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SURFACE SIMULATIONS WITHOUT CRITICAL SLOWING DOWN

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We present new Monte Carlo cluster algorithms which eliminate critical slowing down in surface models of the solid-on-solid type. The algorithms are based on reflecting parts of the surface with respect to appropriately chosen planes. The proper choice of the reflection plane turns out to be crucial.

In the last few years, the development and study of new algorithms that strongly reduce critical slowing down (CSD) has become a major research topic in the field of computer simulations. Our group is presenting within 5 talks at this conference the results we obtained in this area during the last year:

- Development and study of stochastic cluster or multi-grid algorithms without CSD or with strongly reduced CSD for a variety of statistical models and for lattice gauge theories (this talk and [1]);
- Development of a multigrid method for the computation of the fermionic determinant in realistic lattice gauge theories [2];
- Development of stochastic cluster or multigrid methods that eliminate CSD in the simulation of quantum gravity on the lattice (dynamical triangulation algorithms) [3].

In the present contribution, we concentrate on the application of new cluster algorithms for interface models, which have wide applications in crystal growth, telescope mirror alignement, roughening transitions, etc. (note that a different approach to simulating interface models was recently developed in [4]).

Our choice for modeling these physical systems is to consider them as two-dimensional spin systems where the spin m_x at the site x is an integer (Z-spin). The action is a general function of the absolute value of the difference of two spins, $|m_x - m_y|$.

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The connection to a surface model comes from the interpretation of m_x as the height of a surface above the two-dimensional point x. The prototype of such a model is the discrete Gaussian model, but all SOS (solid-on-solid) models and variants thereof are in this class of models[5].

An SOS configuration is a two-dimensional surface without overhangs, embedded in three dimensions. The idea underlying our new algorithms is to take a horizontal plane and reflect "hills" and "valleys" of the surface through that plane. One crucial aspect is the procedure for choosing the reflection plane.

Let us for definiteness discuss the algorithm in terms of the discrete Gaussian model, defined by the partition function

$$\mathcal{Z} = \sum_m \exp\left\{-\frac{1}{2\beta}\sum_{<x,y>}(m_x - m_y)^2\right\}. \quad (1)$$

We take a square lattice, periodic boundary conditions, and nearest neighbour interaction.

Let us denote the height of the horizontal *reflection plane* by M. A reflection of m_x with respect to M means

$$m_x \to 2M - m_x. \quad (2)$$

Obviously, M has to be either an integer or a half-integer. One way of explaining how the clusters are built is in terms of the *embedded Ising variables*[6] $\sigma_x = \pm 1$, defined by the decomposition

$$m_x = \sigma_x |m_x - M| + M. \quad (3)$$

$\sigma_x = 1$ means that m_x is above the reflection plane M, $\sigma_x = -1$ that it is below M. Note that σ_x is not well defined if $m_x = M$; this is not going to cause difficulties, as can be seen from equation (4) below.

In order to define the cluster algorithm we introduce the *deleting* and *freezing* probabilities[7] for a link $<x,y>$ (in the language of [6] the term "activating" is used instead of "freezing"):

$$P_{del}(x,y) = \tag{4}$$

$$q \exp\left\{-\frac{1}{\beta}\,|m_x - M|\,|m_y - M|\,(\sigma_x\sigma_y + 1)\right\}$$

where $q \leq 1$ can explicitly depend on $|m_x - M|$ and $|m_y - M|$, and

$$P_{freeze}(x,y) = 1 - P_{del}(x,y). \tag{5}$$

In contrast to other cluster algorithms investigated in the literature, the possibility of choosing $q \neq 1$ will prove to be useful in our case. Let us however assume for the moment that $q = 1$ (until we explicitly remove this restriction).

After freezing or deleting all the links of the lattice with the above probabilities, two sites are defined to be connected if they are at the endpoints of a frozen link. The clusters are then defined to be the connected components of the lattice.

Notice that $P_{del}(x,y) = 1$ if either $\sigma_x \neq \sigma_y$, i.e. m_x and m_y are on different sides of the reflection plane, or if $|m_x - M|\,|m_y - M| = 0$, i.e. at least one of the points lies on the reflection plane itself. Thus, similarly to the Ising model, the clusters will contain only spins for which the embedded Ising variables have the same value. On the other hand, the spins with $m_x = M$ are always monomers. The most important difference to the Ising model is however the strong dependence of the clusters on the choice of M. Consider for example a situation where M lies above most of the m_x. Since $P_{del}(x,y)$ becomes exponentially small with increasing distance from M, there will be with high probability one very large cluster, containing almost all spins.

Flipping a cluster means flipping the embedded Ising variables. In terms of the original integer variables m_x, this is equivalent to performing the reflection (2) for all spins in the cluster. Notice that the cluster boundaries are not in general exactly at the intersection of the relief landscape with the reflection plane, since $P_{del}(x,y)$ is nonzero also if both m_x and m_y are away from and on the same side of M. Nevertheless, the intuitive picture of clusters as hills or valleys which are flipped through the reflection plane is approximately realized.

In our simulations we used the single cluster algorithm[8], i.e. a cluster is built starting from a randomly chosen site (the *seed*), and it is flipped with probability one.

In order to establish a valid algorithm one has to ensure detailed balance. Once M is given, detailed balance follows from standard arguments[7,8] for the restricted set of configurations related by reflecting the clusters with respect to M. A sufficient condition for detailed balance to hold for the entire procedure is to choose M with an a priori probability prob(M) that is a function of M itself and of the objects that are unchanged by the reflection, i.e. of the values of $|m_x - M|$ for all lattice sites:

$$\text{prob}(M) = f(\{|m - M|\}; M). \tag{6}$$

This condition still leaves a lot of freedom in the choice of M. The proper way to choose the reflection plane strongly depends on some of the physical properties of the model, and it will turn out to be the crucial ingredient in eliminating CSD.

The model (1) is the dual of the two-dimensional XY model with Villain (heat kernel) action. For $\beta < \beta_c$ the global Z-symmetry is spontaneously broken. As a consequence, there is a nonzero mass gap, and the surface thickness, which we define as the square root of $\lim_{|x-y|\to\infty} < (m_x - m_y)^2 >$, is finite. According to the Kosterlitz-Thouless (KT) scenario[9], the correlation length diverges exponentially as β approaches β_c. In the SOS terminology this is due to the fact that the surface fluctuates more and more. At the critical point the surface becomes rough; for all $\beta > \beta_c$ the surface thickness diverges logarithmically with the volume of the system. The large-β phase corresponds to the spin wave (massless) phase of the XY model.

The first important remark about physical properties of the model that strongly influence our algorithm is that, for all practical purposes, the surface is *thin*. We considered systems on a lattice of size L^2. For $L = 256$, the surface thickness was still less than 1 at $\beta = .68$, which is in the smooth (broken) phase very close to β_c, and ≈ 1.4 at $\beta = 1$, which is deep in the massless phase. Both these situations are well within the region where the critical properties are clearly exhibited (KT behaviour for $\beta < \beta_c$ and massless free field theory for $\beta = 1$).

For thin surfaces, it is not trivial to choose the

reflection plane M such that it lies within the vertical bounds of the surface. We tried to ensure this by taking M close to the value m_{x_o} of the spin at the seed x_o of the cluster. The simplest possibility that leads to an ergodic algorithm is to take $M = m_{x_o} \pm \frac{1}{2}$, each of the two possibilities with probability $\frac{1}{2}$, and $q = 1$ (see eq. (4)). Taking $M = m_{x_o}$ is not helpful for $q = 1$ since all the links starting from x_o would be deleted with probability one. Let us denote the procedure just described as the **H-algorithm** (H for half-integer).

We tested the H-algorithm extensively. In order to make sure that we do observe the slowest modes of the Markov matrix[10], we measured a whole range of quantities: mean energy and specific heat, surface thickness, various block spin correlation functions, and the order parameters $\mathcal{M}_\alpha \equiv < L^{-2} |\sum_x \exp(2\pi i \alpha m_x)| >$ for $\alpha = 0.1, 0.2, \ldots, 0.5$ ($\mathcal{M}_\alpha$ is an approximation for the square root of $\lim_{|x-y|\to\infty} < \exp\{2\pi i \alpha (m_x - m_y)\} >$ which becomes exact in the thermodynamic limit).

For all these quantities we studied the autocorrelation function and tried to determine the *exponential autocorrelation time* τ. Note that τ should in principle be the same for all our quantities, since it only depends on the second largest eigenvalue of the Markov matrix[10]. In practice, there always were quantities that did not couple well to the slow modes and exhibited a misleadingly small τ. Sometimes some quantities showed a clear crossover from one clean exponential regime to a slower second one. In other instances there were quantities that did not decay at all exponentially until the limits of our precision were reached. These difficulties notwithstanding, we were usually able to reach a clearcut conclusion with respect to the "true" value of τ because there was a whole set of "slowest decaying quantities" which exhibited this value.

The autocorrelation time τ is always quoted in "work units" (sweeps). A work unit is the work necessary to build a cluster of the size of the entire lattice. Each of our runs consisted of between 100000 and 500000 work units.

Determining the errors on τ is a very delicate business and we were very careful with this point. Details of the problems we encountered are discussed elsewhere[11].

The results for the autocorrelation times of the H-algorithm are shown in tables 1 and 2. The algorithm was not successful in eliminating CSD in either of the two situations.

Table 1: Autocorrelation times for $\beta = 1$ ($\xi = \infty$).

L	H	IH	QH	QM
16	13.5(3.5)	–	–	–
32	60(20)	7(1)	–	–
64	82(18)	8(1)	12.5(1.5)	26.5(4.5)
128	165(33)	11.5(1.5)	13(1.5)	58(12)
256	–	11(2)	–	–

In the massless (rough) phase, where the correlation length ξ of the model is infinite, the dynamical critical exponent z can be defined[6,8,10] by $\tau \sim L^z$. The results of table 1 suggest that z is around 1 at $\beta = 1$. This is an improvement on the $z \approx 2$ of local algorithms, but it is not what we expected.

In the broken (smooth) phase, the two values of τ shown in table 2 suggest that the algorithm performs even less well than at $\beta = 1$. We had problems in determining z here. In principle, it can be defined by the finite size scaling law $\tau = \xi^z F(\xi/L)$ [10]. We tried to estimate ξ by analysing the exponential decay of the two-point function $< (m_x - m_y)^2 >$ (appropriate subtractions, Fourier transforms, etc., were done in standard fashion). In this phase the particles states are *kinks*[12], which correspond to one-dimensional (time-zero) configurations that have an integer value n at minus infinity and $n+1$ at plus infinity. With periodic boundary conditions however, there are only states containing kink-antikink pairs in the Hilbert space of the problem. Thus we tried to determine the correlation length from properties of two-particle states, not one-particle states, and we regard our values for ξ as potentially unreliable (therefore the symbol $\approx$ in table 2). Nevertheless, we can only underestimate ξ, so our conclusions regarding CSD in the smooth phase are not spoiled.

The fact that we do not give reliable values for z should not disturb us in the case of the H-algorithm. What we are after are algorithms that (almost) completely eliminate CSD. Instead of wasting our time with an algorithm that clearly does not satisfy this criterion, we should go on to the description of the more successful algorithms.

A careful analysis of the cluster size distribution revealed that the H-algorithm produces both small

Table 2: Autocorrelation times for $\beta < \beta_c$.

β	ξ	L	H	IH
0.65	≈14	64	12.3(1.5)	9(2)
0.65	≈14	128	–	9(3)
0.68	≈44	64	–	8(2)
0.68	≈44	128	41.5(7.0)	11(2)
0.68	≈44	256	–	13(2)

and very large clusters quite frequently, while intermediate size clusters are comparatively rare. Nearly half of the work is spent in clusters larger than 90% of the lattice, which, similarly to the Ising model studies, do not considerably change a configuration. In view of the above remark that the surface thickness is rather small for all situations we simulated, we can readily understand what is going on: the reflection plane M often lies above or below the bulk of the surface.

A natural attempt to improve the situation is to include reflections with respect to integer valued planes M. In order to get clusters of sizes larger than one site (which cannot happen when M equals the seed spin m_{x_o} and $q = 1$), but still assure that the reflection plane lies frequently enough within the (rather narrow) vertical bounds of the surface, we devised the following two algorithms:

- **algorithm Q:** $M = m_{x_o}$, i.e. the the reflection plane equals the seed spin, but $q = q_o$ for the case that $\mathrm{T}|m_x - M||m_y - M| = 0$, with q_o some constant strictly smaller than 1, and $q = 1$ otherwise.
- **algorithm I:** $M = m_{y_o}$, where y_o is a randomly chosen lattice site which is different from the seed x_o, and $q = 1$ always.

Both these algorithms are nonergodic, since they only change the spins by even amounts. Therefore they have to be combined with other procedures. We studied the combinations IH and QH of the I and Q algorithms with the H-algorithm.

Notice that for the Q-algorithm, a cluster grown from the seed x_o may contain spins that are above, below and equal to M. This is a quite unusual situation in the context of embedded Ising variables, but is perfectly allowed within the framework for cluster algorithms that we used here[7].

From the values of τ displayed in table 1, one can conclude that the value of z for the IH algorithm is very small, possibly even zero, at $\beta = 1$. The results for $\beta < \beta_c$ also suggest a very small value of z (but more data are necessary to reach a definite conclusion; see table 2). Thus the IH algorithm turned out to be *extremely efficient in eliminating* CSD. Furthermore, the results in table 1 show that there is no significant difference between the performance of the IH algorithm and that of the QH algorithm.

By varying the ratio of the number of I and H clusters (within reasonable bounds) the autocorrelation times did not change significantly. In tables 1 and 2 we only presented the results of runs where this ratio was one-to-one. Similarly, changing the value of q_o such that the mean cluster size ranged between a quarter and a third of the lattice (q_o was around 0.7) did not have a significant impact on the performance of the QH algorithm.

The IH and QH algorithms generate considerably more medium-size clusters and less large clusters than the H-algorithm alone. This confirms our expectation that choosing the reflection plane equal to one of the spins, not at a distance of $\pm\frac{1}{2}$ away, is very helpful in the case of a thin SOS surface. However, the good performance of these algorithms is not a function of the cluster size distribution alone, it is also sensitive to other details of the configuration changes that occur when the various types of clusters are flipped.

Let us attempt an explanation of why the IH and QH algorithms work so well.

At small β the important configurations consist of a large flat surface, with a few two-dimensional regions that are *one* unit higher or lower. We shall call these regions *single-step-islands* (SSI). In Hamiltonian (transfer matrix) language, the SSI's correspond to the surface between the world lines of a kink-antikink pair (remember that the kinks are the small β particle excitations[12]). As β_c is approached, SSI's become larger, more frequent, and are more often on top of one another. Their condensation causes the SOS surface roughening at β_c.

If we have an SSI on top of a flat background of height M, there is a large probability that the I or Q algorithms reflect it with respect to that background. Since the original and the reflected configuration have the same Boltzmann weight, the reflection of the SSI is a kind of microcanonical move. Such low-energy-cost large-scale changes in

the configurations are usually very efficient in decreasing the autocorrelation time. We believe that this is the main reason why the cluster flips with respect to an integer valued reflection plane M improve the situation so dramatically.

The I and Q algorithms have to be combined with another algorithm in order to ensure ergodicity. We now ask the question whether, in order to overcome CSD, it is crucial to combine I or Q with the H-algorithm, or whether we may also use a local ergodic algorithm. If M is an integer, no large SSI's can be created or destroyed by cluster reflections. The H-algorithm on the other hand can achieve this easily. Of course, a local algorithm like Metropolis cannot create or destroy any large scale objects. We may therefore expect that a combination IM or QM of I or Q with a Metropolis procedure *will* exhibit CSD. The study of the QM algorithm, whose results are also shown in table 1, clearly shows that this is indeed what happens. Note that for the QM algorithm we did one Metropolis sweep for, roughly, one work unit of the cluster part. The values of τ quoted in table 1 disregard the contribution of the Metropolis sweeps to the total amount of work.

We conclude that our picture of the SSI's as the relevant objects for understanding our cluster algorithms is correct, and that it is absolutely crucial to use both the integer *and* half-integer reflection planes. The situation is entirely satisfactory: we have both devised efficient algorithms and understood the physical reason for this efficiency.

Our algorithms can now be applied to the study of the roughening transition in a variety of SOS models. With modifications, they can also be used for SOS models with restrictions, and for scalar field theories in two dimenisons like e.g. the Sine-Gordon model.

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