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LETTER TO THE EDITOR

Monte Carlo simulations of random walks and surfaces in parallel

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Abstract. The theory of Monte Carlo simulation of random geometric objects such as random walks and random surfaces is considered on a sequential and a parallel computer. The partition functions generated for simple Monte Carlo rules are derived and the difference between sequential and parallel computing is discussed for the case of random walks with fixed endpoints or for random loops. The implications for random surface calculations in parallel is considerd in short.

The increasing availability of parallel computers in the physicist's armoury has made big improvements possible in the statistical simulation of physical systems. The Monte Carlo (MC) (Metropolis *et al* 1953) approach in particular has been applied extensively to all kinds of problems in many different fields (Binder 1979). In this letter we consider the specific application of this process to the restricted problem of generating ensembles of geometric objects like random walks and loops (Berg and Foester 1981, Aragao de Carvalho *et al* 1983), random surfaces (Jurkiewicz *et al* 1986, Billoire and David 1986) and in surface physics (see, e.g., Binder 1979 and references therein).

As an illustration we consider the generation of Brownian random walks with fixed endpoints on a hypercubical lattice using a link-shifting scheme. This problem was considered first by Berg and Foester (1981) using a sequential machine and by Janse van Rensburg (1986) using a parallel computer. The elementary MC process is defined in figure 1. A link is selected at random and shifted perpendicular to itself in any of $2(d-1)$ directions to generate a new configuration. To preserve the condition of detailed balance it is clear that transitions like that in figure 2 must be forbidden. It is easily seen that this process connects the space of random walk configurations.

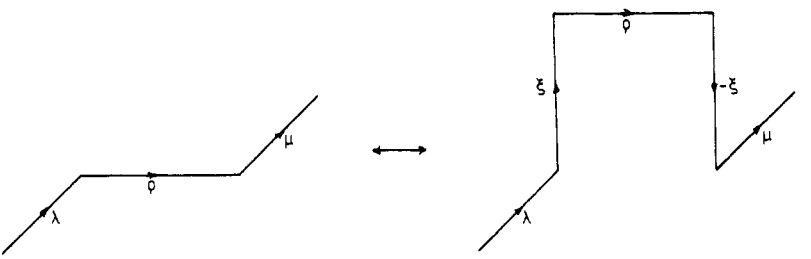

Figure 1. The elementary process defined for the Monte Carlo algorithm. If the link ξ is equal to $-\lambda$ or μ, the formed spike is deleted.

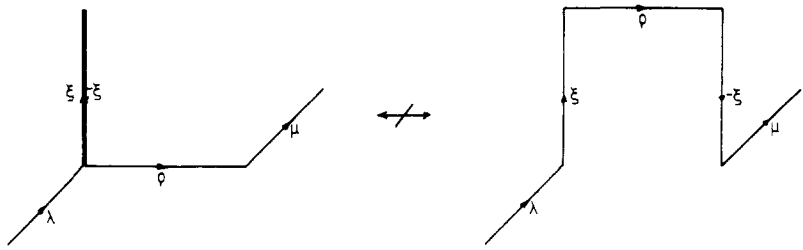

Figure 2. Under the elementary process defined in figurre 1 we have not got detailed balance. Transitions such as this must be forbidden because they are not reversible under the rule in figure 1.

The partition function for Brownian random walks is typically of the form

$$Z_B = \sum_{\omega: x \to y} e^{-b|\omega|} \tag{1}$$

where ω is a random walk connecting the lattice sites x and y with $|\omega|$ links and b is the inverse temperature. This equation suggests a MC transition probability

$$P(|\omega| \to |\omega'|) = \begin{cases} e^{-2b} & \text{if } |\omega| < |\omega'| \\ 1 & \text{otherwise.} \end{cases} \tag{2}$$

Ensembles of random walks are then generated by applying the elementary process and accepting new configurations into the ensemble with the rule (2).

When this algorithm is implemented on a sequential computer, an ensemble P of n random walks are generated as a sequence $(\omega_1 \to \omega_2 \to \ldots \omega_n)$. The *a priori* probability of selecting a link in configuration ω_i is $1/|\omega_i|$ and the probability of a transition $\omega_i \to \omega_{i+1}$ is thus given by

$$P(\omega_i \to \omega_{i+1}) = \frac{1}{|\omega_i|} P(|\omega_i| \to |\omega_{i+1}|). \tag{3}$$

The condition of detailed balance is then easily shown to be

$$\frac{P(\omega \to \omega')}{P(\omega' \to \omega)} = \frac{|\omega'|}{|\omega|} \exp(-b(|\omega| - |\omega'|)). \tag{4}$$

It is thus obvious that the partition function generated by this process is given by (Berg and Foester 1981)

$$Z'_B = \sum_{\omega: x \to y} |\omega| e^{-b|\omega|}. \tag{5}$$

This problem is overcome by Aragao de Carvalho *et al* (1983) by modifying the transition probabilities in equation (2) to $(1/|\omega|)P(|\omega| \to |\omega'|)$. This modification can then be shown to generate the correct partition function but it slows the process down near the critical point of the theory where the lengths of the random walks become very long.

The implementation of the algorithm on a parallel computer with P independent processors is identical to that of the sequential computer except that, for practical reasons, the *a priori* probability that a link on any of the P walks is selected is $1/(|\omega|_{max})$ where $|\omega|_{max}$ is the longest walk in the ensemble P. The ensemble of random walks is

then updated many times. We show that it converges to a Boltzmann distribution. Suppose that we have updated the ensemble m times and call the new ensemble P'. Let

$$X = \prod_{i=1}^{m} \frac{1}{|\omega|_{\max,i}} \tag{6}$$

where $|\omega|_{\max,i}$ is the longest walk in the configuration at the ith update. Then it is clear that

$$P(\omega \to \omega') = \frac{1}{X} P_c(|\omega| \to |\omega'|) \tag{7}$$

where $P_c(|\omega| \to |\omega'|)$ is the product of the elementary probabilities (2) along every configuration in the m updates. Since X is the same for all members of the ensemble, it is easy to show that the walks in the ensemble are distributed over the correct partition function (1). This approach has as a main advantage over the sequential method that longer walks are not overweighted, and one may thus explore the critical region more accurately without the problem that the walks may become so long that they are statistically uncontrolable. As a small example that the parallel MC program generates the correct partition function (1), the algorithm was coded into the ICL DAP, a machine with 4096 parallel elements, to generate an ensemble of self-avoiding random walks in two dimensions. If the correct distribution is obtained over the random walks, we can predict the number of states with lengths 3, 5, 7, 9, 13, etc, statistically and compare the results to known values. The results are listed in table 1. The exact values for the numbers of self-avoiding random walks were obtained from the results of Janse van Rensburg (1986) and the number of walks of length 9 (128) connecting two neighbouring sites was enumerated explicitly.

Table 1. Numbers of self-avoiding random walks connecting (0, 0, 0) to (1, 0, 0). The MC process on the ICL DAP was used to enumerate self-avoiding walks joining the origin with (1, 0) in two dimensions. The comparison to predicted numbers indicates that the parallel program does indeed generate the correct partition function (1) for self-avoiding random walks. The measurements were made over 12 ensembles of 4096 random walks in parallel (i.e. 49 152 walks) and the statistical error was calculated in the usual way.

Length	Theoretical	Measured
1	1	1
3	2	1.92 ± 0.29
5	6	5.70 ± 0.49
7	26	26.91 ± 2.22
9	128	135 ± 11
11	—	739 ± 77

This same problem may haunt the generation of random surfaces. Consider, for example, the model discussed by Jurkiewicz *et al* (1986). A random surface is considered in tetrahedral space. New configurations are generated by the addition (or deletion) of tetrahedra. This model is of course closely related to studies of crystal growth or dissolution in surface physics (Binder 1979). In all these studies the *a priori* probability of selecting a site for the addition or deletion of a tetrahedron or a molecule is inversely proportional to the surface area, and care must therefore be taken to ensure

that the correct partition function is generated if the goal is to generate an ensemble of surfaces or crystals to calculate statistical averages (for example the average crystal size or the average surface area of crystals in solution for a given surface-solvent interaction).

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