

The Loop-Cluster Algorithm for the Case of the 6 Vertex Model

Hans Gerd Evertz^a and Mihai Marcu^b
^aSupercomputer Computations Research Institute, Florida State Univ., Tallahassee, FL 32306, USA

^bSchool of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, 69978 Tel Aviv, Israel

We present the loop algorithm, a new type of cluster algorithm that we recently introduced for the F model. Using the framework of Kandel and Domany, we show how to generalize the algorithm to the arrow flip symmetric 6 vertex model. We propose the principle of least possible freezing as the guide to choosing the values of free parameters in the algorithm. Finally, we briefly discuss the application of our algorithm to simulations of quantum spin systems. In particular, all necessary information is provided for the simulation of spin $\frac{1}{2}$ Heisenberg and xzx models.

1. INTRODUCTION

Cluster algorithms, originally introduced for the Ising model [1] and then generalized to various other situations [2, 3], are one of the promising ways of overcoming critical slowing down. Recently [4, 5] we introduced algorithms for vertex models [6, 7], which are the first cluster algorithms for models with constraints. While [4] is an adaptation of an algorithm originally devised for solid-on-solid models, the loop algorithm introduced in [5] does not resemble any existing scheme.

In [5] we presented the loop algorithm for the F model. This enabled us to present our idea as clearly as possible. Here we shall show how to generalize it for the 6 vertex model, which has an additional coupling and a richer phase structure (see below). The framework of [3] proves to be an extremely useful tool here.

Our scheme is devised such as to take into account the constraints automatically, and to allow a simple way to construct the clusters. After defining the relevant probabilities, we find that we still have some free parameters. In order to optimize the algorithm, we introduce the principle of minimal freezing. As seen from the example of the F model, this choice of parameters is of utmost importance.

The loop algorithm can be further generalized to more complicated vertex models. However, as it stands, there are already important applications: quantum spin systems can be simulated by

mapping them to vertex models [8]. In particular, the loop algorithm for the 6 vertex model presented here can be used to simulate spin $\frac{1}{2}$ Heisenberg ferromagnets and antiferromagnets, and xzx models, even in more than one dimension.

2. THE 6 VERTEX MODEL

The six vertex model [6, 7] is defined on a square lattice. On the bonds there lives an Ising-like variable that is usually represented as an arrow. For example, arrow up or right means plus one, arrow down or left means minus one. At each vertex, there are two incoming and two outgoing arrows. In fig. 1 we show the six possible configurations at a vertex, numbered as in [6, 7].

The statistical weight of a configuration is given by the product over all vertices of the vertex weights $\rho(u)$. For each vertex there are 6 possible weights $\rho(u)$, $u = 1, \dots, 6$. We assume the vertex weights to be symmetric under reversal of all arrows. So in standard notation [6, 7] we have:

$$\begin{aligned} \rho(1) &= \rho(2) = a, \\ \rho(3) &= \rho(4) = b, \\ \rho(5) &= \rho(6) = c. \end{aligned} \tag{1}$$

The six vertex model basically has two types of phase transitions: of Kosterlitz-Thouless type and of KDP type [6, 7]. A sub-model exhibiting the former is the F model, defined by $c = 1$, $a = b = \exp(-K)$, $K \geq 0$. For the latter transition an example is the KDP model itself, defined by $a = 1$, $b = c = \exp(-K)$, $K \geq 0$.

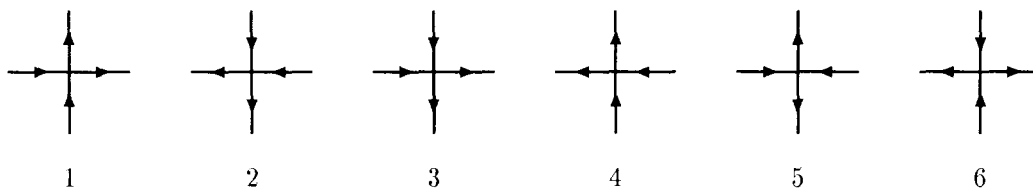


Figure 1. The six vertex configurations, $u = 1, \dots, 6$ (using the standard conventions of [6]).

3. THE LOOP ALGORITHM

If we regard the arrows on bonds as a vector field, the constraint at the vertices is a zero-divergence condition. Therefore every configuration change can be obtained as a sequence of *loop-flips*. By “loop” we denote an oriented, closed, non-branching (but possibly self-intersecting) path of bonds, such that all arrows along the path point in the direction of the path. A loop-flip reverses the direction of all arrows along the loop.

Our cluster algorithm performs precisely such operations, with appropriate probabilities. It constructs closed paths consisting of one or several loops without common bonds. All loops in this path are flipped together.

We shall construct the path iteratively, following the direction of the arrows. Let the bond b be the latest addition to the path. The arrow on b points to a new vertex v . There are two outgoing arrows at v , and what we need is a unique prescription for continuing the path through v . This is provided by a *break-up* of the vertex v . In addition to the break-up, we have to allow for *freezing* of v . By choosing suitable probabilities for break-up and freezing we shall satisfy detailed balance.

The *break-up* operation is defined by splitting v into two pieces, as shown in fig. 2. The two pieces are either two corners or two straight lines. On each piece, one of the arrows points towards v , while the other one points away from v . Thus we will not allow e.g. the ul-lr break-up for a vertex in the configuration 3. If we break up v , the possible new configurations are obtained by flipping (i.e. reversing both arrows of) the two

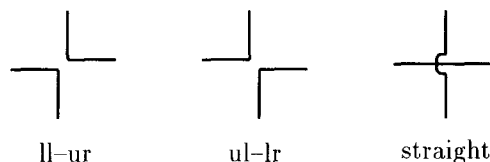


Figure 2. The three break-ups of a vertex: ll-ur (lower-left-upper-right), ul-lr (upper-left-lower-right), and straight.

pieces independently. On the other hand, if we freeze v , the only possible configuration change is to flip all four arrows.

The break-up and freeze probabilities are conveniently described within the general framework for cluster algorithms proposed by Kandel and Domany [3]. It is sufficient to give them for one vertex, which is in the current configuration u . We define 6 new interactions (weight functions) ρ_i , $i = 1, \dots, 6$, corresponding to specific break-up and freeze operations. (The labelling of the new interactions is completely arbitrary, and the fact that we have six of them is just a coincidence). For each vertex in configuration u , we replace with probability $p_i(u)$ the original interaction ρ by the new interaction ρ_i . Detailed balance and the proper normalization of probabilities require that for every u

$$p_i(u) = q_i \frac{\rho_i(u)}{\rho(u)}, \quad \sum_i p_i(u) = 1, \quad (2)$$

where $q_i \geq 0$ are parameters.

As discussed in [3] (see also table 1), *freezing* is described by introducing one new interaction for each different value of $\rho(u)$. For example, to

i action	1 freeze 1,2	2 freeze 3,4	3 freeze 5,6	4 ll-ur	5 ul-lr	6 straight
$\rho_i(\tilde{u})$	1, $\rho(\tilde{u})=a$ 0, else	1, $\rho(\tilde{u})=b$ 0, else	1, $\rho(\tilde{u})=c$ 0, else	0, $\rho(\tilde{u})=a$ 1, else	0, $\rho(\tilde{u})=b$ 1, else	0, $\rho(\tilde{u})=c$ 1, else
$p_i(u)$	q_1/a , $\rho(u)=a$ 0, else	q_2/b , $\rho(u)=b$ 0, else	q_3/c , $\rho(u)=c$ 0, else	0, $\rho(u)=a$ $q_4/\rho(u)$, else	0, $\rho(u)=b$ $q_5/\rho(u)$, else	0, $\rho(u)=c$ $q_6/\rho(u)$, else

Table 1. New interactions $\rho_i(\tilde{u})$ and the probabilities $p_i(u)$ to choose them at a vertex in current configuration u . See eq. (2).

freeze the value a , we choose the interaction ρ_1 to be $\rho_1(u) = 1$ if $\rho(u) = a$, and $\rho_1(u) = 0$ otherwise. In other words, if u is 1 or 2, the Boltzmann weight $\rho_1(u)$ is one, so transitions between 1 and 2 cost nothing; the vertex configurations 3, 4, 5, and 6 are however not allowed with ρ_1 .

Each *break-up* is also described by one new interaction. As an example take the ul-lr break-up. It is given by the new interaction number five, with $\rho_5(u) = 1$ if $\rho(u) = a$ or c , and $\rho_5(u) = 0$ if $\rho(u) = b$. In other words, with the new interaction ρ_5 , transitions between 1, 2, 5 and 6 cost nothing, while the vertex configurations 3 and 4 are not allowed. This corresponds precisely to allowing independent corner flips in a ul-lr break-up (see figs. 1,2).

The full list of new weights $\rho_i(u)$ and probabilities $p_i(u)$ to choose them are given in table 1. From (2) we also obtain:

$$\begin{aligned} q_1 + q_5 + q_6 &= a, \\ q_2 + q_4 + q_6 &= b, \\ q_3 + q_4 + q_5 &= c. \end{aligned} \quad (3)$$

Assume now that we have broken or frozen all vertices. Starting from a bond b_0 , we proceed to construct a closed path by moving in the arrow direction. As we move from vertex to vertex, we always have a unique way to continue the path. At broken vertices the path enters the vertex through one bond and leaves it through another. If the last bond b added to the cluster points to a frozen vertex v , the path bifurcates in the directions of the two outgoing arrows of v . One of these directions can be considered as belonging to the loop we came from, the other one as belonging to a new loop. Since we also have to flip the second incoming arrow of v , we

are assured that this new loop also closes. The two loops have to be flipped together. In general, the zero-divergence condition guarantees that all loops will eventually close.

We have now finished describing the procedure for constructing clusters. In order to specify the algorithm completely, we must choose values for the constants q_i , and decide how the clusters are flipped. The former problem is of utmost importance, and it is the object of the next chapter. For the cluster flips, we may use both the Swendsen-Wang procedure and the single cluster flip [2]. In [5] we used the latter, and obtained a drastic reduction of critical slowing down.

4. OPTIMIZATION

We have seen that freezing forces loops to be flipped together. Previous experience with cluster algorithms [2] suggests that it is advantageous to be able to flip them independently. We therefore introduce the principle of *minimal freezing* as a guide for choosing the constants q_i : we shall minimize the freezing probabilities, given the constraints (3) and $q_i \geq 0$. In [5] we report that for the case of the F model, optimization by minimal freezing does indeed minimize critical slowing down. Here we discuss optimization for the 4 phases of the 6 vertex model, usually denoted by capital roman numerals [6, 7].

Let us first look at phase IV, where $c > a + b$. To minimize the freezing of weight c we have to minimize q_3 . From (3), $q_3 = c - a - b + q_1 + q_2 + 2q_6$. With $q_i \geq 0$ this implies $q_{3,\min} = c - a - b$. The minimal value of q_3 can only be chosen if *at the same time* we set $q_1 = q_2 = 0$, i.e. mini-

mize (in this case do not allow for) the freezing of the smaller weights a and b . The optimized parameters for phase IV are then:

$$\begin{aligned} q_1 = 0, \quad q_2 = 0, \quad q_3 = c - a - b, \\ q_4 = b, \quad q_5 = a, \quad q_6 = 0. \end{aligned} \quad (4)$$

In phase I the situation is technically similar. Here $a > b + c$, and we minimize freezing with $q_1 = a - b - c$ and $q_2 = q_3 = 0$. The same holds for phase II, $b > a + c$, where we obtain minimal freezing for $q_2 = b - a - c$ and $q_1 = q_3 = 0$.

Phase III (the massless phase) is characterized by $a, b, c < \frac{1}{2}(a + b + c)$. Here we can set all freezing probabilities to zero. Thus,

$$\begin{aligned} q_1 = 0, \quad 2q_4 = b + c - a, \\ q_2 = 0, \quad 2q_5 = c + a - b, \\ q_3 = 0, \quad 2q_6 = a + b - c. \end{aligned} \quad (5)$$

The F model is obtained from (4) and (5) as the special case $a = b \leq 1, c = 1$. One can easily see that for this case we recover the discussion of [5]. (Notice that since $a = b$, in the F model the straight break-up will be called freezing).

5. APPLICATIONS, CONCLUSIONS

We have presented a new type of cluster algorithm, the loop algorithm, for the case of the six vertex model. For the F model, the algorithm has been shown in [5] to beat critical slowing down.

Particularly promising is the possibility of *accelerating Quantum Monte Carlo simulations* [8, 9]. Quantum spin systems in one and two dimensions can be mapped into vertex models in $1 + 1$ and $2 + 1$ dimensions via the Trotter formula and suitable splittings of the Hamiltonian [8]. The simplest example is the spin $\frac{1}{2}$ xzx quantum chain, which is mapped directly into the 6-vertex model. For higher spins, more complicated vertex models result (e.g. 19-vertex model for spin one).

For $(2 + 1)$ dimensions, different splittings of the Hamiltonian can lead to geometrically quite different situations [8, 9]. We can e.g. choose between 6-vertex models on a complicated $2 + 1$ dimensional lattice, and models on a *bcc* lattice with 8 bonds (and a large number of configurations) per vertex. Notice that for the simulation

of the 2-dimensional Heisenberg antiferromagnet using the former splitting, all relevant formulas have been worked out in the present paper.

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