

Empirical Relations between Static and Dynamic Exponents for Ising Model Cluster Algorithms

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(Received 10 September 1991)

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

PACS numbers: 64.60.Ht, 05.50.+q, 11.15.Ha

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 (for reviews of cluster algorithms, see Refs. [3,4]). There is little theoretical understanding of the dynamics of these algorithms. In particular, little is known as to why they seem to eliminate critical slowing down completely in some cases and not others. There is no known theory which can predict the value of the dynamic critical exponent z for any spin model, although a rigorous bound on z for the SW algorithm for Potts models 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 2D Potts model [6], but have very different behaviors for other models, such as the Ising model in more than two dimensions [7,8].

The measurement of dynamic critical exponents is notoriously 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 $z \approx \frac{1}{3}$ for both the SW and Wolff algorithms [1,8]. Further work [7] gave $z \approx \frac{1}{4}$, 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, Brower, and Klein [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 they are also fitted well by a logarithm, so that $z=0$ is also a possibility.

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.

Because of the discrepancies between the various measurements of the dynamic critical exponents, we have done numerical simulations of the Ising model in two, three, and four 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 dynamic exponents. We measured the time correlation function $\rho(t)$ for the energy, and extracted the integrated autocorrelation time [3] $\tau = \frac{1}{2} + \sum_{t=1}^{\infty} \rho(t)$. The dynamic critical exponent z is given by $\tau \sim L^z$, where τ for the different lattice sizes is measured 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 $\beta_c = \ln(1 + \sqrt{2}) \approx 0.8813736$ [13]. For the 3D model we used the value 0.443308 [14], while in the 4D case we used 0.29962 [15]. A detailed account of the methods we used to do the measurements, fits, and error estimates is given in Ref. [6].

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 $\langle |c_{\text{W}}| \rangle$ and the number of lattice sites L^d . The scaled autocorrelation time

$$\tau = \tau' \langle |c_{\text{W}}| \rangle / L^d \quad (1)$$

is what we present for the Wolff autocorrelations. Since this scaling ratio is an estimator for the susceptibility [2], the dynamic critical exponent z' for the unscaled autocorrelations is given by $z' = z + (d - \gamma/\nu)$, where ν is the critical exponent for the correlation length, and γ is the critical exponent for the susceptibility, which diverges as $L^{\gamma/\nu}$.

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. For the other lattice sizes, we ran multiple simulations in parallel using smaller shared-memory machines and networks of work stations.

Results for $\tau_{int,E}$, the integrated autocorrelation time for the energy, are shown in Figs. 1(a)-1(c) for $d=2, 3$, and 4, respectively. For $d=3$ we have used a log-log

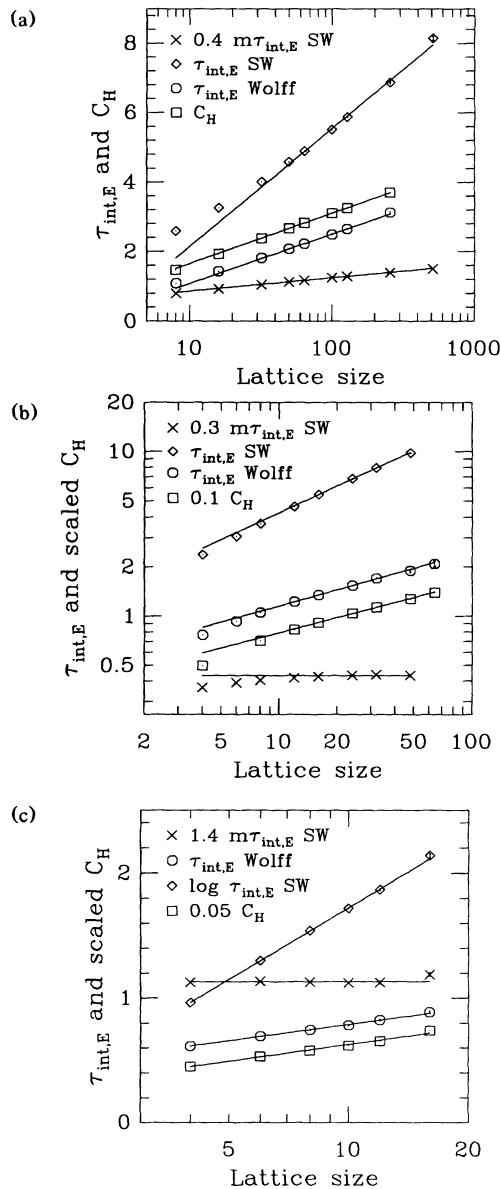


FIG. 1. Autocorrelations $\tau_{int,E}$ for the Wolff and SW algorithms plotted against lattice size L for the Ising model in (a) 2D, (b) 3D, and (c) 4D. Also shown is the specific heat C_H , and the SW autocorrelations scaled by the average maximum cluster size m . The latter two quantities are also scaled by an arbitrary constant. 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 with a power law, logarithm, or constant.

TABLE I. Measured dynamic critical exponents for Ising model cluster algorithms. Asterisks indicate that the data are also consistent with a logarithmic divergence ($z_{int,E} = 0$).

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

plot, with the straight lines representing χ^2 fits with a power law, while for $d=2$ and 4 we have used a log-linear plot, with the straight lines representing χ^2 fits with 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 I. For the Wolff algorithm in all dimensions, and the SW algorithm in two dimensions, it is very difficult to distinguish between a small exponent and a logarithmic increase in the autocorrelations (which would imply that $z = 0$).

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],

$$\tau_{int,E} \geq \text{const} \times C_H, \quad z_{int,E} \geq \alpha/\nu, \quad (2)$$

is indeed satisfied by the SW algorithm. Here α is the critical exponent for the specific heat ($C_H \sim L^{\alpha/\nu}$). 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.

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

$$\tau_{int,E}^W = a + b \times C_H, \quad z_{int,E}^W = \alpha/\nu, \quad (3)$$

where a and b are constants. In Fig. 2 we plot the difference $\tau_{int,E}^W - (a + b \times C_H)$ 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 (1 standard deviation). In two dimensions the best fit is obtained with $a \approx -0.474$ and $b \approx 0.957$ (the data do not exclude the possibility that $b=1$, which would imply that $\tau_{int,E}^W$ is just a constant plus C_H). For the 3D model the additive constant a is consistent with zero, so that the autocorrelation time may be just a mul-

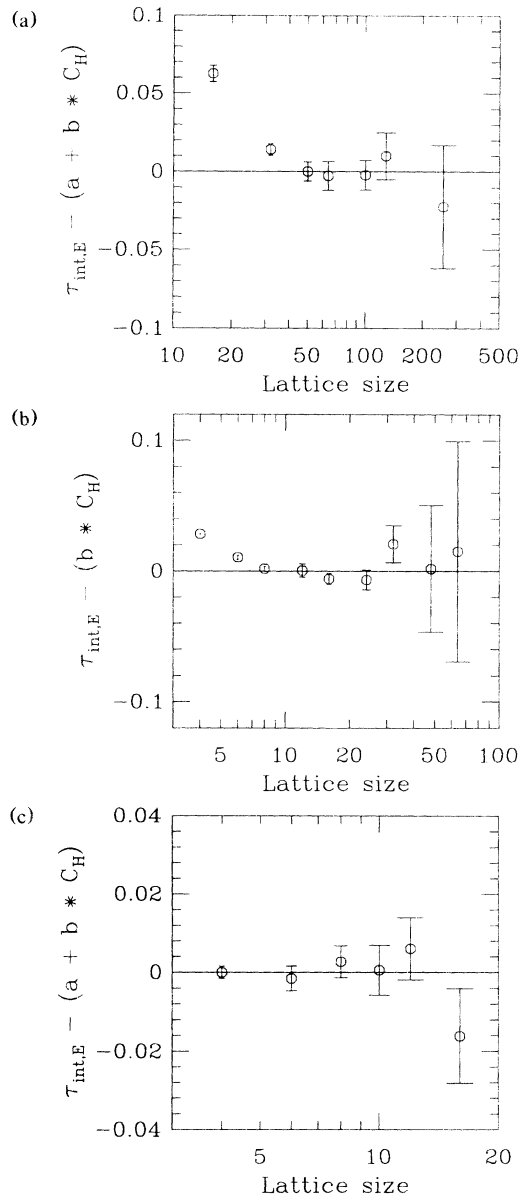


FIG. 2. The difference $\tau_{int,E}^W - (a + b * C_H)$ between the Wolff autocorrelations and a simple linear function of the specific heat for the Ising model in (a) 2D, (b) 3D, and (c) 4D. The values of a and b are chosen so as to minimize the χ^2 , except in three dimensions, where we have taken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

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, $m = \langle |c_{SW}^{max}| \rangle / L^d$, is an estimator of the magnetization [18], and the exponent β/v characterizing the divergence of the magnetization has values which are similar to our measured values for

the dynamic exponents of the SW algorithm. To investigate this further, we have scaled the SW autocorrelations by m , in a manner similar to the scaling of the Wolff autocorrelations in Eq. (1). If this gives a constant or a logarithm, then $\tau_{int,E}^{SW}$ diverges like the magnetization, and so we have $z_{int,E}^{SW} = \beta/v$.

The SW autocorrelations scaled by m (and by an additional arbitrary constant, 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 with a logarithm than do the unscaled data, as can be seen in Fig. 1(a), and fit very poorly with a power law. The data therefore support the assertion that

$$m \tau_{int,E}^{SW} = a + b \times \log L, \quad z_{int,E}^{SW} = \beta/v. \quad (4)$$

Our measurements of $z_{int,E}^W$ in 3D and $z_{int,E}^{SW}$ in 4D give results which are very different from the accepted values of a/v ($\approx 0.10-0.20$) [19,20] and β/v ($=1$) [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 3D and the magnetization in 4D, we get results which are also very different from the actual exponents, but which are very close to the measured values of the corresponding dynamic exponents, as expected from relations (3) and (4). Thus although we may not be able to measure the asymptotic behavior of the autocorrelation times, finding simple relations between the autocorrelations and static quantities whose asymptotic behavior is known enables us to infer the true values of the dynamic critical exponents.

This is especially useful for the 2D 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 relation (3) seems to be the most compelling evidence so far that $z_{int,E}^W$ is in fact zero for the 2D Ising model, while the relation (4) would imply that $z_{int,E}^{SW}$ is actually $\frac{1}{8}$, which is not apparent from the usual fits with either a logarithm or a power law.

We have measured the autocorrelations and dynamic critical exponents of the SW and Wolff cluster algorithms for the Ising model in two, three, and four dimensions. We have found what appear to be surprisingly simple empirical relations between the autocorrelation times of these algorithms and simple static quantities (the magnetization and specific heat). These relations could perhaps stem from the fact that the dynamics of cluster algorithms are closely linked to 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 relations (3) and (4) are certainly not general results, since for the 2D $q=3$ 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 2D Ising model, whereas the two appear to be equal for the 2D $q=3$ Potts 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 simulations were done using an nCUBE/10, a Symult S2010, an Encore Multimax, a BBN GP1000 Butterfly, and a network of SPARC stations, DEC stations, and IBM RS-6000 work stations. We would like to thank the North-East Parallel Architecture Center at Syracuse University, the Caltech Concurrent Supercomputer Facility, Michigan State University, and the Sandia National Laboratories for the use of these machines, as well as the Center for Research in Parallel Computing for allowing us access to most of these computers. P.D.C. was sponsored in part by Department of Energy Grants No. DE-FG03-85ER25009 and No. DE-AC03-81ER40050, and by a grant from the IBM corporation. C.F.B. is supported by Air Force Office of Scientific Research Grant No. AFOSR-89-0422 and by the Department of Energy under Contract No. DE-AC02-86ER40253. We would also like to thank Alan Sokal for useful discussions.

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