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CLUSTER ALGORITHMS FOR SURFACES

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ABSTRACT

We discuss a new cluster algorithm that completely eliminates critical slowing down for surface models of the SOS (solid-on-solid) type.

Keywords: SOS models; Critical slowing down; Cluster algorithm; Kosterlitz-Thouless transition

1. Introduction

Cluster algorithms are one of the two main successful methods for overcoming critical slowing down (CSD) (the other method is multigrid). They first occured in the pioneering work of Swendsen and Wang[1] on the Ising model. For reviews on the current status of cluster algorithms see Refs. 2-4, for generalizations of the formalism see Ref. 5. In particular, we mention the successful algorithms for $O(N)$ models and ϕ^4 theories,[6−8] which are generally referred to as Wolff algorithms.

Here we are interested in solid-on-solid (SOS) models,[9] which are important in the study of crystal interfaces. We shall describe a class of algorithms for such models with no CSD whatsoever.[10] As in the case of other cluster algorithms, this success can be explained in terms of what is being done to the relevant degrees of freedom. The main aim of the present lecture is to explain the algorithm from this point of view.

After briefly reviewing the definition and some properties of SOS models in section 2, we shall present the cluster algorithm in section 3. We shall concentrate on the algorithmic problems, giving only a single example for the physical results obtained using the new simulation technique (more results will be presented elsewhere[11]). Our cluster algorithm can be easily adapted for many two-dimensional lattice field theories with continuous fields. It is interesting to note that, as opposed various claims,[12] there is no CSD even in the case of the massless free field theory.

While SOS models are defined in two dimensions, we can investigate the behaviour of our algorithm for similar models in three dimensions. Most surprisingly (since the situation is different for the Swendsen-Wang and the Wolff algorithms), it turned out that in this case CSD was not eliminated at all. In section 4 we try to explain this result in terms of the physical properties of the model. The discussion will shed some new light on cluster algorithms in general.

In section 5 we present our conclusions.

2. SOS Models

An SOS model is a two-dimensional spin system with integer valued spins and with the global symmetry of adding an integer to all spins. A configuration can be viewed as a surface without overhangs, embedded in three dimensions. The surface is defined by giving its (integer) height h_x above each base point x. For simplicity we shall assume that the base points form an $L \times L$ square lattice. The interaction Hamiltonian is a sum over nearest neighbour ($<x, y>$) interactions:

$$H(h) = \sum_{<x,y>} f(|h_x - h_y|) \ . \tag{2.1}$$

Extension to the case of more remote neighbours is trivial, but we shall not discuss here the case of interactions between more than two spins, like e.g. the BCSOS model.[9] Of special interest in the literature are:

- the discrete Gaussian model (DGSOS):

$$f(|h_x - h_y|) = \frac{1}{2}(h_x - h_y)^2 \ ; \tag{2.2}$$

- the ASOS model ("A" stands for "absolute value"):

$$f(|h_x - h_y|) = |h_x - h_y| \ ; \tag{2.3}$$

- the dual of the XY model:

$$\exp\left\{-\frac{1}{T}f(|h_x - h_y|)\right\} = \frac{I_{|h_x-h_y|}(\beta^*)}{I_0(\beta^*)} \quad . \tag{2.4}$$

Here T is the temperature of the SOS model, β^* is the inverse temperature of the two-dimensional XY model,[13] and I_n are imaginary argument Bessel functions.

Let us briefly review the physics of these models.[9,14,15] At low temperatures the global symmetry is broken. This follows from the fact that any *hills* and *valleys* are very costly from the point of view of the Boltzmann weight (this observation is the basis for the convergent expansion that exists in this region). The SOS surface is smooth, i.e. the surface thickness σ,

$$\sigma^2 := < (h_x - \overline{h})^2 > \quad , \tag{2.5}$$

is finite ($\overline{h}$ is the average over the lattice of the h_x). With constant fixed boundary conditions, the expectation value of the average height is, in the thermodynamic limit, an integer (pure states). Notice that with periodic boundary conditions, which we choose for improving the statistics in the simulations, we may only consider quantities like (2.5) that are invariant under the global symmetry.

As the temperature is increased, the SOS surface fluctuates more and more. At high temperatures the discreteness of the spins is hardly felt. The surface thickness is infinite (in the thermodynamic limit), and the large distance behaviour is that of the massless free field theory (i.e. the model (2.2) with real instead of integer spins). The global symmetry is not broken (actually an enhancement of the symmetry probably occurs[15,16]). For a finite lattice size L we thus have the large L prediction

$$\sigma^2 = \frac{T_{\rm eff}}{\pi}\ (\ln L + \text{const}) \quad , \tag{2.6}$$

with the constant $T_{\rm eff}$ defined such that in the free field theory $T = T_{\rm eff}$. The other constant in (2.6) is in practice small.

The phase transition separating the two regions described above is the Kosterlitz-Thouless (KT) transition.[14] We shall not review the KT theory here . One remark is in place however: the surface thickness and related quantities diverge as a power when the transition temperature $T_{\rm KT}$ is approached from below. The correlation length ξ on the other hand diverges as $\exp \sigma^2$, as can be seen heuristically from the following simple argument. Assume we are at a temperatute just below $T_{\rm KT}$. For lattice sizes $L < \xi$, there is no real difference from the situation in the high temperature phase, and thus the behaviour (2.6) is true. Let us now increase L without changing the temperature. As $L \sim \xi$, (2.6) roughly reads: $\sigma^2 \sim \ln \xi$. If we further increase L, the surface thickness changes only insignificantly, since we already are close to the thermodynamic limit. Thus $\sigma^2 \sim \ln \xi$ remains true.

The numerical test of a power law behaviour is easier than that of an exponential behaviour. For this reason it is probably a good idea to test the KT scenario in the SOS representation rather than in the dual XY representation.[11]

In the case of the Ising model the phase transition can be viewed as the condensation of Peierls contours. What the Swendsen-Wang cluster algorithm[1] does with great efficiency is to remove existing and create new Peierls contours. Let us now concentrate on the picture of the SOS phase transition as the "condensation" of objects that occur in the low temperature expansion.

The Boltzmann weight for a height difference $\mathrm{d}h_{xy} := h_x - h_y$ between nearest neighbours is one for $\mathrm{d}h_{xy} = 0$. At low temperatures it decreases very fast with increasing $|\mathrm{d}h_{xy}|$. Thus close to $T = 0$, the dominant configuration is a flat surface (all h_x equal). The next important configurations have small regions that are one unit above or below the flat background. Let us call such regions *single-step-islands* (SSI's). As T_{KT} is approached, SSI's become larger, more frequent, and are more often on top of one another. It is their "condensation" that causes the SOS surface roughening at $T = T_{\mathrm{KT}}$.

It is instructive to understand the meaning of SSI's in transfer matrix (Hamiltonian) language. Close to $T = 0$, the eigenstates of the transfer matrix are to a good approximation spin configurations restricted to one row of the lattice (a row is a one-dimensional line perpendicular to the Euclidean time direction). The state corresponding to the highest eigenvalue of the transfer matrix is that where all spins in the row have the same value. The next eigenvalue corresponds to a *kink*,[17] i.e. all spins to the left of of a given point have one value, and all spins from that point on to the right have another value which differs from the first one by ± 1 (kink or antikink). With periodic boundary conditions, states with one kink are not allowed, but kink-antikink pairs are. The SSI's correspond to world lines of such pairs.

3. The Cluster Algorithm

The idea for the cluster algorithm came from the picture of the SOS configurations as landscapes with hills and valleys. In a somewhat similar manner to the Wolff algorithm,[6–8] we perform large scale changes of a configuration by choosing a horizontal *reflection plane*, considering the connected regions above (hills) and below (valleys) the plane, and reflecting them through the plane ("flipping" them) independently, with an appropriate probability.

If this were the whole story, our algorithm would be little more than a variant of the Wolff algorithm. We shall show that this is in fact not the case. What always happened with cluster algorithms in the past was that each new model required a conceptually new trick, which ensures efficient moves in the space of the degrees of freedom relevant to criticality. In our case the trick is the *proper choice of the reflection plane*.

Let us first describe the technical details of our algorithm. We shall do this in the language of the DGSOS model (2.2), but everything can be easily translated for other SOS models. Let us denote the height of the horizontal *reflection plane* by M. A reflection of h_x with respect to M means

$$h_x \to 2M - h_x \ . \tag{3.1}$$

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 *embedded Ising variables*[6,1–4] $s_x = \pm 1$, defined by the decomposition

$$h_x = s_x \, |h_x - M| + M \ . \tag{3.2}$$

$s_x = 1$ means that h_x is above the reflection plane M, $s_x = -1$ that it is below M. Note that s_x is not well defined if $h_x = M$; this is not going to cause difficulties, as can be seen from equation (3.3) below.

In order to define the cluster procedure we introduce the *deleting* and *freezing* probabilities[5] for a link $< x, y >$ (in the language of [1–4] the term "activating" is used instead of "freezing"):

$$P_{\rm del}(x,y) = \, q \, \exp\left\{ -\frac{1}{T} \, |h_x - M| \, |h_y - M| \, (s_x s_y + 1) \right\} \ , \tag{3.3}$$

where $q \leq 1$ can explicitly depend on $|h_x - M|$ and $|h_y - M|$, and

$$P_{\rm freeze}(x,y) = 1 - P_{\rm del}(x,y) \, . \tag{3.4}$$

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 $q = 1$.

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 $P_{\rm del}(x,y) = 1$ if either $s_x \neq s_y$, i.e. h_x and h_y are on different sides of the reflection plane, or if $|h_x - M| \, |h_y - M| = 0$, 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 $h_x = M$ 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 h_x. Since $P_{\rm del}(x,y)$ 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 h_x, this is equivalent to performing the reflection (3.1) for all spins in the cluster. Notice that the cluster boundaries are not in general exactly at the intersection of the hills-and-valleys landscape with the reflection plane, since $P_{\rm del}(x,y)$ is nonzero also if both h_x and h_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,[7,2] i.e. a cluster is built starting from a randomly chosen site x_o (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[1-8] 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 $|h_x - M|$ for *all* lattice sites:

$$\mathrm{prob}(M) = f(|h - M|; M) \ . \tag{3.5}$$

This condition still leaves a lot of freedom in the choice of M. Note that if one starts with an unnormalized distribution of the form (3.5), one has to make sure that the normalization constant (the sum over M in the last equation) does not depend on the configuration h.

Let us now turn to the choice of the reflection plane M. For all practical purposes, the SOS surface thickness is small, as can be seen from table **3.1** at the end of this section. Even in the rough phase, at values of T that are not very large in comparison to T_{KT}, and for $L = 256$, σ hardly exceeds a value of two. Thus the first thing we have to take care of is that the reflection plane lies *within the vertical bounds of the SOS surface.*

The H-algorithm. One very simple way to ensure this is to choose M in the neighbourhood of the height of the seed spin h_{x_o}. Typically x_o will neither correspond to the top of a hill, nor to the bottom of a valley, but to a point on a slope. If the reflection plane is close to h_{x_o}, there is a good chance that the cluster algorithm will cut a hill or a valley of reasonable size from the landscape and flip it. Since we assume $q = 1$ in (3.3), there is no point in allowing $M = h_{x_o}$, as all links starting from x_o are deleted, and the reflection of the monomer at x_o does not change the configuration at all. However, since the surface thickness is small, we would like to have $|h_{x_o} - M|$ as small as possible, in order to avoid as much as possible the reflection plane falling outside the vertical bounds of the surface. We thus choose

$$\mathrm{prob}(M) = \frac{1}{2} \quad \text{for} \quad M = h_{x_o} \pm \frac{1}{2} \ , \quad \mathrm{prob}(M) = 0 \quad \text{else} \ . \tag{3.6}$$

We denote this procedure as the H-algorithm, "H" standing for "half-integer" choice of the reflection plane. The H-algorithm is ergodic.

We tested this algorithm extensively. For details on the numerical problems connected to the analysis of autocorrelations we refer the reader to Ref. 10. Here we only report the conclusion of this analysis for the DGSOS model at $T = 1$ in the rough phase: for the dynamical exponent z we have $z \approx 1$. Thus *CSD is only partly overcome.* While z increases somewhat with decreasing temperature, even at T_{KT} the value of one is the right order of magnitude.

Let us mention that it is quite difficult to measure z in the smooth phase, since in this case we would have to use the finite size scaling formula[3]

$$\tau = L^z F\left(\frac{\xi}{L}\right) \ , \tag{3.7}$$

where τ is the autocorrelation time,[1–8] and F is a universal scaling function. It is however not a priori clear that this formula defines a unique exponent z: if F has a zero at an infinite value for its argument, there may be one z for the regime $L > \xi$ and another one for $L < \xi$. For the Ising model, such a phenomenon does not happen, but the T-dependence of z in the rough phase suggests that it may happen in our case. We did not do an analysis using (3.7) since accurate measurements of the correlation length ξ are in practice unfeasible, the reason being that for periodic boundary conditions the first excited states are kink-antikink states, i.e. two-particle states.[10] As alternatives, we might either compute ξ in the dual model[18], or use the surface thickness to estimate ξ (see the discussion of section 2).

We did however perform autocorrelations measurements in the smooth phase too, and, close to $T_{\rm KT}$ and for lattices of up to $L = 256$, there was no significant difference as compared to the results at and above $T_{\rm KT}$.

A careful analysis of the cluster size distribution revealed that the H-algorithm produces both small 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. This indicates that the surface thickness is so small that taking the reflection plane only half an integer away from the seed spin may still too often be a bad choice. It might help to be able to take the reflection plane equal to the seed height itself, without adding anything.

On the other hand, the cluster size distribution for small clusters was quite similar to that of the Ising model, so there may be a different reason for the failure of the H-algorithm to completely remove CSD. To understand more, we have to consider the action of the reflections on the SSI's. Consider an SSI on top of a flat background of integer height M_o, and a reflection plane of height $M = M_o + \frac{1}{2}$. The H-algorithm may produce such an SSI or annihilate it in case it already exists. What it cannot do is to reflect such an SSI through the background M_o. But in the name of efficiency, such an operation should be possible, since it costs nothing at all in terms of Boltzmann weights! So we should supplement our algorithm with *reflections through integer-valued planes* to make such " microcanonical moves" possible. Of course, in a real-life configuration, there may be some difference between the Boltzmann weight of the original and integer-reflected-SSI configuration, but this is not a significant effect.

The I-algorithm. We can choose an integer reflection plane M by simply setting it equal to the height at *a point different from the seed*:

$$M = h_{y_o} \ , \quad y_o \neq x_o \ . \tag{3.8}$$

In our simulations we chose y_o randomly, after having chosen x_o randomly too. We remind that we still assume $q = 1$ in (3.3). This procedure ensures that M is strictly within the vertical bounds of the hills-and-valleys landscape. Since the I-algorithm is not ergodic, we *combined it with the H-algorithm.* For the combined algorithm we found *no CSD whatsoever* both in the rough and in the smooth phase. We took

lattice sizes from $L = 8$ to $L = 256$.

The I-algorithm produced a cluster size distribution with larger relative weight for intermediate size clusters than was the case for the H-algorithm. The question arises whether this is the relevant issue in overcoming CSD, or whether the above considerations about SSI's play a more fundamental role. In order to settle this issue we performed simulations where we combined the I-algorithm with a standard local Metropolis algorithm. For this case CSD was still partly present, similarly to the H-algorithm case. So we learned that we need both the H-algorithm to create or destroy SSI's, and the I-algorithm to do "almost microcanonical" reflections of SSI's. Thus once again, the problem of removing CSD was tied to the problem of understanding how to move efficiently in the space of relevant degrees of freedom.

The Q-algorithm. A different way of implementing reflections through integer-valued planes is to take the value of the reflection plane equal to the height of the seed spin, but to allow $q < 1$ in (3.3):

$$M = h_{x_o} \ , \quad q = q_o < 1 \quad \text{for} \quad |h_x - M|\,|h_y - M| = 0 \ , \quad q = 1 \quad \text{else} \ . \tag{3.9}$$

In our numerical investigations, values of q_o between 0.7 and 0.8 turned out to be optimal. The efficiency of the Q-algorithm is comparable to that of the I-algorithm, and combining it with the H-algorithm also *eliminates CSD completely*.

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.[5]

For large values of the surface thickness, we could have found the "correct" cluster algorithm much more easily: it suffices to take e.g. a discretized Gaussian a priori distribution of the reflection plane M around the height of the seed spin. The (integer and half-integer) values of M need not be very close to the seed height in this case. By tuning the width of the a priori distribution we can optimize the performance of such an algorithm. If we allow M to be continuous, we can use this algorithm even for the massless free field theory. As expected from the fact that the SOS models in the rough phase and the massless free field theory have similar infrared properties, the cluster algorithm for the free field theory also eliminates CSD completely (we tested this!).

Let us complete this section by giving an example of the quality of results that can be obtained using our cluster algorithm. Table 1 presents our values for the surface thickness in the DGSOS model at $T = 1$ (contrary to Ref. 12, we succeeded in vectorizing the cluster algorithm in a very simple fashion[19]). Eq. (2.6) fits all data perfectly. Using only the values of σ^2 for $L \geq 32$ we obtained $T_{\text{eff}} = 0.9965(8)$. We fitted the data with other functional forms too. We first replaced in (2.6) $\ln L$ by $(\ln L)^a$. The fitted value for a was one within errorbars. Then we allowed for an additional term proportional to $\ln\ln L$. The fitted value for the coefficient of this term was zero (within errorbars). Finally we fitted with a constant times a power of L plus a another constant. There were no good fits at all. We have thus confirmed

Table **3.1**: The surface thickness for the DGSOS model at $T = 1$.

L	σ^2
8	0.75471(36)
16	0.97523(36)
32	1.19415(34)
64	1.41442(32)
128	1.63364(39)
256	1.85396(42)

the validity of (2.6) with a high degree of accuracy.

4. The Case of Three Dimensions

In three dimensions, the discrete Gaussian model is defined through (2.1)-(2.2) too, the only difference being that we consider an L^3 lattice. The physics however is very different from the two-dimensional case.[20] The global symmetry is broken at any finite temperature. The critical point is $T \to \infty$, and the correlation length ξ increases exponentially with T. The large distance properties are described by a massive rather than a massless free field theory. The relevant degrees of freedom are long wavelength spin waves, which correspond to fluctuations of large block spins. On a finite lattice, there are two distinct regimes: for $L > \xi$ we effectively have, as just said, a massive free field theory, while for $L < \xi$ we effectively have a massless free field theory, similarly to the two-dimensional case (of course, interaction is present, so there will be corrections to this effective behaviour, which are larger for shorter distances).

We studied our cluster algorithms in both these regimes for lattices up to $L = 64$. For the more interesting regime $L > \xi$ we measured the exponent z using (3.7) and the known dependence of ξ on the temperature.[20] We took temperatures from 1.4 to 2.3, which correspond to correlation lengths from 3 to 23. Although we would need more statistics and maybe larger systems, it definitely seems that even for the combination of the H- and I-algorithms, which gave the shortest autocorrelations, *z is consistent with two.* In the other regime, $L < \xi$, we got the same result for $T = 3$, which corresponds to $\xi \approx 120$. For $T = 10$, i.e. an astronomical correlation length, we did not see CSD.

These results were surprising, since up to now the successful cluster algorithms dramatically reduced CSD in all dimensions. Let us attempt to understand what is going on.

The first remark concerns the quantity σ^2 of (2.5): is quite small, even at $T = 3$ (notice that in three dimensions this quantity does not have a very pronounced

volume dependence, since the inverse Laplacian decreases with distance). Thus for $T \leq 3$ there is no point in choosing a wider a priori distribution for the reflection plane M than what we described when defining the H- and I-algorithms.

We investigated the cluster size distribution for these algorithms, and, while clusters of all sizes do occur, we found a marked difference from the behaviour in two dimensions. From percolation theory one expects[21] that for clusters C which are small enough as not to feel the finiteness of the lattice, the cluster size distribution $\rho(|C|)$ should be of the form

$$\rho(|C|) = |C|^{-b} \ . \tag{4.1}$$

Now, in two dimensions we found $b \approx 1$, and in three dimensions $b \approx 2$. This means that in three dimensions the relative weight of small clusters is enhanced, and thus the relevant large distance degrees of freedom are not updated efficiently enough.

A possible explanation for this phenomenon is the following. As a general rule in quantum field theory, the ultraviolet, i.e. short distance, fluctuations increase with increasing dimension. For the Discrete Gaussian model we actually saw this happening in our data. But if the *amplitude of short distance fluctuations* is larger, the reflection plane will cut out smaller "hills" and "valleys". If the amplitude of the long range fluctuations is smaller or comparable to that of the short range fluctuations, the latter will obscur the former for the purpose of cluster formation. This is a new phenomenon in the framework of cluster algorithms, which may play a role whenever unbounded fields are used (NB: a field may be bounded by a potential too, as in the case of ϕ^4 theories).

At $T = 10$ (4.1) is still true, but we saw no CSD (of course, here only the regime $L < \xi$ is accessible). As discussed in the previous section, this result should imply that our cluster algorithm has no CSD for the massless free field theory too. This expectation was fully confirmed by simulation results. A better understanding of this result is still needed. On the one hand, at $T = 10$ σ^2 is large, so we are in the regime where the reflections of hills and valleys do comparatively more changes in the configuration. On the other hand, the fact that (4.1) is still true sheds a shade of doubt on the explanation for the presence of CSD at smaller T that we attempted in the previous paragraph.

5. Conclusions

We described a new class of cluster algorithms which eliminate critical slowing down for SOS models. We also provided the physical intuition for understanding why this kind of algorithms are successful.

Furthermore, the type of cluster algorithms we described can be adapted for continuous-spin models (two-dimensional scalar field theories), like the Sine-Gordon model, the dipole gas, and the massless free field theory. Actually, for the massless free field theory and for the Sine-Gordon [11] model we already have results that show (almost) no critical slowing down.

Detailed numerical investigations of the KT transition in SOS models and in the Sine Gordon model are in progress.[11]

In Ref. 22 a related surface-cluster-algorithm is described for the interface of the three-dimensional Ising model with mixed boundary conditions.

Finally, our study of the three-dimensional Discrete Gaussian model sheds new light onto properties of cluster algorithms in general. In order to make further progress here, we are thinking of cluster algorithms that act on block spins.

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18. Such a computation was performed very recently by Jahnke and Nather, FU-Berlin preprint.
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    See also e.g.: M. Karliner and G. Mack, Nucl. Phys. B225 (1983) 371.
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