Scaling *Ansatz* for Swendsen-Wang Dynamics

W. Klein

IBM Bergen Scientific Centre, N-5007 Bergen, Norway, and
Physics Department[a] and Center for Polymer Studies, Boston University, Boston, Massachusetts 02215

T. Ray and P. Tamayo

Physics Department and Center for Polymer Studies, Boston University, Boston, Massachusetts 02215

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Using cluster and percolation concepts, we obtain a relation between relaxation times at critical points obtained from a new dynamical model introduced by Swendsen and Wang and those obtained from Glauber dynamics. This relation, which involves only static critical exponents, provides new insight into the physics underlying cluster acceleration methods such as the one introduced by Swendsen and Wang.

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It has been known for some time that percolation and cluster concepts are useful tools for understanding thermal phase transitions. Critical points in Ising models[1-3] and in Potts models[4] as well as in nucleation[5-7] are phenomena that have been elucidated with the ideas of clusters and percolation. The application of these geometric concepts has been, for the most part, to equilibrium or quasiequilibrium problems. Recently, however, Swendsen and Wang[8] (SW) have applied these cluster ideas to define a new simulation dynamics with the same conservation laws as Glauber dynamics.[9] The essential difference is that in SW dynamics, clusters rather than single spins are flipped. The flipping of clusters results in a decrease in critical slowing down, which reduces substantially the time requird to obtain equilibrium properties near critical points.

Although this method is intriguing and can be very useful, there is no understanding of why it works, or why critical slowing down is not eliminated altogether. We propose a first step in the direction of constructing a theory of the SW dynamics. Specifically, we present a scaling argument from which we obtain a good approximation to the value of the dynamical exponent z obtained by SW as well as insight into the physics underlying the method.

The exponent z can be defined through dynamical correlation functions. For example, if we denote the magnetic correlation function $\theta(t)$, then z is defined by $\theta(t)\sim\exp(-t/\tau)$ and $\tau\sim\xi^z$, where t is the time and ξ is the correlation length. For Glauber dynamics, $z\sim 2$ for Ising models (see Table I) and about 2.2 for the $q=3$ Potts model in two dimensions.[10] It has been shown[11] that algorithms with local dynamics have a lower bound for z of γ/ν. In SW dynamics this limitation is avoided by flipping clusters rather than spins thereby constructing nonlocal dynamics.

In order to make the argument for our scaling *Ansatz* more transparent, we present a slightly different description of SW dynamics than that presented in Ref. 8. We begin with the q-state dilute Potts model with the Hamiltonian H_1 given by

$$-\beta H_1 = J\sum_{ij}(\delta_{\sigma_i\sigma_j}-1)n_i n_j + K\sum_{ij} n_i n_j - \Delta\sum_i n_i\,, \qquad (1)$$

where β is the inverse temperature, δ is the Kronecker delta, σ labels the Potts states, the occupation numbers n_i are 0 or 1, Δ is the chemical potential, and the sum is over all pairs. The second two terms on the right-hand side are the lattice-gas Hamiltonian and the first term is a Potts interaction between sites which are both occupied.

The Hamiltonian in Eq. (1) can be used to describe a percolation problem.[1] Specifically, if we differentiate the corresponding free energy with respect to q and take the limit $q\to 1$, we obtain the generating function for the random-bond correlated-site percolation model. In this model the distribution of occupied sites is governed by the lattice-gas Boltzman factor and the bonds are distributed at random between occupied sites with a probability

$$p_b = 1-\exp(-J)\,. \qquad (2)$$

Clusters are defined as sets of occupied sites connected, either directly or indirectly, by bonds. If J is chosen to

TABLE I. The line designated by z_{SW} contains the values obtained by SW with the exception (Ref. 21) of the $d=4$ Ising model. The notation $z_{SW}^{(d)}$ and $z_{SW}^{(d_f)}$ denote values obtained from Eq. (6) with d_m equal to d and d_f, respectively. Values for the static exponents are from Refs. 22–24 and z_G for the $d=3$ Ising is taken from Ref. 25.

	Ising $d=2$	Ising $d=3$	Ising $d=4$	Potts ($q=3$) $d=2$
$z_{SW}^{(d)}$	0.39 ± 0.05	0.73 ± 0.02	1.0	0.45 ± 0.05
z_{SW}	0.35 ± 0.01	0.75 ± 0.01	0.97 ± 0.09	0.6 ± 0.01
$z_{SW}^{(d_f)}$	0.27 ± 0.05	0.45 ± 0.04	0.667	0.32 ± 0.05

be equal to $K/2$, then it can be shown[1] that the percolation transition is the same as the Ising or lattice-gas transition. That is, the Ising critical point is also the percolation transition, and the critical exponents of the two problems are identical. The divergence of the correlation length and the connectedness length are described by critical exponents with the same numerical value. The same is true for the susceptibility and the mean cluster size as well as all other singular quantities. Equivalently this mapping selects the "Fisher droplets"[12] for the Ising critical point, i.e., a set of noninteracting clusters or modes which describe the critical point.

We can define another Hamiltonian, βH_2, where holes rather than particles interact so that the n_i in Eq. (1) are replaced by $1-n_i$. Clearly the above discussion still applies. If we now define a Hamiltonian $H=H_1+H_2$, the above discussion still applies except the value for J is shifted to K so that the bond probability is $p_b=1-\exp(-K)$. This symmetrized model is the one used by Swendsen and Wang. Consequently, SW take as their fundamental objects clusters at the percolation threshold, rather than single spins. This argument can be generalized to Hamiltonians similar to Eq. (1), where the lattice-gas Hamiltonian is replaced by a q-state Potts interaction.[4]

In order to understand how the SW algorithm results in a modification of z, we need to examine the expression $\tau\sim\xi^z$ with more care. At a critical point there are two important lengths, the correlation length and the smallest length scale in the problem, ℓ. For systems on a lattice where a local algorithm is used ℓ is clearly the lattice constant. All times, such as the time associated with critical slowing down, are functions of ℓ. Nonlocal algorithms modify ℓ in a nontrivial manner and hence ℓ must be treated carefully. In the development of Fourier acceleration techniques by Batrouni *et al.*,[13] this idea is treated in some detail. We take as our starting assumption that the SW algorithm modifies z by modifying ℓ.

In order to obtain the dependence of τ on ℓ, we need a model for the dynamics of equilibration near critical points. We argue that a plausible mechanism for equilibration in the Glauber model is the diffusion of domain walls. This mechanism is clearly the case in one-dimensional Potts models, since the probability of flipping a spin in the interior of a domain vanishes as $\exp(-J/k_BT)$ as T approaches the critical point $T_c=0$, while the probability of flipping a spin at the boundary of a domain remains $\frac{1}{2}$ independent of T.

Additional support for the domain-wall diffusion mechanism can be obtained from considering the dynamics of critical slowing down in mean-field Glauber models. One approach is to investigate tunneling in a ϕ^4 theory near the critical point for long-range interactions.[14] In this limit the tunneling process can be treated with saddle-point techniques.[15] For this model it is straightforward to show that the growth or decay of domains is centered on the domain surface.[15]

These considerations suggest the *Ansatz* that equilibration is dominated by diffusion of domain walls. In turn this assumption implies that $\tau\sim l^2/D$, where D is a diffusion constant which contains information about the domain wall and l is the distance that the domain wall diffuses. In the vicinity of the critical point decorrelation occurs when $l=\xi$. On physical grounds one would expect that since the domain wall is correlated on a length scale ξ, D will vanish as the critical point is approached, leading to anomalous diffusion.

Our *Ansatz* is that Glauber dynamics can be described as a diffusion process of the domain walls in a "background" of the interior domain spins. If *all* length scales in the problem are rescaled so that ℓ is no longer the lattice constant, the diffusion constant will remain unchanged and the time will be rescaled only by the rescaling of l, or at the critical point, ξ. If we take ℓ to be the lattice constant for single spin-flip dynamics, then after rescaling the fundamental length to ℓ we have

$$\tau\sim D^{-1}\xi^2/\ell^2\sim\xi^z/\ell^2. \tag{3}$$

In order to obtain values for z in the SW dynamics, we need to know how ℓ varies as the critical point is approached. As discussed previously, in SW dynamics the clusters are flipped at the percolation threshold. The largest length is the correlation length, which is the linear size of the incipient infinite cluster.[1] The smallest length in the problem is more complicated. Since clusters of various sizes are flipped, there is no unique fundamental smallest length. However, since the clusters are independent, we can treat the problem as a collection of clusters all of the same size with mean linear dimension ℓ_0. We denote the minimum length $\ell=\ell_0$.

In order to determine ℓ_0 we employ the following scaling argument. The mean mass of the finite clusters diverges as $\Delta T^{-\gamma}$, where $\Delta T=(T-T_c)/T_c$, T_c is the critical temperature, and γ is the Ising susceptibility exponent.[1] We have then

$$\Delta T^{-\gamma}\sim\ell_0^{d_m}, \tag{4}$$

where d_m is the mean fractal dimension of the finite clusters. Unfortunately, we do not know the value of d_m. However, we can reasonably assume that it lies between d, the spatial dimension, and $d_f=d-\beta/\nu$, the fractal dimension of the incipient infinite cluster. These bounds follow from the idea that clusters with a strictly finite length (i.e., $\ell<A<\infty$) should have $d_m=d$ and arbitrarily large finite clusters should have a structure approaching that of the incipient infinite cluster.[16]

If we now replace ℓ by ℓ_0 in Eq. (3) and use Eq. (4) and $\xi=\Delta T^{-\nu}$ we obtain

$$\tau\sim\xi^{z-2\gamma/d_m\nu} \tag{5}$$

or

$$z_{SW} = z_G - 2\gamma/d_m\nu, \quad (6)$$

where z_{SW} and z_G are the SW value and Glauber value for z, respectively.

For the $d=1$ Ising model, $z_G=2$ and since $d=d_f=1$, $z_{SW}=0$,[17] consistent with Eq. (6). Table I summarizes the numerical values of z_{SW} calculated from Eq. (6) for Ising models in 2D, 3D, and 4D and the $q=3$ Potts model in 2D. The numerical values found by Swendsen and Wang are included for comparison.

Our scaling argument explains why z_{SW} increases with dimension rather than decreasing like z_G. Second, the numerical values for $d_m=d$ are quite good. If the argument is correct, $z_{SW}^{(d)}$ is an upper bound for z_{SW} and $z_{SW}^{(d_f)}$ is a lower bound. The value for $z_{SW}^{(d)}$ for the $q=3$ Potts would appear somewhat low. This value could be caused by the value of z_G that was used.[10] If, for example, we take the average of the measured values of z_G quoted in Table I of Ref. 10, the value of $z_{SW}^{(d)}$ increases to 0.62. Clearly a better value of z_G would be of interest.

The basic assumption we have made to obtain these results is that the SW algorithm works by modifying the basic fundamental length in the problem. Specifically, the lattice constant is replaced by the size of the finite clusters. The agreement with the numerical calculations of SW would indicate that the assumption is fundamentally correct. This argument then implies that an attempt to develop a theory of SW dynamics should address itself to "renormalizing" the smallest length in the problem. It should also help in understanding the generalization of SW to continuum models.[18]

In addition to what can be learned from these considerations about SW, several points can be made about critical dynamics. If, as seems plausible from the numerical results, Eq. (6) is exact for some value of d_m (either d or something close to d), then information about Glauber dynamics can be obtained much more readily from SW and translated back to Glauber dynamics via Eq. (6). Moreover, there would appear to be a different type of universality classification for critical dynamics then previously expected. The assumption, invalidated by SW, was that universality classes in critical dynamics were determined by the usual parameters associated with static critical phenomena and the conservation laws. Our results imply that the new universality class generated by SW is in fact related to Glauber by static critical exponents. This raises the possibility that the same is true for other acceleration methods such as Fourier acceleration,[13] the SW multigrid hybrid proposed by Kandel *et al.*,[19] and the extended SW algorithm of Edwards and Sokol.[20] Clearly more work is needed to understand what might be called static-equivalent universality.

This work also raises the following extremely intriguing possibility. That is, Eq. (6) can be rewritten as $z_G - z_{SW} = 2\gamma/d_m\nu$, where the right-hand side is a static quantity. The value of z_G is determined by equilibration on all length scales, but z_{SW} contains information only about modes of equilibration on length scales greater than $\mathscr{l} = \xi^{\gamma/d_m\nu}$. The difference $z_G - z_{SW}$ should then contain information about equilibration length scales less than $\mathscr{l}$. Equation (6) implies that this equilibration is described by static quantities only and hence may be independent of conservation laws. It would be of great interest to have a procedure equivalent to SW in models with different conservation laws.

Clearly what we have presented is not a theory. However, we think that the insight this work provides into the physics underlying the SW method will help in the development of a theoretical basis for cluster acceleration algorithms. In addition, we believe that the development of such algorithms will lead to a deeper understanding of critical dynamics.

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[a]Permanent address and address to which inquiries should be sent.

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