is reduced. Typically time scales may be found to grow at best exponentially with inverse temperature and as consequence it is often extremely difficult to probe the long time dynamics of such systems through means of numerical simulation. One way to help alleviate this problem is the use of rejection free algorithms such as the “n-fold way”, or continuous time (CT) Monte Carlo [1, 2]. However, even CT can become an inefficient tool to study some extremely slow systems.

A more recent generalization of the CT approach is Novotny’s Monte Carlo with Absorbing Markov Chains (MCAMC) [3]. This technique has been successfully used in the study of magnetic reversal and nucleation in systems such as the Ising model, see e.g. [3, 4, 5]. In a recent paper [6] we show how to apply the MCAMC method for the simulation of a variety of kinetically constrained models. In this paper we summarize our findings focusing on the particular example of the East model in one dimension. For this simple facilitated spin model we have shown that the MCAMC method allows computational speed gains of several orders of magnitude.

The paper is organized as follows. In Section 2 we outline the workings of the MCAMC technique. Section 3 provides a detailed analysis of its application to the one-dimensional East model. In section 4 we present quantitative results on the algorithms performance and in section 5 we discuss the application of MCAMC to other models with specific reference to the 2-spin facilitated Frederick-Anderson (FA) model in 2 dimensions.

2. Outline of the MCAMC Method

Rejection free algorithms, such as continuous time, can improve on MC for systems where the majority of moves are rejected due to energy or kinetic constraints [2]. Using a knowledge of all the possible moves the algorithm is able to choose one and accept it at each iteration. For slow systems the most likely next move will be to undo the previous step, the system becoming trapped in a small area of the phase space. An MCAMC algorithm can improve further by forcing the system to leave this subspace in one step. To keep the dynamics exact and maintain detailed
balance one must use the formalism of absorbing Markov chains [3] (see [7] for a pedagogical review).

A MC algorithm is an example of a Markov process [8] and is characterized by the Markov matrix \( \mathbf{M} \). If the vector \( \vec{x}_T(m) \) indicates the probability distribution of the system after iteration \( m \), the probability distribution at the next step \( m + 1 \) is given by \( \vec{x}_T(m + 1) = \vec{x}_T(m)\mathbf{M} \). An absorbing Markov chain is now defined by separating the available states into \( s \) transient states and \( r \) absorbing ones [3, 7] so that the general state vector becomes an \((r + s)\)-dimensional vector \( \vec{x}_T = (\vec{u}_T, \vec{v}_T) \) where \( \vec{v}_T \) contains the transient states. With this structure the Markov matrix can be written in the form,

\[
\mathbf{M} = \begin{pmatrix}
\mathbf{I}_{r \times r} & 0_{r \times s} \\
\mathbf{R}_{s \times r} & \mathbf{T}_{s \times s},
\end{pmatrix}
\tag{1}
\]

where \( \mathbf{I} \) is the identity matrix, \( \mathbf{0} \) is the zero matrix and subscripts indicate the size of each matrix. The positions of the identity and zero matrices guarantee that if the system falls into an absorbing state then it does not leave. The transient matrix, \( \mathbf{T} \), gives the probabilities for moving between transient states and the recursive matrix, \( \mathbf{R} \), gives the probabilities for moving from the transient states to the absorbing states. We now list some important results, for a full derivation see [7].

For a given starting vector \( \vec{v}_T \) the probability of still being in the transient subspace, \( p_{\text{trans}} \), after \( m \) steps is

\[
p_{\text{trans}} = \vec{v}_T \mathbf{T}^m \vec{e},
\tag{2}
\]

where \( \vec{e} \) is a vector with all elements equal to 1. The probability of absorbing to a particular state after \( m \) steps is given by summing over the probabilities of absorbing at each time step. This gives the vector \( \vec{p}_{\text{abs}}. \)

\[
\vec{p}_{\text{abs}. \text{after } m} = \vec{v}_T (\mathbf{I} + \mathbf{T} + \cdots + \mathbf{T}^{m-1}) \mathbf{R}.
\tag{3}
\]

If the exit has taken place at step \( m \), then the probabilities of absorbing into the different exit states is given by:

\[
\vec{p}_{\text{abs. at } m} = \frac{\vec{v}_T \mathbf{T}^{m-1} \mathbf{R}}{\vec{v}_T \mathbf{T}^{m-1} \mathbf{R} \vec{e}}
\tag{4}
\]

Here it is convenient to introduce the fundamental matrix

\[
\mathbf{N} = (\mathbf{I} - \mathbf{T})^{-1} = \mathbf{I} + \mathbf{T} + \mathbf{T}^2 + \cdots,
\tag{5}
\]

which can be used to obtain the probability that the system will absorb to a particular state irrespective of when it exits,

\[
\vec{p}_{\text{abs.}} = \vec{v}_T \mathbf{N} \mathbf{R}.
\tag{6}
\]

The fundamental matrix can also be used to determine the average time to leave the transient subspace [3, 7]

\[
\langle \tau \rangle = \vec{v}_T \mathbf{N} \vec{e}.
\tag{7}
\]

Once our system is in the initial state we can generate an exit time by solving the inequality

\[
\vec{v}_T \mathbf{T}^m \vec{e} < \tau \leq \vec{v}_T \mathbf{T}^{m-1} \vec{e},
\tag{8}
\]

where \( \tau \) is a random number between 0 and 1. Next, we use a second random number to choose an absorption state from the distribution in equation (4) and then we can update the system appropriately.
3. Application of MCAMC to Kinetically Constrained Models

Kinetically constrained models (KCMs) are widely used to study the dynamical behaviour of glass formers [9]. These systems often fall into deep energy traps from which it can be difficult to escape. For a given system there may be a multiplicity of trapping states which change as the system evolves dynamically. In order to apply the MCAMC method to KCMs one needs to identify the nature of the transient states in these systems.

As an example consider the East model in one-dimension [10, 9]. The East model consists of a chain of Ising spins, \( n_i = \{0; 1\} \), upon which a directional facilitation constraint is imposed: a given spin \( n_i \) may only flip if its nearest neighbour to the left is in the excited state, \( n_{i-1} = 1 \). The rates for allowed moves are such that the equilibrium distribution is that corresponding to the energy function \( H = J \sum_i n_i \) (we set \( J = 1 \) from now on),

\[
10 \xrightarrow{\epsilon} 11, \quad 11 \xrightarrow{1/N} 10,
\]

where \( \epsilon \equiv e^{-\beta} \) and \( \beta \equiv 1/T \). The result is a model in which excitations propagate in the eastward direction. The East model has been found to reproduce the dynamic behaviour of fragile glassy materials [9, 11, 12].

Consider a configuration with only isolated excitations:

\[
\cdots 100 \cdots 100 \cdots 100 \cdots
\]

This arrangement acts as an effective energy trap. Here one has no choice but to excite a spin and pay the accompanying energy penalty, i.e. it is overwhelmingly likely that the spin will then be relaxed immediately. It is possible to identify two classes of transient state for the system, the isolated configuration shown above and all states in which only a single excitation pair exists. The absorbing states of the system correspond to all arrangements in which two spins have been excited, either forming two isolated doubles or a triplet state,

\[
\cdots 110 \cdots 110 \cdots 100 \cdots
\]

\[
\cdots 111 \cdots 100 \cdots 100 \cdots
\]

In order for the algorithm to be classified by two transient states the initial state must not contain any pair of excitations separated by less than two unexcited spins.

It is possible to classify each lattice site according to its local neighbourhood. Taking a site along with its nearest and next-nearest neighbour to the right, each site can be classed according to a binary labelling scheme, i.e. \( 100 \equiv 4, 110 \equiv 5 \), etc., where the number of sites in each class is, \( N_4, N_5 \), etc. Using this notation we define the entry condition for the algorithm with \( s = 2 \) transient states as the point at which the number of sites in class 4 equals the total number of excitations present in the lattice, \( M \), i.e. \( N_4 = M \).

The transient and recursive states may be labelled as follows,

\[
v_1 = \cdots 100 \cdots 100 \cdots \quad u_1 = \cdots 110 \cdots 110 \cdots \\
v_2 = \cdots 110 \cdots 100 \cdots \quad u_2 = \cdots 111 \cdots 100 \cdots
\]

with the following transition probabilities

\[
P(v_1 \rightarrow v_2) = \frac{\epsilon N_4}{N}, \quad P(v_1 \rightarrow u_2) = 0, \\
P(v_2 \rightarrow v_1) = \frac{1}{N}, \quad P(v_2 \rightarrow u_1) = \epsilon \frac{N_4 - 1}{N}, \\
P(v_1 \rightarrow u_1) = 0, \quad P(v_2 \rightarrow u_2) = \frac{\epsilon}{N}.
\]
where $N$ is the system size.

These transition probabilities are then used to build the transient and recursive matrices for the system

$$T = \begin{pmatrix} 1 - x & x \\ y & 1 - x - y \end{pmatrix} \quad (10)$$
$$R = \begin{pmatrix} 0 & 0 \\ x - \epsilon y & \epsilon y \end{pmatrix} \quad (11)$$

where $x = \frac{\epsilon N}{N^4}$ and $y = \frac{1}{N}$.

The absorption probabilities for the $u_1$ and $u_2$ states can be found by solving equation (4) giving

$$P(u_1) = 1 - \frac{1}{N_4}, \quad (12)$$
$$P(u_2) = \frac{1}{N_4}, \quad (13)$$

where we have used an initial state vector $\vec{v}_T = (1 \ 0)$.

The algorithm then goes as follows: Run the system using a CT ($s = 1$) algorithm until the entry condition is met. Next choose a random number between 0 and 1 and use this to generate an exit time by iteratively solving the inequality in (8). Using another random number an exit state is chosen from the distribution given by equations (12) and (13). Finally all system variables are updated and CT used until the entry condition is met once more.

Computationally the most expensive part of this process is generating the exit time. There are a number of approximations available, the fastest of which is to use the average exit time calculated using equation (7). This does mark a departure from the exact Monte Carlo algorithm, but in most cases it turns out to be a reasonable simplification (it is analogous to the approximation made when going from the n-fold algorithm [1] to the CT one [2]).

It is possible to further the application of the MCAMC technique well beyond the simple $s = 2$ example outlined above. In general, one may construct higher order algorithms by successively adding more and more states of the system into the transient subspace and updating the absorption states in accordance, e.g $s = 3$, $s = 4$ etc. This process can help achieve increasingly large time steps, once again the computational enhancement is offset by the added algorithmic complexity.

4. Speed Tests
In order to compare the performance of the MCAMC algorithm to that of both CT and standard MC it was chosen to compute equilibrium trajectories of length $10^7 \times e^{2\beta}$ for the East model in one dimension. For such simulations the average CPU time for a $s = 1$ CT simulation is independent of $T$, thus providing a benchmark measure. Fig. 1a shows a comparison between the temperature dependence of the CPU time, for all simulations the system size was fixed at $N = 10^5$. At high temperatures MC is the most efficient algorithm due to the likelihood of accepting a move. However, as $T$ is lowered CT is quickly outperforms MC. At lower temperatures the $s = 2$ MCAMC becomes fastest algorithm, outperforming CT by an approximate factor $e^{2\beta}$. By further reducing $T$ we find that the $s = 7$ algorithm provides a further improvement of $e^{2\beta}$.

The performance of the $s = 2$ algorithm can be considered as follows. In comparison to CT it obtains a speed up of $e^{\beta}$, however this is then suppressed by a factor of $N_4$. Consequently the efficiency of the $s = 2$ algorithm is affected by the system size. This not only determines the probability of entering the isolated state, the larger the system the less likely it is that all excitations will be isolated, but also the exit time, i.e. in a large system there are far more facilitated sites available. In order to maximize performance for all $s > 1$ algorithms it is desirable to use the smallest system size possible. Fig. 1b shows the dependency of the CPU time on system size. Simulations were performed using an equilibrium trajectory of time $t = 3 \times 10^{12}/N$. 
Figure 1. (a) Temperature dependence of CPU time for equilibrium East model trajectories of total Monte Carlo time $t = 10^7 \times e^{2\beta}$ and system size $N = 10^5$, for MC, CT, and MCAMC algorithms. The straight lines indicate the approximate speed-up of the MCAMC simulations. CPU time shown relative to the average time needed when using CT dynamics. (b) System size dependence of CPU time (relative to that for CT) for equilibrium East model trajectories of MC time $t = 3 \times 10^{12}/N$ at $T = 0.2$.

5. Other Models

The East model in one dimension has proven to be ideally suited to the method of MCAMC. The algorithm has been successfully extended to the East model in dimensions more than one, and also to a cross over model between the East and the Frederick-Anderson (FA) model [6]. Another group of models that we have considered are the $f$-spin FA models [13, 9, 14] with specific focus on the 2-spin facilitated model with dimension $d = 2$. Here we outline how we attempted to construct an algorithm for this model.

The 2-spin FA model has the same Hamiltonian as the East model and has the kinetic constraint that a site may only change if at least two of its neighbours are excited. This kinetic constraint has the effect that the model is extremely slow, making simulation difficult, particularly at lower temperatures. Any improvement on CT for this model would be very useful.

The first decision one must make is to choose the initial transient state for the algorithm. It must be a state that the system regularly falls into but also the immediate transient subspace surrounding it has to be small enough so that the Markov matrix remains manageable. The state that we chose is one where there are no facilitated excited spins and further to that there are no excited spins that can be facilitated by a single spin flip. This greatly restricts the number of neighbouring transient states as required because once the first move has been made the only way for the system to relax is to go back to the initial state.

From the entry state a facilitated spin may become excited and in turn either facilitate one, two or no other sites. These three possibilities each represent a distinct transient state and so including the entry state constitute an $s = 4$ MCAMC algorithm. The variables required inside the transient matrix are the numbers of spins that fit into each of the three categories above. Along with the entry condition these variables must be monitored at all times and this is what makes up the extra bookkeeping cost for this algorithm.

So far the MCAMC algorithm outlined above has been unable to make an improvement on standard CT. This is for a number of reasons: Firstly, due to the slow nature of the model, the temperature range we are interested in is such that the potential exponential in $\beta$ gains from excitation rates are very modest. Another problem with working in this temperature range is it appears that the entry condition is an unlikely state for the system to fall into and so most of
the time is spent using the CT algorithm. The speed increase that is achieved is therefore not enough to make up for the increased algorithmic complexity that this scheme requires.

6. Discussion

We have shown that the method of MC with absorbing Markov chains, MCAMC, of Novotny [3] can be used to dramatically speed up simulations of facilitated spin models of glasses, such as the East and FA models. Even the simplest \( s = 2 \) algorithm can improve simulation times at low temperature by a factor of \( e^{23} \) over the n-fold or continuous time MC. By increasing the number of transient states \( s \) even larger computational gains can be achieved. One could imagine an algorithm where the number of transient states is variable, and at each iteration the \( s \) with the largest number of transient states allowed by the current configuration, the smallest distance between excitations, is used.

The method of MCAMC has been adapted for \( f \)-spin facilitated FA models with \( f = 2 \) and has proved problematic due to the more complicated nature of the model. The next step for future work would be to find a way to use a MCAMC algorithm without the cost due to bookkeeping outweighing the speed gain. This includes applying the method to other interesting KCMs, such as all \( f \)-spin facilitated FA models with \( f > 1 \) and constrained lattice gases [15, 16, 9, 17, 18, 19]. Constrained lattice gases have many of the same problems that the \( f \)-spin facilitated FA models have. Since the barriers are purely entropic the problem of balancing algorithmic complexity with the speed gain becomes even more difficult. In any case, given that the high density or low temperature dynamics of these systems is in general so much slower than that of East models, a clever MCAMC algorithm which overcomes these hurdles could prove extremely useful.

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