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## LETTER TO THE EDITOR

# A rapid dynamical Monte Carlo algorithm for glassy systems

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**Abstract.** In this letter we present a dynamical Monte Carlo algorithm which is applicable to systems satisfying a clustering condition: during the dynamical evolution the system is mostly trapped in deep local minima (as happens in glasses, pinning problems etc). We compare the algorithm to the usual Monte Carlo algorithm using, as an example the Bernasconi model. In this model, a straightforward implementation of the algorithm gives an improvement of several orders of magnitude in computational speed with respect to a recent, already very efficient, implementation of the algorithm of Bortz *et al.*

Direct dynamical simulations have traditionally played an important role in statistical physics. Investigations have covered a large range of problems, from dynamical phase transitions (e.g. the spinodal decomposition and the glass transition) to detailed, realistic simulations of polymers and long proteins in the sub-nanosecond regime.

The macroscopic evolution of the system is always much slower than its microscopic Monte Carlo dynamics. This simply means that the problem of dynamical simulations is, almost by definition, a very difficult enterprise.

In dynamical Monte Carlo simulations one considers Markov sequences of configurations

$$\sigma_1(\tau_1) \rightarrow \sigma_2(\tau_2) \cdots \rightarrow \sigma_i(\tau_i) \rightarrow \sigma_{i+1}(\tau_{i+1}) \cdots \quad (1)$$

where the symbols mean that the system will remain in the configuration  $\sigma_i$  during the time  $\tau_i$ . For concreteness we imagine the configuration to stem from a spin model  $\sigma = (S_1, S_2, \dots, S_N)$  with  $S_i = \pm 1$ . In the single-spin flip Metropolis dynamics, the system can move from configurations  $\sigma_i$  to any configuration which differs from it by the flip of a single spin  $m$ , which we denote by  $\sigma^{[m]}$ . The probability of making a move is then given by

$$p(\sigma \rightarrow \sigma^{[m]}, \Delta\tau) = \frac{\Delta\tau}{N} \begin{cases} 1 & \text{if } E(\sigma^{[m]}) < E(\sigma) \\ \exp[-\beta(E(\sigma^{[m]}) - E(\sigma))] & \text{otherwise} \end{cases} \quad m = 1, \dots, N \quad (2)$$

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where  $E(\sigma)$  is the energy of the configuration  $\sigma$ . Usually, the sequence in (1) is directly simulated (with a *finite* time-step  $\Delta\tau$ ) by means of a rejection method. In that case, the time intervals  $\tau_i$  in (1) are multiples of  $\Delta\tau$ :  $\tau_i = M\Delta\tau$ . At each time-step a flip of a randomly chosen spin  $m$  is attempted, and a uniform random number is drawn. Then

$$\sigma(\tau + \Delta\tau) = \begin{cases} \sigma^{[m]} & \text{if } p(\sigma \rightarrow \sigma^{[m]}) > \text{ran } 0 < \text{ran} < 1 \\ \sigma & \text{otherwise.} \end{cases} \quad (3)$$

At low temperatures, the MC dynamics often encounters the problem of small acceptance probabilities: as soon as the temperature is such that the available phase space is dominated by low-lying minima, the system will take a long time to move from a low-lying state to an excited one. The problem of small acceptance probabilities is certainly a nuisance, but not a true impediment to the simulation. Almost 20 years ago, Bortz, Kalos and Lebowitz [1] (BKL) showed how to circumvent it: in a nutshell, their algorithm consists of giving up the rejection method in favour of a direct calculation of waiting times, which can be calculated from the knowledge of all the transitions. In the above example, the time  $\tau_i$  the system will stay in a configuration  $\sigma_i$  can be directly sampled from its probability distribution  $p(\tau_i) = \lambda \exp(-\lambda\tau_i)$  with  $\lambda = \sum_{m=1,N} p(\sigma_i \rightarrow \sigma_i^{[m]})$ . The BKL algorithm has been used repeatedly (e.g. in [2, 3]) over the last few years. A recent, very efficient implementation [4] has given improvements in computational speed of the order of  $10^3$ – $10^5$  for glassy systems at low temperatures.

If the problem of small acceptance probabilities has thus been effectively solved by the BKL algorithm, it is usually accompanied by another one, which we may call ‘futile’ dynamics: if the dynamical evolution is dominated by isolated deep local minima, the system will get trapped even though we force it to make transitions out of them: very shortly after having escaped a minimal configuration (by means of the BKL algorithm), the system simply falls back into it. This means that, at low temperature, the dynamics consists mostly of short cycles.

The purpose of the present letter is to show that this problem can also be eliminated, and the power of the BKL algorithm increased by at least a few orders of magnitude. To give an illustration of the problem we are concerned with and to introduce the model which will serve as an example for our presentation, we show in figure 1 the result of a very long

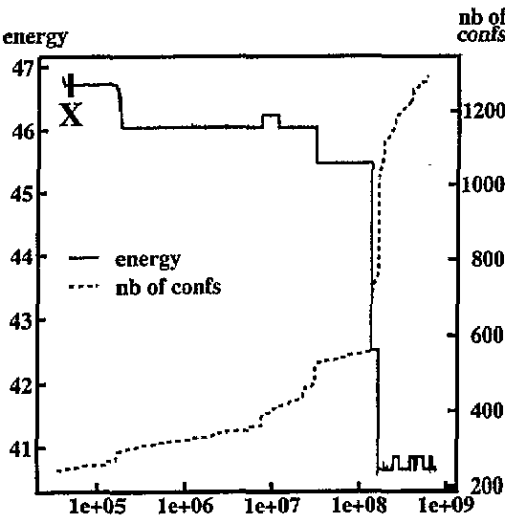


Figure 1. Energy versus  $\log t$  for the Bernasconi model at  $T = 0.05$  for a single realization. The calculation was performed using the BKL algorithm in a very efficient implementation [4]. The point marked ‘X’ serves as a starting point for subsequent simulations (cf figure 3). The second curve gives the total number of different configurations visited (scale to the right). When on a ‘plateau’, the number of configurations increases roughly linearly in  $\log t$ .

simulation of a single run of the Bernasconi model [5], defined by the Hamiltonian

$$\mathcal{H} = \frac{1}{N} \sum_{k=1}^{N-1} \left[ \sum_{i=1}^{N-k} S_i S_{i+k} \right]^2. \quad (4)$$

The model defined in (4) has acquired some fame during the last years as an example of a 'tough' optimization problem. An inkling of why this is so can immediately be found from figure 1, in which we show the temporal evolution of a system of size  $N = 400$  at a temperature  $T = 0.05$ . The simulation has gone over a time  $t = 3.9 \times 10^8$ , (i.e. has performed the equivalent of  $3.9 \times 10^8$  Monte Carlo steps *per spin*). The total number of accepted moves is around  $N_{\text{acc}} = 2.1 \times 10^9$ , but the total number of different configurations visited,  $N_{\text{diff}} = 1290$ , is very small. In an effort to be completely explicit, we restate that the small acceptance probability ( $N_{\text{acc}}/(Nt) \ll 1$ ) is related but not identical to the 'futility' expressed by  $N_{\text{diff}}/N_{\text{acc}} \ll 1$ . On the second curve in figure 1 we display the total number of different configurations visited as a function of time. One can clearly see that this number grows very slowly whenever the system is within a given plateau of the energy. Many of the configurations are thus visited a large number of times. It should be evident that the total time the system spends in any of these configurations can be evaluated in a much more efficient way than by visiting them repeatedly. It can in fact be deduced from the Boltzmann distribution. We have extensively tested this fundamental hypothesis of our method in simulations using the BKL algorithm.

Now consider the schematic view of the algorithm presented in figure 2. This algorithm completely avoids the computational slowdown associated with repeated visits to the same configuration. In fact, it visits one *new* configuration per iteration. At any given time, there is an active set of configurations which make up the 'cluster'  $\mathcal{C}$ . For any configuration  $i$  in  $\mathcal{C}$ , we have stored, besides the energy  $E(i)$ , the total probability to move from site  $i$  to a configuration outside the cluster

$$p_{\text{ext}}(i) = \sum_{j \notin \mathcal{C}} p(i \rightarrow j). \quad (5)$$

Now we suppose that the configurations in  $\mathcal{C}$  are in quasi-equilibrium, i.e. we assume that the system visits configuration  $j$  with the probability given by its normalized Boltzmann weight

$$p_{\text{eq}}(i) = \frac{\exp(-\beta E(i))}{\sum_{k \in \mathcal{C}} \exp(-\beta E(k))}. \quad (6)$$

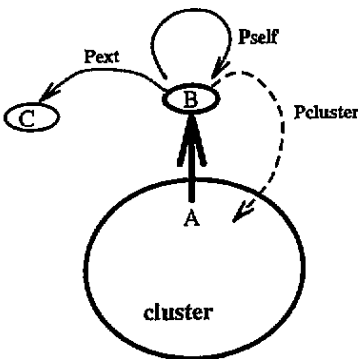


Figure 2. Schematic view of the cluster Monte Carlo algorithm presented in this letter.

The (normalized) probability to move from any configuration in  $C$  to a configuration outside  $C$  is thus given by  $\sum_{i \in C} p_{\text{eq}}(i) p_{\text{ext}}(i)$ . In direct analogy to the BKL algorithm, we then sample the time  $\tau$  the system will stay in  $C$  from its probability distribution

$$p(\tau) = \lambda \exp(-\lambda \tau) \quad \text{with} \quad \lambda = \sum_{i \in C} p_{\text{eq}}(i) p_{\text{ext}}(i). \quad (7)$$

As before,  $\lambda$  is the parameter of the exponential distribution of waiting times in the cluster. It should be evident that  $\lambda$  can very quickly become a small quantity, which needs to be calculated with high-precision arithmetic. In the calculation presented later on (figure 4),  $\lambda^{-1}$  routinely takes on values of  $\lambda^{-1} \sim 3 \times 10^9$ , which simply means that a *single* iteration of the algorithm (at very large times of the simulation) corresponds to  $3 \times 10^9$  Monte Carlo steps per spin! After this time, sampled from (7), the system moves outside  $C$ . Now, in analogy with the BKL algorithm, we are able to sample in its turn the configuration of  $C$  (denoted by  $A$  in figure 2) from which this move will be made (this probability is simply proportional to  $p_{\text{eq}}(j) p_{\text{ext}}(j)$ ). Finally, having identified the configuration  $\sigma_i$  ( $\equiv A$ ), we can sample the configuration outside  $C$ , according to (2), after having excluded all the moves which stay within  $C$ . This then produces the configuration denoted by  $B$  in figure 2.

In our current implementation of the algorithm, we then calculate the probability  $p_{\text{cluster}}$  to return to the cluster from  $B$ , or to move directly to configurations outside the cluster,  $p_{\text{ext}}$ . In both cases, the amount of time spent on  $B$  is sampled from  $p_{\text{self}} = 1 - p_{\text{ext}} - p_{\text{cluster}}$ . We then add  $B$  to the cluster and update all the probabilities  $p_{\text{ext}}(i)$  for all members of  $C$ , whose size, in the meantime, has been incremented.

A little thought shows that the algorithm just sketched can be implemented recursively, and that a single iteration consists of two passes through the cluster. Furthermore, besides the configurations (which we keep in external memory), we only need the tables  $E(i)$  and  $p_{\text{ext}}(i)$ , i.e. there is no need for tables which grow faster than the cluster size. In the example treated, we can presently, for  $N = 400$ , allow up to  $10^4$  members in  $C$ .

To show that the algorithm works, we have tested it against the BKL algorithm. In fact, for both algorithms, we have started 300 samples on the same configuration (marked 'X' in figure 1), and have determined the histogram of trapping times (times after which the system accesses a new plateau with lower energy). This histogram is shown in figure 3. As can be clearly seen, the distributions of waiting times are identical, which indicates that the algorithm is correct for all intents and purposes. Furthermore, it should be evident that,

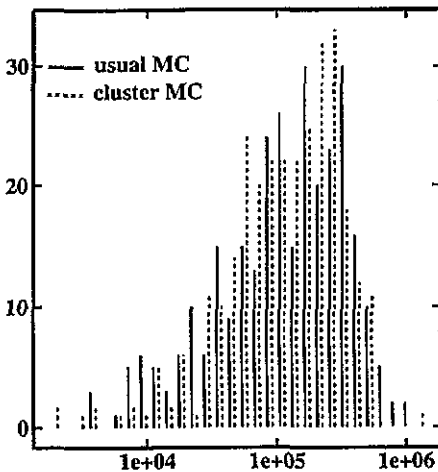


Figure 3. Histograms of trapping times for the two algorithms. For this figure, both the BKL algorithm and the cluster algorithm presented in this letter were started at the point marked 'X' in figure 1. 300 runs of both algorithms were done, and the time after which a new plateau of lower energy was found was typically between  $t = 10^4$  and  $t = 10^6$ .

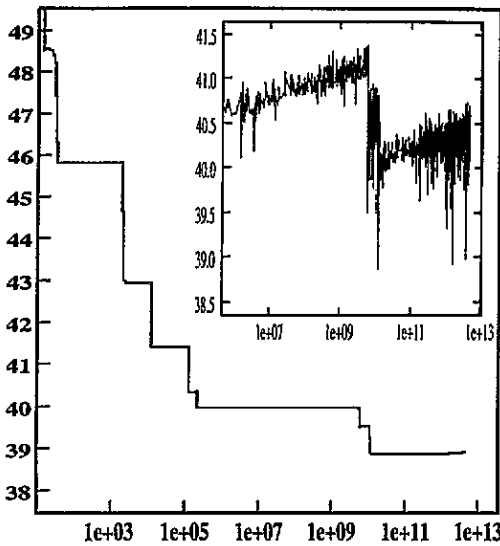


Figure 4. Mean energy of the cluster versus  $\log t$  for the Bernasconi model at  $T = 0.05$  (single run of the cluster algorithm). The inset displays the energy of new configurations which enter the cluster.

once an old plateau has been left, and a new configuration of minimal energy found, the original members of  $\mathcal{C}$  drop out of the picture. At this point, a new cluster can be started.

In figure 4 we show the result of a simulation for the same system as in figure 1, but this time with the new algorithm. Using the same amount of computer time, we reach physical times which are about 10 000 times larger. The inset in figure 4 shows the energy of the new configurations which enter the cluster. This energy drops as a new plateau is found, and then increases (approximately logarithmically in time), as more and more remote configurations are encountered during the thermal exploration process. The main plot in figure 4 shows the mean energy of the cluster. Note that many more quantities are accessible, such as correlation functions, or more detailed properties of the dynamical process.

Finally we would like to discuss whether the algorithm, as presented, and as sketched in figure 2 can be made rigorous. In the present state, we increase the size of the cluster by one at any iteration. Clearly, a more rigorous approach would be to add point 'B' to the cluster only if  $p_{\text{ext}} \ll p_{\text{int}}$ , say if  $p_{\text{ext}}/p_{\text{int}} < \gamma$ . The algorithm is equivalent to the BKL algorithm for  $\gamma = 0$ , but certainly retains some asymptotic validity as  $\gamma \gtrsim 0$ . The issue at hand is that the configurations in the cluster should satisfy a quasi-equilibrium condition, which basically means  $p_{\text{ext}} \ll p_{\text{int}}$ , and which may be implemented with various degrees of rigour.

A second question of course concerns the criterion for abandoning the cluster and growing a new one. In our present case we have simply adopted an energy criterion: each time a new lowest energy was found, the old cluster was abandoned, and a new one grown. The precise criterion will depend on the particular problem. Whenever geometry plays an important role, the cluster may have to be scrapped as soon as the geometrical distances between members of the cluster become too large.

In conclusion, we have presented in this letter an algorithm for the Monte Carlo dynamics of glassy systems, which is able to produce enormous gains in efficiency if configurations are visited over and over again. In a natural way, the algorithm forms a cluster of a certain number of configurations, which are close in energy. These configurations are then assumed to be in thermal equilibrium, an assumption which was very well satisfied in the example we treated.

Finally, we indicate that a FORTRAN source code for the algorithms used in this work may be obtained by e-mail.

We acknowledge helpful discussions with M Mézard.

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