Virtual Bond Percolation for Ising Cluster Dynamics

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**Abstract**

The Fortuin-Kasteleyn mapping between the Ising model and the site-bond correlated percolation model is shown to be only one of an infinite class of exact mappings. These new cluster representations are a result of “renormalized” percolation rules correlated to entire blocks of spins. For example these rules allow for percolation on “virtual” bonds between spins not present in the underlying Hamiltonian. As a consequence we can define new random cluster theories each with its own Monte Carlo cluster dynamics that exactly reproduce the Ising model. By tuning parameters on the critical percolation surface, it is demonstrated numerically that cluster algorithms can be formulated for the 2-d and 3-d Ising model that have smaller autocorrelations than the original Swendsen-Wang algorithm.
1. Introduction

Our understanding of the Ising model has been greatly enhanced by the study of Coniglio-Klein \[1\] critical percolation clusters and the classic work of Fortuin-Kasteleyn \[2, 3\] on the exact mapping of the Ising model into the random cluster model for site-bond correlated percolation. With the work of Swendsen and Wang \[4\] this cluster representation has also lead to accelerated Monte Carlo dynamics with very small autocorrelation times \[5, 6, 7\].

In all of these endeavors the underlying clusters representation appeared to be unique — the probability of bond percolation, the only free parameter, being fixed by detailed balance or the requirement of scaling in the critical region. However, a central mystery of this beautiful formalism remains concerning the incompletely decoupling of clusters as manifest in divergent autocorrelations at the phase transition. It appears to us that a “perfect” representation of normal modes via clusters (analogous to fourier modes for a pure Gaussian theory) should in principle exhibit no critical slowing down \((z = 0)\).

Here we show that the underlying Fortuin-Kasteleyn map is not unique.

By introducing longer range correlated percolation, we show that there are additional free parameters (in the null vector space transverse to the critical percolation surface) which are not fixed by the requirement of an exact mapping between the Ising and the random cluster partition functions. The percolation process is extended to longer length scales without leaving the critical surface on which the pair connectedness function coincides identically with the Ising correlation function. The new freedom to define “renormalized” critical clusters may help to understand the residual cluster interactions and lead to even more efficient Monte Carlo methods. By removing the rigid constraints of earlier methods, we also hope to formulate new cluster methods for more complex systems such as spin glasses \[8\]. Even generalizations to continuous molecular systems now appear less daunting.

In the present article our new cluster methods will be explained exclusively in the context of the Ising model, although it should be obvious that they apply equally to all the recent extensions of the Swendsen-Wang algorithm such as those made by Brower and Tamayo \[5\] for the Landau-Ginzburg theory, by Wolff \[6\] for spin models and others \[3, 5, 7\]. While shorter autocorrelations evidently can result, in all probability the dynamical universality class and the critical exponent \(z\) will not be changed unless we go to recursive methods that introduce virtual bonds on all length scales. Such extensions of our methods will be considered in future publications.
The organization of this article is as follows. Section 2 presents the block percolation scheme through two simple examples, with illustrations of possible extensions. Section 3 defines the resulting cluster dynamics and computes autocorrelations and cluster distributions. The renormalized clusters are shown numerically to lead to reduced autocorrelations relative to the Swendsen-Wang method. Appendix A presents the general construction of our block correlated decomposition and the proof of equilibrium for the resultant cluster dynamics. Although the general argument is important both for its rigor and for the extraordinary range of alternative cluster methods it implies, the specific examples are probably easier to understand.

2. Blocking Schemes for the 2-d and 3-d Ising Model

Let us begin by studying in detail the simplest extension of the Fortuin-Kasteleyn (F-K) mechanism from blocks of 2 spins to blocks of 3 spins. This modest generalization already encounters several qualitatively new features.

The conventional F-K mapping has two steps. The first step decomposes the Ising Hamiltonian into a sum over bonds (or 2 spin blocks) so that the Ising probability distribution is seen as a product of factors.

\[ P^{Ising}(s_i) = \frac{1}{Z} \prod_{<i,j>} e^{-\beta(1-s_i s_j)} \]  (1)

The second step decomposes each factor into two terms,

\[ e^{-\beta(1-s_1 s_2)} = \sum_{n=0,1} p_n \Delta_n(s_1, s_2) = e^{-2\beta} + (1 - e^{-2\beta})\delta_{s_1, s_2} \]  (2)

with the probabilities,

\[ p_0 = e^{-2\beta}, \quad p_1 = 1 - e^{-2\beta}, \]  (3)

uniquely determined by the requirement that probabilities for aligned vs unaligned spins be correct. The deletion (n=0) and percolation (n=1) terms have been designated by \( \Delta_0(s_1, s_2) = 1 \) and \( \Delta_1(s_1, s_2) = \delta_{s_1, s_2} \) respectively to accommodate a more general expansion for larger blocks.

2.1 Three Spin Blocks

The general expansion for a block of spins B takes the form,

\[ e^{-\beta V_B(s_i)} = \sum_{n=0,\ldots,n_{max}-1} p_n \Delta_n(s_i). \]  (4)
Each of the \( n \) terms is a unique product of delta functions representing one of the many possible ways to break it up into clusters. The only requirement is that the entire Hamiltonian be given by the sum over the set of blocks and that the expansion of the block into delta functions be complete. (See Appendix A for the proof and an even larger class of options.)

For example, the 3-spin block for a nearest neighbor Ising lattice (See Figure 1 and 2), \( B = (s_1, s_2, s_3) \), can be split into 5 terms,

\[
e^{-\beta(2-s_1s_2-s_2s_3)} = p_0 + p_1 \delta_{s_2,s_3} + p_2 \delta_{s_1,s_3} + p_3 \delta_{s_1,s_2} + p_4 \delta_{s_1,s_2} \delta_{s_2,s_3}
\]

(5)

However, this most general 3-spin expansion is no longer unique. Since there are 5 independent \( p \)'s and only 4 independent equations, for \( (s_1, s_2, s_3) = (+, +, +), (-, +, +), (+, -, +), (+, +, -) \), the linear equations must have a non-trivial null space. The general solution, \( p_i = p_i^{FK} + p_i^{null} \), is the sum of an original inhomogeneous F-K solution \( p_i^{FK} \) and one null vector, \( p_i^{null} = (-1, 1, 1, 1, -2) \).

\[
\begin{align*}
p_0 & = e^{-4\beta} - \zeta \\
p_1 & = e^{-2\beta}(1 - e^{-2\beta}) + \zeta \\
p_2 & = \zeta \\
p_3 & = (1 - e^{-2\beta})e^{-2\beta} + \zeta \\
p_4 & = (1 - e^{-2\beta})^2 - 2\zeta 
\end{align*}
\]

(6)

This null vector expresses the simple fact that at least two Ising spins must be in the same state.

\[
(1 - \delta_{s_1,s_2})(1 - \delta_{s_2,s_3})(1 - \delta_{s_3,s_1}) = 0
\]

(7)

No new solutions are present for the \( q \) state Potts model for \( q > 2 \) without going to larger blocks. The parameter \( \zeta \) has been chosen to represent a virtual bond connecting \( s_1 \) to \( s_3 \) so that at \( \zeta = 0 \) this solution reverts to the standard Fortuin-Kasteleyn decomposition. As the parameter \( \zeta \) is increased the “real” bonds are reduced and the longer range “virtual” bond increased moving along the critical surface of the mapping. The remarkable simplicity of percolation relative to most critical phenomena is seen in the ability to find the critical surface analytically as a function of the critical Ising temperature.

For Monte Carlo cluster algorithms, it will turn out that the only requirement is to make all the probabilities non-negative, which in the neighborhood of the critical temperature restricts \( \zeta \) to \( 0 \leq \zeta \leq e^{-4\beta_c} \). For the 2-d Ising at the critical temperature, the limiting case,

\footnote{Note that the identity, \( \delta_{s_1,s_2} \delta_{s_2,s_3} = \delta_{s_1,s_3} \delta_{s_2,s_3} \), implies that the last term is actually a symmetric cluster of all three spins.}
\[ \zeta = e^{-4\beta c} = (1 - \sqrt{2})^2 \] has the remarkable property that both the no percolation term \( p_0 \), and the fully percolated term \( p_4 \), are exactly zero. Consequently any 3 spins must have precisely one percolated bond with 100% probability.

To illustrate a little the range of options we have considered a variety of ways of partitioning the 2-d lattice into 3 spin (or two bond) blocks (See Figure 1). It is instructive to consider the limiting case \( \zeta = e^{-4\beta} \) for lattice 1a with the three spin blocks centered on all the “black sites”. If we start with a checkerboard and use our limiting case again, \( \zeta = e^{-4\beta c} \), the lattice will immediately percolate into two sublattices with infinite clusters on the “red” sites and single clusters on the “black” sites. The study of such extreme non-equilibrium configurations shows how different our clusters are relative to Coniglio-Klein site-bond correlated percolation clusters.

It is easy to extend this example to the most general three spin blocks,

\[ e^{-\beta_{12}(1-s_1 s_2)-\beta_{23}(1-s_2 s_3)-\beta_{31}(1-s_3 s_1)} = p_0 + p_1 \delta_{s_2,s_3} + p_2 \delta_{s_1,s_3} + p_3 \delta_{s_1,s_2} + p_4 \delta_{s_1,s_2} \delta_{s_2,s_3} \quad (8) \]

appropriate for continuous spin models on cubic or triangular lattices. Again the general solution can be expressed as \( p_i = p_i^{FK} + p_i^{null} \), where the inhomogeneous solution is given by the F-K prescription applied to each bond separately and the null vector is unchanged. If we consider a red-black decomposition of the triangular lattice \( (\beta_{ij} = \beta) \), the limiting case , \( \zeta = e^{-6\beta c} = \sqrt{3} \) at the critical point again has the remarkable property that one and only one bond is percolated with 100% probability.

In the remainder of the paper we will consider in greater detail the resultant random cluster model and its Monte Carlo dynamics for the 3-spin block and plaquette blocking schemes. However as the reader will readily note, we have opened a Pandora box of alternative schemes. As the blocks are increased in size, there are more and more free parameters and neither the blocks nor the choice of these parameters have to be chosen to respect the symmetries of the underlying lattice. Consequently the exact constraint of mapping the Ising model into a random cluster scheme is far less restrictive than we might expected.

2.2 Plaquette Blocking for the Ising Model.

As a second additional example we briefly describe a scheme corresponding to 4 spin blocks or plaquettes. The energy can be expanded either, as a sum over all plaquettes dividing the interaction \( \beta \) for each bond by the number of ways it is shared \( (2 \text{ in 2-d or 4 in 3-d}) \), or by breaking the lattice up into a sum over over red (or black) plaquettes on the lattice. As in the 3-spin block case the Boltzmann factor for each plaquette is decomposed in a weighted
sum over products of delta functions $\Delta_n$ that constrain different subsets of spins inside the plaquette.

$$e^{-\beta V_{\text{plaq}}} = p_0 + p_1 (\delta_{s_1,s_2} + \delta_{s_3,s_4} + \delta_{s_1,s_3} + \delta_{s_1,s_4}) +$$

$$p_2 (\delta_{s_3,s_1} \delta_{s_1,s_2} + \delta_{s_1,s_2} \delta_{s_2,s_4} + \delta_{s_2,s_4} \delta_{s_4,s_3} + \delta_{s_4,s_3} \delta_{s_3,s_1}) +$$

$$p_3 (\delta_{s_1,s_3} \delta_{s_2,s_4} + \delta_{s_1,s_2} \delta_{s_3,s_4}) + p_4 \delta_{s_1,s_2} \delta_{s_2,s_4} \delta_{s_4,s_3} \delta_{s_3,s_1} +$$

$$p_5 \delta_{s_1,s_4} \delta_{s_2,s_3} + p_6 (\delta_{s_1,s_4} + \delta_{s_2,s_3}),$$

(9)

where $s_1, s_2, s_3$ and $s_4$ are the four spins that define the plaquette (see figure 3). Notice that the probabilities $p_5$ and $p_6$ represent virtual percolation bonds across the diagonals that freeze spins which do not interact in the Ising Hamiltonian.

This expansion is not the most general however, since we have imposed rotational symmetry in the spins $(s_1, s_2, s_3, s_4)$. For example the use of three spin blocks as shown in figure 1d offers a legitimate example of a four spin expansion as well, which violates rotational symmetries on the plaquette. The most general four spin expansion has 15 parameters and only 7 constraints. The number of solutions grows faster than exponential as the size of the block increases — for a 5 spin block there are already 52 parameters but only 16 constraints. Our 5 spin star blocking (fig 1a) could be expanded with 36 adjustable parameters!

Imposing rotational symmetry for the Ising model, there are four independent linear equations for $(s_1, s_2, s_3, s_4) = (+, +, +, +), (-, +, +, +), (-, -, +, +), (-, +, -, +)$ and their solution is expressed again as the sum of the F-K inhomogeneous solution plus the null space — this time with three free parameters $(\zeta_1, \zeta_2, \zeta_3)$ for three null vectors.

$$p_0 = e^{-8\beta} - 4\zeta_2 - 2\zeta_3$$

$$p_1 = e^{-6\beta}(1 - e^{-2\beta}) + \zeta_1 + 3\zeta_2 + \zeta_3$$

$$p_2 = e^{-4\beta}(1 - e^{-2\beta})^2 - 2\zeta_1 - 2\zeta_2 - \zeta_3$$

$$p_3 = e^{-4\beta}(1 - e^{-2\beta})^2 - 2\zeta_1 - 2\zeta_2$$

$$p_4 = 4e^{-2\beta}(1 - e^{-2\beta})^3 + (1 - e^{-2\beta})^4 + 8\zeta_1$$

$$p_5 = 4\zeta_2$$

$$p_6 = \zeta_3$$

(10)

The parameters $\zeta'$s are constrained by the condition that all probabilities must be positive numbers in the range $(0, 1)$. These three parameters give us additional flexibility to tune the percolation process in different ways. For example, one can increase or decrease the
probability of diagonal bonds with respect to horizontal or vertical bonds and, as we will see in section 5, in this way change cluster properties and decorrelation times. The plaquette example can also be applied to the 3 state Potts model with the result that the rotational symmetric solutions has only one null vector, \( p_{null} = (1, -1, 2, 1, -6, 1, -1) \), expressing the fact that in a 3 state Potts model the four spins of a plaquette can all reside in different states. In general it appears likely that for a \( q \)-state Potts model on \( e \) must resort to blocks bigger than \( q \) spins to find a non-trivial null space.

Finally we would like to emphasize that rather elegant blocking schemes exist whereby bonds are shared between adjacent blocks with the energy divided between the two blocks. Even for the F-K map this is allowed due to the trivial identity on each shared bond that \( ((1 - p)\delta_{s_1,s_2} + p) \times ((1 - p')\delta_{s_1,s_2} + p') = (1 - pp')\delta_{s_1,s_2} + pp' \). For example in our blocking schemes, we can restore translational symmetry for the 2-d triangular and square lattices simply by the replacement \( \beta \to \frac{1}{2}\beta \) throughout eq. 8 and eq. 10 respectively. Each bond is split into two equal pieces. For the Plaquette percolation method this has the appealing feature that all the symmetries of the original theory are preserved with next-to-nearest neighbor virtual bond percolation allowed over the entire lattice. We feel that the more symmetric forms are more likely to express the proper scaling of critical clusters and thus lead to more efficient algorithms.

3. Cluster Dynamics.

In order to define a dynamics based on the percolation mappings described in the previous section one has to introduce for every blocking scheme, a set of auxiliary percolation variables \( n_B = 0, 1, ... \) on each block. Then the Monte Carlo cluster dynamics is chosen to be a Markov process for the joint distribution \( P_{joint}^{B}(s_i, n_B) \), in which one alternatively chooses the percolation variables \( n_B \) at fixed spins \( s_i \) and the spins for each cluster at fixed \( n_B \) (see Appendix A).

We outline our algorithm in the following steps.

1. Choose a local blocking scheme in such way that all spin-spin interactions are accounted for in the ensemble of blocks. Expand each block into a fixed percolation representation to define the joint distribution, \( P_{joint}^{B}(s_i, n_B) \).

2. For each block obtain its spin configuration \( (s_i) \) and choose a value for the “percolation”
variable \( n \equiv n_B \) with normalized probability:

\[
p(n|s_i) = \frac{p_n \Delta_n(s_i)}{\sum_n p_n \Delta_n(s_i)}
\]  

(11)

3. Label the connected components for the percolation graph using a cluster finding algorithm such as breadth-first search [10], the Hoshen-Kopelman algorithm [11], or a parallel algorithm [12].

4. Flip all of the spins in each cluster coherently with 50% probability and return to step 2.

Basically this is very similar to the standard Swendsen-Wang algorithm except that the percolation step involves probabilities correlated to entire blocks of spins. The variations on Swendsen-Wang suggested by Wolff [9] can be adapted to these clusters as well. There is a slight increase in complexity in the percolation step compared with Swendsen-Wang but the algorithm is still very straightforward. The values for the \( \zeta \)'s parameters can be taken to have different values for different block in the system. In our simulations we choose all of them to be fixed at a uniform value and then generate a look-up table of probabilities to be employed in the percolation process. The 3-spin and 4-spin block dynamics at \( \zeta_i = 0 \) are identical to the original Swendsen-Wang algorithm.

### 3.1 Numerical Results

Due to their simplicity we have implemented the 3-spin and plaquette blocking schemes as described in the previous section. In this section we analyze the autocorrelation times for equilibrium simulations and the dynamics of cluster distributions as the system relaxes to equilibrium.

**Autocorrelation times analysis**

All our simulations were carried out at the critical point of the infinite system. We studied the autocorrelation function for the squared magnetization as an average over Monte Carlo time \( (2.5 \times 10^5 \) steps). Figure 4 shows two autocorrelation functions for a system of size \( 64 \times 64 \) using the 3-spin block dynamics with the star blocking shown in figure 1a. The two curves correspond to the values of \( \zeta \) at the two extremes of the interval \((0, \ e^{-4\beta_c})\) of allowed values. The two functions show exponential relaxation but the extreme case farthest from the Swendsen-Wang point is faster by a noticeable amount. Moreover, the data in figure 5 appears to exhibit a monotonic decrease in autocorrelation times as the probability of virtual
bonds increases. A similar picture appears for the 3-spin block dynamics in three dimensions where for $\zeta = e^{-4\beta c}$, $\tau_{m^2}$ is almost twice as fast as Swendsen-Wang.

For the red-black plaquette dynamics we explored different regions of the solution space. We have not done an exhaustive search but it is clear that the autocorrelation times decrease as $\zeta_1$ decreases and the other two parameters, $\zeta_2$ and $\zeta_3$, increase. The fastest dynamics, the one with smallest autocorrelation times, we were able to find is the one corresponding to $\zeta_1 = -0.056349$, $\zeta_2 = 0.00245$, $\zeta_3 = 0.0098$ which is about 1.6 times faster than the Swendsen-Wang dynamics. Similar increases in speed are obtained for the symmetric form which expands both red and black plaquettes simultaneously using eq. 10 with $\beta \to \frac{1}{2}\beta$.

A general trend is seen in all these cases, as one might expect, increasing the probability of long range virtual bonds reduces the autocorrelation times.

Figure 6 shows the scaling of autocorrelation times with system size for the 3-spin block, plaquettes and Swendsen-Wang dynamics in two dimensions. If indeed the scaling is the same for all these dynamics, then they will have the same dynamic exponent $z$ as the original Swendsen-Wang and consequently would belong to the same dynamic universality class\cite{4, 13}. A more comprehensive and systematic study of these dynamics is required to settle this question but all our numerical results appear to be consistent with universality.

Cluster relaxation analysis

In addition to the standard autocorrelation times analysis we studied the equilibrium cluster distributions and the dynamics of cluster relaxation (see Stauffer, Kertesz and Miranda\cite{14}). Figure 7 shows the equilibrium cluster distributions for a $32 \times 32$ system using the plaquette blocking and Swendsen-Wang. Notice that the two cluster distributions are not identical but have very similar scaling behavior. The fastest plaquette dynamics having larger probabilities for virtual bonds favors larger clusters. It is clear that the cluster distributions follow a power law with identical or similar exponents. These exponents are related to the fractal dimension, $d_f$, of the clusters by the relation, $n_{eq}^s \sim s^{-(1+d/d_f)}$ with the implication that our extended percolation clusters have the same or similar fractal dimension as the Coniglio-Klein clusters.

In order to study cluster relaxation, a large number of simulations were performed in which the system relaxes to equilibrium at the critical point from an initial state with all spins up. Cluster histograms were accumulated at every time step and a logarithmic binning used to reduce fluctuations. Bin $n_s$ contains contributions from clusters sizes in the interval $(2^s, 2^{s+1} - 1]$. \end{proof}
1. Clusters numbers are assumed to relax exponentially to equilibrium,

\[ n_s(t) \sim (1 - e^{-t/\tau_s}) n_s^{eq}. \]

The scaling of the cluster decorrelation time \( \tau_s \) with cluster size defines a critical exponent \( r \),

\[ \tau_s \sim s^r \sim s^{z/d_f} \]

where \( z \) is the standard critical slowing down exponent and \( d_f \) is the fractal dimension of the clusters \( (d_f = d - \beta/\nu) \). For the 2-d Ising model, \( d_f = d - \beta/\nu = 1.875 \).

We have performed this analysis for two values of \( \zeta \) in the 3-spin block dynamics. We used a system of size \( 256^2 \) and sampled over 400 experiments. Figures 8 shows the relaxation of \( n_s(t) \) as a function of time for the Swendsen-Wang and the \( \zeta = e^{-4\beta_c} \) dynamics. It is clear that the \( \zeta = e^{-4\beta_c} \) dynamics produces a much more rapid relaxation process for the cluster numbers, perhaps by a factor of 5. This is surprising in view of the much smaller change for the equilibrium autocorrelation time (a factor of about 1.5), and gives an indication that the non-equilibrium dynamics may depend very sensitively on the strength of virtual bonds. In fact, the relaxation is so fast that it is hard to extract the scaling behavior by computing relaxation times for different cluster numbers. A more thorough study of the effects of these dynamics on cluster properties would help us to understand how to tune the \( \zeta \) parameters to have more control over the cluster relaxation process.

All the numerical experiments confirm the validity of these dynamics as equilibrium Monte Carlo processes and their potential to reduce autocorrelation times.

4. Conclusions

The main purpose of this article was to demonstrate the existence of a new class of exact percolation mappings not allowed in the original methods of Fortuin and Kasteleyn. To clarify the discussion we have studied in detail 3 spin and 4 spin blocking schemes applied to the nearest neighbor Ising model on a cubic lattice. However as we demonstrate in Appendix A, the freedom to invent new cluster algorithms within this framework is extraordinarily unencumbered. Not only is the Fortuin-Kasteleyn mapping not unique, one can find exact mappings which have peculiar properties such as not respecting the exact symmetries of the underlying model. We also note as illustrated by eq. 7 that these new mappings can not in general be extended analytically to the entire q state Potts model. The lower the value of q the larger the class of solutions. Now the problem is no longer the difficulty of finding
percolation mappings but the problem of choosing the most interesting or efficient straw in the haystack.

It is difficult not to be reminded of the analogous freedom in blocking schemes for the real space Renormalization Group (RG). In spite of this analogy several differences remain. For example the real space Renormalization Group has the following properties not shared by our approach: (i) the Hamiltonian has fewer degrees of freedom so that only the longer length scales are described correctly, (ii) the blocking procedure gives renormalized parameters that are automatically tuned to respect the scale change and (iii) the blocking is applied recursively. With respect to the first feature concerning the use of a semi-group, perhaps our approach offers an improvement in that we have an exact isomorphism. However the second two features we would like to emulate more closely, in the belief that they might be the key to better cluster methods. For example, it appears likely to us that the optimal choices for our $\zeta_i$ parameters (ie those with shortest autocorrelations) can be “derived” from scaling arguments. We are also looking at recursive blocking schemes — in particular a class of recursive algorithms based on iterative block decomposition in the spirit of the Migdal-Kadanoff renormalization group, which may be able to reduce $z$ below the value given by the Swendsen-Wang multi-cluster or Wolff single-cluster algorithms. Progress on these issues will be published in the future.

It is also interesting to consider the possibilities that virtual bond percolation parameters may be able to tune percolation processes in cases in which the standard Swendsen-Wang percolation does not produce acceleration such as in spin-glasses. Work is also proceeding on this problem. In summary the use of virtual bond dynamics in its most general form may be able to open new perspectives for cluster methods both to understand critical domains or droplets and to design faster algorithms for Monte Carlo simulations in statistical mechanics and quantum field theory.

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Figure Captions

• Figure 1. Examples of the variety of blocking schemes for 3-spins. The blocking used in our numerical experiments is shown in a). This blocking can be seen as a special case of a 5-spin “star” blocking. It is also interesting to notice that c) is an asymmetrical blocking and that d) produces plaquette-like structures.

• Figure 2. The expansion of the interaction between 3-spins in terms of percolation variables.

• Figure 3. Different percolation schemes for the 4-spin plaquette block mapping.

• Figure 4. Magnetization squared autocorrelation functions for the 3-spin block dynamics in two (a) and three (b) dimensions with different parameters $\zeta$. The two values shown correspond to the extremes of the interval of allowed values.

• Figure 5. Variation of the magnetization squared autocorrelation time as a function of $\zeta$ for the 3-spin block dynamics in two dimensions. The value of $\tau_{m^2}$ decreases as $\zeta$, the probability of virtual bonds, increases.

• Figure 6. Scaling of $\tau_{m^2}$ as a function of system size $L$ for the 3-spin block, plaquettes and Swendsen-Wang dynamics in two dimensions.

• Figure 7. Equilibrium cluster distributions for Swendsen-Wang and plaquette dynamics (with $\zeta_1 = -0.056349, \zeta_2 = 0.00245$ and $\zeta_3 = 0.0098$) in two dimensions. The slopes are nearly identical but large clusters are favored by the plaquette dynamics.

• Figure 8. Relaxation of cluster numbers for Swendsen-Wang (a) and the 3-spin block (for $\zeta = e^{-4\beta}$) (b) dynamics in two dimensions.
Appendix A: General Formulation of Block Percolation

Our generalization of the Fortuin-Kasteleyn percolation map has a strong similarity to blocking methods used for the real space Renormalization Group transformations. To bring out this similarity and to prove the correctness of the resulting dynamics, we follow the suggestion of Kandel et al[8] by introducing effective block potentials, \( U_{B}^{\text{eff}}(s_i, n_B, \beta) \), instead of the delta function constraints \( \Delta_{n_B}(s_i) \) considered above. Also we note that the delta functions can be recovered as a limiting case. For example, in this approach the original F-K map is replaced by the following two terms,

\[
e^{-\beta(1-s_1 s_2)} = p_0 e^{-J_0(1-s_1 s_2)} + p_1 e^{-J_1(1-s_1 s_2)}
\]

(A.1)

where \( U_{B}^{\text{eff}}(s_i, n, \beta) = J_n(1 - s_1 s_2) + \log(p_n) \). If we adjust the two weights correctly,

\[
p_0 = \frac{(e^{-2\beta} - e^{-2J_1})/(e^{-2J_0} - e^{-2J_1})}{},
\]

\[
p_1 = \frac{(e^{-2J_0} - e^{-2\beta})/(e^{-2J_0} - e^{-2J_1})}{},
\]

(A.2)

this is in itself a (new) legitimate mapping of the Ising bond at temperature \( \beta^{-1} \) into two randomly chosen terms with effective temperatures \( J_i^{-1} \). We can recover the standard F-K map by taking the limit of the effective inverse temperatures to zero (\( J_0 \to 0 \)) and to infinity (\( J_1 \to \infty \)) for the deletion and freezing (ie percolation) terms respectively (see eq.2). It is also interesting to view percolation methods in this way as the limiting extreme of a random mapping of a fixed temperature Ising system into a heterogeneous mixture of high and low temperature interactions.

Our general blocking scheme has two steps:

1. The Hamiltonian is expressed as a sum over blocks \( B \) of spins,

\[
H(s_i) = \sum_{B} V_B(s_i).
\]

(A.3)

2. The corresponding factor in the partition function is decomposed into a sum of terms,

\[
e^{-\beta V_B(s_i)} = \sum_{n_B=0,1,...,n_{max}-1} e^{-U_{B}^{\text{eff}}(s_i, n_B, \beta)}
\]

(A.4)

The products over all the resulting terms \( (A.4) \) forms a new joint probability distribution, \( P_{\text{joint}}(s_i, n_B) \) so that our generalized map is

\[
P^{\text{Ising}}(s_i) = \sum_{\{n_B\}} P_{\text{joint}}(s_i, n_B),
\]

(A.5)
The Ising model is represented as a marginal distribution by summing over the generalized percolation variables, \( n_B \). Alternatively the sum over the Ising variables yields the generalized “random cluster” (RC) model,

\[
P^{RC}(n_B) = \sum_{\{s_i\}} P^{joint}(s_i, n_B).
\]  

(A.6)

Lastly by taking the limiting case for effective potentials to freeze or delete clusters of spins in each block, we can among others obtain the entire class of virtual bond (or extended) percolation models. The fundamental identity for this class of percolation models, that guarantees criticality of the random cluster model at the Ising fixed point, is

\[
\langle s_i s_j \rangle \equiv \sum_{\{s_i\}} s_i s_j P^{Ising}(s_k) = \sum_{\{n_B\}} \gamma_{i,j} P^{RC}(n_B)
\]

(A.7)

where \( \langle s_i s_j \rangle \) is the Ising correlation function and the connectedness function, \( \gamma_{i,j} \), is 1 if \( i \) and \( j \) are in the same random cluster and 0 otherwise. From this identity it follows that the Ising spin-spin correlation length and the cluster connectedness length are equal and therefore that the critical scaling of both the Ising model and the corresponding random cluster model are identical.

**Equilibrium for cluster Monte Carlo**

To prove that all static quantities are given correctly by the Monte Carlo cluster algorithm in Section 3, one must show that the Markov process preserves the equilibrium distribution,

\[
P^{Ising}(s'_i) = \sum_{\{s_i\}} W(s'_i \leftarrow s_i) P^{Ising}(s_i).
\]  

(A.8)

This equilibrium balance condition is weaker than the full detailed balance satisfied by many Monte Carlo algorithms, but it is sufficient. To prove it recall that in our cluster Monte Carlo algorithm the percolation variables \( n_B \) in each block were first chosen according to the conditional probability,

\[
p(n_B | s_i) = \frac{e^{-U^{eff}_B(s_i, n_B; \beta)}}{\sum_{n_B} e^{-U^{eff}_B(s_i, n_B; \beta)}} = e^{-(U^{eff}_B(s_i, n_B; \beta) - \beta V_B(s_i))}
\]

(A.9)

and “clusters” of spins were subsequently chosen at fixed values of \( n_B \). Clearly this implies that the full transition matrix is a product of two conditional distributions,

\[
W(s'_i \leftarrow s_i) = \sum_{\{n'_B\}} P^{joint}(s_i | n'_B) P^{joint}(n'_B | s_i).
\]  

(A.10)
To complete the last step in demonstration one explicitly performs the sums in eq. A.10 and eq. A.8 by applying Bayes theorem,

\[ P(a, b) = P(a|b)P(b) \quad P(b) \equiv \sum_b P(a, b), \quad \text{(A.11)} \]

for each of the marginal distributions in eq. A.5 and eq. A.6. While there is nothing fundamentally new in this proof relative to that needed for the Swendsen-Wang algorithm it is necessary to see that it still goes through. Moreover this more general derivation illuminates a striking feature of cluster methods that the stochastic replacement of the full potential by a particular effective potential bears a very close resemblance to the Metropolis algorithm. Put into the context of blocks of spins, the similarity to the multigrid concept of “stochastic coarsening” is also transparent.