Figure captions

Fig. 1. Autocorrelations $\tau_{int,E}$ for the Wolff and SW algorithms plotted against lattice size L for the Ising model in (a) 2-d, (b) 3-d and (c) 4-d. Also shown is the specific heat C_H, and the SW autocorrelations scaled by the average maximum cluster size m. The latter two quantities are also scaled by an arbitrary factor. The plots are log-linear for (a) and (c), and log-log for (b). All error bars are shown, but are usually smaller than the points. The lines are fits to a power law, logarithm, or constant.

Fig. 2. The difference $\tau^W_{int,E} - (a + b \times C_H)$ between the Wolff autocorrelations and a simple linear function of the specific heat, for the Ising model in (a) 2-d, (b) 3-d and (c) 4-d. The values of a and b are chosen so as to minimize the χ^2, except in three dimensions, where we have taken $b = 0$. The errors shown are almost all less than 1% of $\tau^W_{int,E}$.

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relation (3) between the Wolff autocorrelation times and the specific heat seems to be the most compelling evidence so far that $z^W_{int,E}$ is in fact zero for the 2-d Ising model, while the relation (4) would imply that $z^{SW}_{int,E}$ is actually 1/8, which is not apparent from the usual fits to either a logarithm or a power law.

4. Conclusions

We have measured the autocorrelations and dynamic critical exponents for the SW and Wolff cluster algorithms for the Ising model in 2, 3 and 4 dimensions. We have found what appear to be very simple empirical relations between the autocorrelation times of these algorithms and simple static quantities (the magnetization and specific heat).

The simplicity of the relations (3) and (4) between static and dynamic quantities is very surprising. It could perhaps be due to the fact that the dynamics of these algorithms are closely linked with the physical properties of the system, since the Swendsen-Wang clusters are just the Coniglio-Klein-Fisher droplets [22] , or "physical clusters" [18], from which the critical behavior of the system may be described. The simplicity of these relations indicates that a quantitative theoretical understanding of the dynamic critical behavior of cluster algorithms in terms of fundamental static quantities should be attainable, at least for the Ising model. It is of course possible that these relations are not exact, but merely good approximations. We are currently collecting more data in order to check whether these results hold up with larger lattices and better statistics, and we will present more detailed results in a future publication [23] .

The relations (3) and (4) are certainly not general results, since for the 2-d $q = 3$ Potts model we find that $z^W > \alpha/\nu$ and $z^{SW} > \beta/\nu$ [5][6]. Also, it is quite surprising that these empirical relations imply that z^{SW} is not equal to z^W for the 2-d Ising model, whereas the two appear to be equal for the 2-d $q = 3$ Potts model. However it is interesting to note that for this model $(\alpha + \beta)/\nu = 8/15 \approx 0.5333$, which is very close to the measured values for $z_{int,E}$, of 0.55(1) for SW and 0.57(1) for Wolff [6].

It would be interesting to investigate whether simple relations between the autocorrelations of cluster algorithms and static quantities such as the specific heat and the magnetization can also be found for other spin models, such as Potts and $O(N)$ models.

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obtained with $a \approx -0.474$ and $b \approx 0.957$, and this is what we show in Fig. 2(a). For the 3-d model the additive constant a is consistent with zero, so that the autocorrelation time may be just a multiple of the specific heat, with $b \approx 0.148$. In four dimensions we find $a \approx 0.167$ and $b \approx 0.050$.

The surprising simplicity of the result (3) led us to look for a similar relation for the SW algorithm. The power of cluster update algorithms comes from the fact that they flip large clusters of spins at a time. The relative average size of the largest SW cluster, $m =< |c_{SW}^{max}| > /L^d$, is an estimator of the magnetization [18] , and the magnetization exponent β/ν has values which are similar to our measured values for the dynamical exponents of the SW algorithm. To investigate this further, we have scaled the SW autocorrelations by m, in a similar manner to the scaling of the Wolff autocorrelations in equation (1). If this gives a constant or a logarithm, then $\tau_{int,E}^{SW}$ diverges like the magnetization, and so we have $z_{int,E}^{SW} = \beta/\nu$.

The SW autocorrelations scaled by m (and by an additional arbitrary factor, so that these points are not entangled with others in the plots) are also shown in Fig. 1. For $d = 4$ the results are very close to a constant, while for $d = 3$ they seem to approach a constant as L increases. In two dimensions the scaled autocorrelations are not constant, but they fit very much better to a logarithm than does the unscaled data, as can be seen in Fig. 1(a). The data therefore supports the assertion that

$$m \ \tau_{int,E}^{SW} = a + b \times \log L, \qquad z_{int,E}^{SW} = \beta/\nu. \tag{4}$$

We are still faced with the problem that it is difficult to tell if the scaled autocorrelations increase as a logarithm or a small power, so that unless $b = 0$ we can only say with any certainty that $z_{int,E}^{SW} \approx \beta/\nu$. However the scaled 2-$d$ data fit very much better to a logarithm than to a power law.

Our measurements of $z_{int,E}^{W}$ in 3-d and $z_{int,E}^{SW}$ in 4-d give results which are very different from the accepted values of α/ν ($\approx 0.10 - 0.20$) [19] [20] and β/ν ($= 1$) [15][21] , since corrections to scaling are known to be important for these quantities. If we do a simple power law fit to the specific heat in 3-d and the magnetization in 4-d, we get results which are also very different from the actual exponents, but which are very close to the measured values of the corresponding dynamical exponents, as expected from relations (3) and (4). Thus although we may not be able to measure the asymptotic behavior of the autocorrelation times, if we can find simple relations between the autocorrelations and static quantities whose asymptotic behavior is known, then we can infer the true value of the dynamical critical exponents.

This is especially useful for the 2-d model, for which the autocorrelations grow so slowly that any corrections to scaling could have a big effect. It is therefore very difficult to say with any confidence that $z = 0$, even with data on very large lattices. The apparent

in all dimensions, and the SW algorithm in two dimensions, it is virtually impossible to distinguish between a small exponent and a logarithmic increase in the autocorrelations (which would imply that $z = 0$).

Dimension	$z_{int,E}$ SW	$z_{int,E}$ Wolff
2	0.25(1) or 0	0.25(1) or 0
3	0.54(2)	0.33(1) or 0
4	0.86(2)	0.25(1) or 0

Table 1.
Measured dynamic critical exponents for Ising model cluster algorithms.

In Fig. 1 we also include the measured value of the specific heat C_H, scaled by an appropriate factor, in order to show that the bound of Li and Sokal [5]

$$\tau_{int,E} \geq constant \times C_H, \qquad z_{int,E} \geq \alpha/\nu \tag{2}$$

is indeed satisfied by the SW algorithm. No such bound has been proven for the Wolff algorithm [17] , although it appears from the figures that not only does the bound hold, but that there may actually be equality in the exponents, so that for the Ising model in all dimensions $z_{int,E} = \alpha/\nu$ for the Wolff algorithm.

If we compare the results of fits to C_H and $\tau^W_{int,E}$ (the autocorrelations in the energy for the Wolff algorithm), which correspond to the measured values of α/ν and $z^W_{int,E}$ respectively, then for $d = 3$ we find 0.32(1) and 0.33(1). In two and four dimensions $\alpha = 0$, and $z^W_{int,E}$ is also consistent with zero. Hence the Wolff algorithm for the Ising model seems to satisfy the surprisingly simple relations

$$\tau^W_{int,E} = a + b \times C_H, \qquad z^W_{int,E} = \alpha/\nu, \tag{3}$$

where a and b are constants (i.e. independent of L). In Figure 2 we plot the difference $\tau^W_{int,E} - (a + b \times C_H)$ for the various dimensions, with a and b chosen to minimize χ^2 over a certain range of lattice sizes (smaller values of L are excluded from the fit). We can see that in all cases, values of a and b can be found such that the difference is zero within errors. Note that all the errors shown here are purely statistical (one standard deviation).

It appears from Fig. 1(a) that in 2-d the Wolff autocorrelations and the specific heat share the same multiplicative constant of the logarithm, since the lines of best fit have approximately the same slope. This corresponds to $b = 1$, in which case $\tau^W_{int,E}$ is just a constant plus C_H. From our data this is certainly a possibility, however the best fit is

2. Simulations

Due to the discrepancies between the various measurements of the dynamical critical exponents, we have been performing simulations of the Ising model in 2, 3 and 4 dimensions using the SW and Wolff algorithms, with the aim of obtaining good statistics on fairly large lattices, in order to get reliable values for the dynamical critical exponents. The definitions of the various autocorrelations and dynamical exponents, and an account of the methods we used to do the measurements, fits and error estimates, are given in ref. [6]. We use finite size scaling to determine z, by measuring the autocorrelations for different lattice sizes at the infinite volume critical point. We have used the Potts formulation of the Ising model, for which the critical point in two dimensions is known to be $\beta_c = \log(1+\sqrt{2}) \approx 0.8813736$ [13] . For the 3-d model we used the value 0.443308 [14] , while in the 4-d case we have used 0.29962 [15] .

Autocorrelations are traditionally measured between each update of the entire lattice, so for the single cluster Wolff update, where only a fraction of the lattice sites are updated at each iteration, the measured autocorrelation time τ' needs to be scaled by the ratio of the average Wolff cluster size $< |c_W| >$ and the number of lattice sites L^d. The scaled autocorrelation time

$$\tau = \tau' < |c_W| > /L^d \tag{1}$$

gives a more reasonable comparison between the Wolff and SW algorithms in terms of the amount of work done (or CPU time used), and it is these scaled autocorrelations that we present here for the Wolff algorithm. Since this scaling ratio is an estimator for the susceptibility [2], the dynamical critical exponent z' for the unscaled autocorrelations is given by $z' = z + (d - \gamma/\nu)$.

For the SW algorithm on the larger lattice sizes in two and three dimensions, we used a parallel cluster labeling algorithm which we have developed [16] in order to run on large parallel machines such as the nCUBE hypercube and the Symult S2010. For the other lattice sizes, we ran multiple simulations in parallel, on shared memory machines such as the BBN Butterfly and Encore Multimax, or using networks of workstations.

3. Results

Results for $\tau_{int,E}$, the integrated autocorrelation time for the energy, are shown in Figures 1(a), (b) and (c) for $d = 2$, 3 and 4 respectively. For $d = 3$ we have used a log-log plot, with the straight lines representing χ^2 fits to a power law, while for $d = 2$ and $d = 4$ we have used a log-linear plot, with the straight lines representing χ^2 fits to a logarithm. Note however that for $d = 4$ we plot $\log \tau_{int,E}$ rather than $\tau_{int,E}$ for the SW algorithm, since the SW autocorrelations increase as a power of L. The measured values of the exponents from the fits to the data are shown in Table 1. For the Wolff algorithm

1. Introduction

The Monte Carlo cluster update algorithms of Swendsen and Wang (SW) [1] and Wolff [2] can dramatically reduce critical slowing down in computer simulations of spin models, and thus greatly increase the computational efficiency of the simulations. Since they were introduced, a large amount of effort has gone into studying these algorithms, in an attempt to understand how they work, and how they can be generalized to more complicated models (for reviews of cluster algorithms, see refs. [3] [4]).

So far there has been very little theoretical understanding of the dynamics of these algorithms. In particular, little is known as to why cluster algorithms seem to eliminate critical slowing down completely in some cases, and not in others. There is no known quantitative theory which can predict the value of the dynamical critical exponent z for any spin model, although a rigorous bound on z for the SW algorithm has been derived [5] . Another problem which is not well understood is why the SW and Wolff algorithms give similar values of z for the 2-d Potts model [6] , but have very different behavior for other models, such as the Ising model in more than two dimensions [7] [8] .

A lot of work has been done on measuring the dynamical critical exponents of cluster algorithms for various spin models. These results are very useful "experimental" inputs for any theoretical understanding of these algorithms, since z is a quantity which one would hope to be able to derive, at least approximately, from any comprehensive theory of cluster algorithm dynamics. Unfortunately the measurement of dynamical critical exponents is very difficult, and both very good statistics and very large lattices are required in order to obtain accurate results. This is certainly the case for the Ising model, where a number of different measurements have given conflicting results.

For the two dimensional Ising model, initial results suggested $z \approx 1/3$ for both the SW and Wolff algorithms [1][8]. Further work [7] gave $z \approx 1/4$, and it was later shown that the data were consistent with a logarithmic divergence, suggesting that $z = 0$ [9] . Recent results show that it is very difficult to distinguish between a logarithm and a small power [6]. Measurements on the three dimensional model have proven to be just as difficult, with values of z for the SW algorithm ranging from 0.339(4) to 0.75(1) [1][7][10] . For the Wolff algorithm, Tamayo *et al.* [8] obtained 0.44(10), while Wolff found a value of 0.28(2) for the energy autocorrelations [7]. We have examined Wolff's data and found that it also fits well to a logarithm, so that $z = 0$ is also a possibility. Again it is very hard to tell the difference between a logarithm and a small power. In four dimensions only one result is known, which is $z = -0.05(15)$ for the Wolff algorithm [8]. Simulations have also been done on the mean-field Ising model, which is expected to give the same exponents as the Ising model in four or more dimensions [11] . The mean-field data are consistent with z being 0 for the Wolff algorithm [8] and 1 for SW [12] , with the latter result being supported by theoretical arguments.

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Empirical relations between static and dynamic exponents for Ising model cluster algorithms

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Abstract

We have measured the autocorrelations for the Swendsen-Wang and the Wolff cluster update algorithms for the Ising model in 2, 3 and 4 dimensions. The data for the Wolff algorithm suggest that the autocorrelations are linearly related to the specific heat, in which case the dynamical critical exponent $z^W_{int,E} = \alpha/\nu$. For the Swendsen-Wang algorithm, scaling the autocorrelations by the average maximum cluster size gives either a constant or a logarithm, which implies that $z^{SW}_{int,E} = \beta/\nu$ for the Ising model.