Computer simulations at the fixed point using an inverse renormalization group transformation

Dorit Ron [1]

Department of Computer Science and Applied Mathematics, Weizmann Institute of Science, Rehovot 76100, Israel

Robert H. Swendsen

Physics Department, Carnegie Mellon University, Pittsburgh, PA 15213

Achi Brandt

Department of Computer Science and Applied Mathematics, Weizmann Institute of Science, Rehovot 76100, Israel

Abstract

Following Brandt and Ron's suggestion of inverting the renormalization group transformation used in Monte Carlo renormalization, it is shown that efficient computer simulations of the fixed point of the transformation can be carried out on very large systems without critical slowing down. We illustrate the new method with calculations of critical exponents for the two- and three-dimensional Ising models, based on several different transformations.

Key words: renormalization group transformation, Monte Carlo simulations, fixed point, Ising model, critical exponents, Brandt-Ron representation

PACS: 05.50.+q, 05.10.Cc, 05.10.Ln

1 Introduction

The efficiency of computer simulations in many fields has been enhanced by the introduction of multi-scale techniques. In the study of critical phenomena, Monte Carlo renormalization group (MCRG) simulations have improved the determination of critical exponents,[1] as well as shedding light on the structure of the critical point. The multigrid approach, which exploits the advantages of a multi-scale approach from a different point of view, has long been a leading method for efficiently solving partial differential equations and other computationally difficult problems. Recently, Brandt and Ron have combined some of these ideas in a multiscale analysis of critical behavior in a spin system using a new representation of the renormalized interactions.[2] Ron and Swendsen have used the Brandt-Ron (BR) representation to improve the numerical determination of the properties of renormalized systems [3] and clarify the effects of multispin interactions. [4]

In this paper, we turn the usual renormalization-group (RG) analysis around to use an *inverse* renormalization group (IRG) transformation to generate large systems that correspond to the fixed point of a renormalization group. The striking advantage of this approach is that it is completely free of critical slowing down, even for the three-dimensional Ising model.

[1] Corresponding author: Dorit Ron, *Phone*: +972-8-9342141, *Fax*: +972-8-9342945, *Email address*: dron@wisdom.weizmann.ac.il .

The first use of a kind of inverse RG transformation to generate configurations of the Ising model on a large lattice were carried out by Compagner, Hoogland, and Blöte in the late 1970's.[5] Starting with a configuration of the $d = 2$ nearest-neighbor model at criticality on a small lattice, they replaced each spin by a block of four spins with the same value and performed a few MC sweeps using again the nearest-neighbor Hamiltonian at criticality. By repeating the process, they moved to successively larger lattices. They never published their work, but at conferences they did show a picture of a 1024×1024 lattice that looks like a configuration at criticality. This was quite an achievement at the time, even though it was not as exact criticality as obtained by the method described below. Also, they never used the configurations found with this technique for calculating critical properties.

The first use of inverting the renormalization group to calculate physical observables was done by Brandt and Ron.[2] They performed what they called "coarse-to-fine Monte Carlo acceleration" under the assumption that they knew the structure of the renormalized Hamiltonians at each stage. As an "extremely simple example" they approximated the renormalized Hamiltonians by using the original nearest-neighbor Hamiltonian to demonstrate the absence of critical slowing down, although in this simple case it was not very accurate. They have further increased the accuracy to some extent by using better approximations to the renormalized Hamiltonians.

The basic algorithm used in this paper is essentially the same as that used in the simple approximation introduced by Brandt and Ron.[2] However, instead of simulating the properties of a nearest-neighbor model, we develop approximations for the simulation of the fixed point of an RG transformation. The difference is of great importance in the efficiency of the calculations.

In an earlier Letter,[6] we applied the inverse RG method to some simple cases, using transformations and fixed points that had already appeared in the literature. [7] [8] [9] [10] In this paper, we extend our work by combining the inverse RG method with the Brandt-Ron determination of the renormalized fixed point.

In the following section, we will describe the method we are using for simulations without critical slowing down. We will use the Ising model for all examples, but the method is not limited to this case. The Brandt-Ron representation is reviewed in Section 3, while in section 4 it is used to calculate approximations for the fixed point. Results for the two- and three-dimensional Ising models are presented in Sections 5 and 6.

2 Inverse renormalization group Monte Carlo

In a normal MCRG calculation of an Ising model, an MC simulation is performed on a large system. For each configuration generated, a renormalized configuration can also be generated by grouping the spins into blocks and assigning a single, renormalized spin to each block on the basis of some rule. The rule can be either deterministic or probabilistic. For example, if 2×2 blocks are used (as will be done for the examples in this paper), a "majority-rule" RG transformation would assign a block spin according to the sign of the majority of spins, while a random number would be used to decide a tie.

By such transformations, the linear dimensions of the lattice would be reduced by a factor of $b = 2$, and the number of spins would be reduced by a factor of $b^d = 2^d$. If the original Hamiltonian was at a critical point, the repeated trans-

formations would carry the renormalized Hamiltonians toward the fixed point (FP) of the particular transformation used. If not, the repeated iterations would carry the renormalized Hamiltonians away from the critical sheet.

The nature of the trajectories of the renormalized systems is extremely important for understanding the methods and approximations that we will introduce in this paper. Under renormalization, the trajectories in the space of Hamiltonians will flow toward the fixed point in all directions except one. This means that for a normal MCRG calculation, it is only necessary to determine the critical temperature of the original system to insure that the RG trajectory flows toward the FP.

The inverse RG transformation requires the knowledge of both the RG transformation and the Hamiltonian of the previous renormalization step.[2] The algorithm is quite simple. After equilibration of a small system, each spin is replaced, for example, by a 2^d block of spins of the same sign, and an MC simulation is carried out with the constraint that configurations are restricted to those that are compatible with the unchanged smaller system. If a proposed spin flip would violate the condition that the majority of spins in a block has the same sign as the renormalized spin on the original (smaller) lattice, it is rejected. If the spin flip would result in a block with an equal number of positive and negative spins, the acceptance probability of the move is divided by two. Brandt and Ron called this step "compatible Monte Carlo" (CMC) for obvious reasons.[2] This procedure has a very small correlation time, independent of the lattice size, because of the local nature of the relaxation, even though the system is at criticality. The result of the procedure is a configuration corresponding to a lower level of renormalization on a larger lattice. By repeating this procedure, arbitrarily large lattices can be generated.

Each sequence of inversely renormalized lattices begins with a small lattice with a short correlation time. Thus it is easy to simulate the small lattice long enough to produce an independent configuration. Since the larger lattices are all based on the configuration of the smallest lattice, this means that every configuration at any given lattice size is independent, even for the largest lattices.

Before discussing the approximations necessary for this calculation, first assume that we could carry out this procedure exactly. For the IRG, the deviation from the FP in the relevant direction would *decrease* by a factor of $1/\lambda_1$ (where $\lambda_1 > 1$ is the relevant eigenvalue of the RG transformation), moving the system onto the critical sheet. On the other hand, the deviations from the FP in all irrelevant directions would *increase* by factors of $1/\lambda_j$, where $\{\lambda_j |\ j > 1\}$ is the set of irrelevant eigenvalues, since all irrelevant eigenvalues are less than one. In fact, most of the irrelevant eigenvalues are very small, so that tiny deviations from the FP would be greatly magnified by this procedure.

Curiously enough, while this feature of the exact inverse transformation makes it unsuitable for application to general Hamiltonians, the approximate inverse transformations we will apply to the fixed point are stable and efficient.

The key feature to notice is that while the MC generation of a renormalized configuration requires only the original configuration and a well-defined RG, the inverse process requires not only the coarse configuration, but also the inversely renormalized Hamiltonian. It is the exact inversely renormalized Hamiltonian that develops the pathological expansion of the irrelevant operators.

In this paper, we will apply IRG transformations to the fixed point of the transformation, which eliminates the pathology of inversely renormalized Hamiltonians. The approximations that we will use also eliminate instabilities that could arise from the divergence of irrelevant operators under the IRG. A final advantage of this approach is that it uses the *same* Hamiltonian at every level.

Although we cannot calculate the FP Hamiltonian exactly for any known RG transformation, several methods have been developed for approximating such Hamiltonians. Swendsen developed a method for calculating renormalized and fixed point Hamiltonians. Brandt and Ron developed methods for approximating renormalized Hamiltonians in terms of tables of conditional probabilities. These calculations can be aimed at systematically finding better and better approximations for the FP as discussed below in Section 3. Blöte et al developed an optimized RG transformation and found a good approximation for its FP. In Sections 5 and 6, we apply the results of all of these calculations to the creation of approximate realizations of the IRG. Gupta and Cordery also developed an elegant method for calculating renormalized Hamiltonians,[11] but since they did not apply it to the determination of fixed points, we have not included it.

The MC simulations presented in this paper were carried out with the *g05caf* random number generator from the NAG library. To check for possible systematic errors due to this choice of random number generator, we have repeated some of the calculations with the *ran2* random number generator from Numerical Recipes, and no systematic deviations were found. Both generators use a multiplicative congruential algorithm with cycle of 2^{59}, while the later also includes random shuffling of the generated sequence. It is of interest to mention that for the high accuracy results we present here, the standard For-

tran random number generator *rand* (which has a cycle of only 2^{32}) was not sufficient and indeed introduced systematic deviations.

3 The Brandt-Ron Representation

The Brandt-Ron representation is described in detail in [2] and [3]. A brief description is given below. The main idea behind the BR representation is to describe the interactions between spins by calculating the conditional probability of a specific spin to be $+1$ given explicit values of a set of its neighboring spins. The set of spins and their values is called a "neighborhood". This conditional probability table is denoted by P_+^m, where m is the number of spins in the neighborhoods under consideration.

The P_+ tables can be easily calculated from a Monte Carlo simulation. In [2] it has been shown for the $d = 2$ Ising model using the majority-rule transformation on 2×2 blocks, that it is only important to achieve local equilibrium, i.e., at a scale comparable to the size of the neighborhood. It has also been confirmed that the calculation of the P_+ table is statistically optimal in the sense that it automatically acquires accuracy ε when the amount of statistics is $O(\varepsilon^{-2})$.

In the rest of this work, all $d = 2$ Ising calculations involve the P_+^{12} table (consisting of 314 distinct neighborhoods) and the P_+^{20} table (consisting of 2826 neighborhoods, where only the *sums* of the 8 most distant spins were taken into account).

The generalization of the BR representation to the $d = 3$ Ising model is straightforward. We have confirmed that the calculation of the P_+ tables does

not suffer from critical slowing down. A very good approximation for the P_+ tables is obtained from just few MC passes, independent of the lattice size.

4 Calculation of P_+ tables at fixed points

We determine the fixed point using a combination of the Brandt-Ron perturbative algorithm and a new fixed-point criticalization (FPC) to be introduced below.

The P_+ tables represent the block-spin conditional probabilities and can be used to run an MC simulation on that level, which in turn can be used to calculate the P_+ table of the next renormalized level. An approximation to the fixed point P^* is obtained by repeating such renormalization steps. Due to the extreme sensitivity to deviations from criticality caused by the truncation errors and statistical errors, each P_+ table needs to be modified by pushing it back to the critical hypersurface. We have first used the BR perturbative iteration method to obtain a P_+ table very close to the FP followed by one FPC.

4.1 Brandt-Ron Fixed Point Perturbative Iterations

The BR perturbative algorithm was first introduced in [2]. We have used a somewhat simplified version in this work.

Let the vector P^0 represent the P_+ table obtained for the current level, also referred to as the fine level. Let q^0 be a normalized approximation to q^* (the exact relevant direction) obtained at the previous stage of the algorithm, i.e.,

$\|q^0\| = 1$, where the weighted norm is defined by $\|t\|^2 \equiv \sum_i w_i t_i^2$, i runs over all the entries of the P_+ table (represented by P^0) and $w_i \sim f_i / [(P^0)_i (1 - (P^0)_i)]$, with $f_i \geq 0$ being the frequency of $(P^0)_i$ and $\sum_i w_i = 1$. We first calculate a better approximation for q^*. This is achieved by applying the RG transformation $\mathbf{R}$ twice: $P^1 = \mathbf{R}[P^0]$ and $P^2 = \mathbf{R}[P^0 + C_q q^0]$, where $C_q \ll 1$ is the perturbation coefficient and P^1 and P^2 are the P_+ tables produced at the renormalized level or coarse level. As $\mathbf{R}$ is applied repeatedly, all irrelevant directions diminish, leaving the relevant direction as the dominant perturbation to P^0. An approximation for λ^*, the eigenvalue associated with q^*, is then given by

$$\lambda_o = \frac{1}{C_q} \sum w_i q_i^o q_i^1 \tag{1}$$

where $q^1 = P^2 - P^1$ and w_i is defined above.

Next we calculate an improved approximation for P^*. We choose

$$P = P^1 + x\lambda q$$

where $q = q^1 / \|q^1\|$, and x is such that $\|P - (P^o + xq)\|^2$ is minimal. Thus x is chosen so that xq nearly cancels any remaining component in the relevant direction still present in P^o.

The next iteration is repeated for $q^o \leftarrow q$ and $P^o \leftarrow P$, applied again on the same grid sizes as the previous iteration.

In principle, such iterations would generate a sequence of systematically improved approximations for the fixed point, each using a larger neighborhood and more statistics than the previous one. Also, it can be used for calculating

λ^* as described in [2]. That is, calculating an approximation for λ^* for a set of decreasing values for C_q, using Eq. (1), and extrapolating towards $C_q = 0$ using a quadratic fit to the data in their paper gives a value of $\lambda = 1.9987$, which is quite close to the exact value of 2.

4.2 Fixed point criticalization

The approximation for the FP, P^o, obtained by the BR perturbative iterations can be further improved by a procedure of fixed point criticalization, which is specifically designed to minimize the deviation of the approximate fixed point from the critical hypersurface. We use P^0 to simulate the fine grid for which we calculate P^1, P^2, P^3, the P_+ tables associated with the coarse grids obtained from the fine grid by applying the RG transformation $\mathbf{R}$ three times. The improved approximation for the FP is then given by

$$P^o \leftarrow \left(\lambda P^2 - P^3\right) / (\lambda - 1)$$

where λ is an approximation to λ^*.

It is easy to show that this criticalization not only moves P^0 towards the critical hypersurface along the relevant direction, but it also moves it closer to the FP. If the approximation to λ is already rather good, the deviation of P^0 from the FP in the relevant direction is greatly reduced, while each irrelevant direction is reduced by a factor proportional to the square of its eigenvalue. We have not used P^1 for the criticalization because P^0 was already too accurate for P^1 to reveal the relevant direction.

An approximate FP, either calculated by the methods in this section or from an alternative approach, can now be used to generate configurations for arbitrarily large lattice using the corresponding IRG transformation discussed in Section 2.

5 Two-dimensional Ising model

As a first application of the IRG method to approximations for the fixed point, we have used finite-size scaling of the large lattices available through these calculations to calculate the critical exponent ratio γ/ν and the value of η. The ratio γ/ν was obtained from a log-log plot of the magnetic susceptibility as a function of the linear system size, since the magnetic susceptibility χ is proportional to $L^{\gamma/\nu}$. The exponent η was obtained from the spin-spin correlation function, which decays as $r^{-(d-2+\eta)}$, using the finite size scaling of the function at $r = L/4$. All simulations started on a 4×4 lattice, employing 20 CMC sweeps (see Section 2) on increasingly larger grids. The largest lattices obtained were 1024×1024, although the method is not limited to this size.

The first approximate realization of the IRG that we have tried uses the nearest-neighbor, two-dimensional Ising model at its critical point as an approximation for the fixed point of the 2×2 majority rule RG. This is clearly a very poor approximation, since the FP of this RG transformation is known to be quite far from the nearest neighbor model. However, the results of this calculation, shown in the first line of Table 1, are surprisingly good. The error in the estimate of γ/ν is only 0.7%.

As a systematic way of calculating successive approximations to the fixed

Table 1

The critical exponents γ/ν and η are calculated for the two-dimensional Ising model using the IRG method with the majority rule as the RG transformation and with an approximation for the FP either by a Hamiltonian presentation or by the P_+ tables.

Fixed-point	γ/ν	η
Nearest-neighbor	1.76195(2)	0.23807(2)
P_+^{12}	1.73227(2)	0.2676(1)
$C(P_+^{12})$	1.75285(3)	0.2469(1)
P_+^{20}	1.74815(2)	0.25183(2)
$C(P_+^{20})$	1.74953(3)	0.2504(2)
7-couplings FP	1.74991(3)	0.25004(4)
Exact	1.75	.25

point, we used the algorithms developed by Brandt and Ron.[2] The entries in Table 1 for "P_+^{12}" and "P_+^{20}" refer to estimates of the fixed point in terms of the Brandt-Ron conditional probability tables using neighborhood of 12 and 20 sites described in Section 3, while the entries marked "$C(P_+^{12})$" and "$C(P_+^{20})$" refer to refinements of the estimates for the FP using the fixed point criticalization introduced in Section 4.2. Although the first estimate using 12 sites is actually worse than that using the simple nearest-neighbor Hamiltonian, after criticalization, the results are very good. The approximation is improved by enlarging the neighborhood to 20 sites and applying another FP criticalization. The "$C(P_+^{20})$" estimate has a systematic error of less than 0.03% for γ/ν.

There are three types of errors involved in calculating γ/ν : One is due to approximations in the fixed point that we used which will be discussed below; the two others are due to the statistical and finite-size effects. It turned out that the finite-size errors in all our tests were much smaller than the statistical errors. Even a 16×16 grid had finite-size errors smaller than 0.0001, and perhaps much less: our statistics (comparing the up to 16×16 results with those of up to 512×512 using the same Hamiltonian) could not resolve smaller errors. We have calculated the statistical error by dividing the total amount of statistics into a few independent runs and measuring the variance between them.

The number of independent configurations needed to obtain high accuracy is rather small: 10^5 configurations of sizes up to 512×512 are sufficient to obtain small statistical errors of about 0.002%, provided the observables of all lattices are measured from the *same* simulation to guarantee the compatibility of their deviations to each other. Because the renormalized configurations are correlated with each other, fluctuations in the ratios needed to calculate critical exponents are much smaller than the fluctuations in the quantities themselves. If the observables are calculated separately from different runs for different lattice sizes, the statistical errors are at least 50 times larger.

After observing how small are the finite-size and the statistical errors, it is clear that the main error is due to the uncertainty of the fixed point Hamiltonians used for the simulations. This error, which is explicitly seen in this case since the analytical solution is known, can generally be estimated by further iterations which either increase the neighborhood and/or perform another criticalization as can be seen in Table 1. Sufficient increase of that or the other will get us as close as we wish to the exact solution. The differences between

two consecutive results in this sequence of experiments, which decrease as the approximations are improved, can serve as a rough estimation to the error in the fixed point Hamiltonian used for the simulation, (in other cases, where the analytical solution is unknown).

Finally, we have used an approximated FP given by a seven-coupling Hamiltonian as calculated by Swendsen[7], using comparisons of different methods for calculating correlation functions. This approximation gives a remarkable small error of only 0.005% for γ/ν as shown in the sixth line of Table 1.

Fig. 1 shows these results in the form of a log-log plot of the susceptibility as a function of the linear size of the system. The first striking feature is the extreme linearity of the plot, reflecting the lack of corrections to scaling. The second feature is that the results for different approximations lie almost exactly on top of each other, reflecting the fact that they all refer to the same majority-rule RG transformation.

Fig. 2 shows data for the spin-spin correlation function, $\langle S_0 S_r \rangle$, as a function of separation, r, for lattices from 4×4 through 512×512. The separation r is divided by L, and the correlation function is scaled by a factor of $L^{0.25}$. Because the lattices differed in size by powers of two and the correlation functions were evaluated at points of the form $L2^{-n}$, points from different lattices coincide completely to demonstrate how well the scaling laws are satisfied. The points corresponding to $r = L/4$ were used in Table 1 to calculate the value of η.

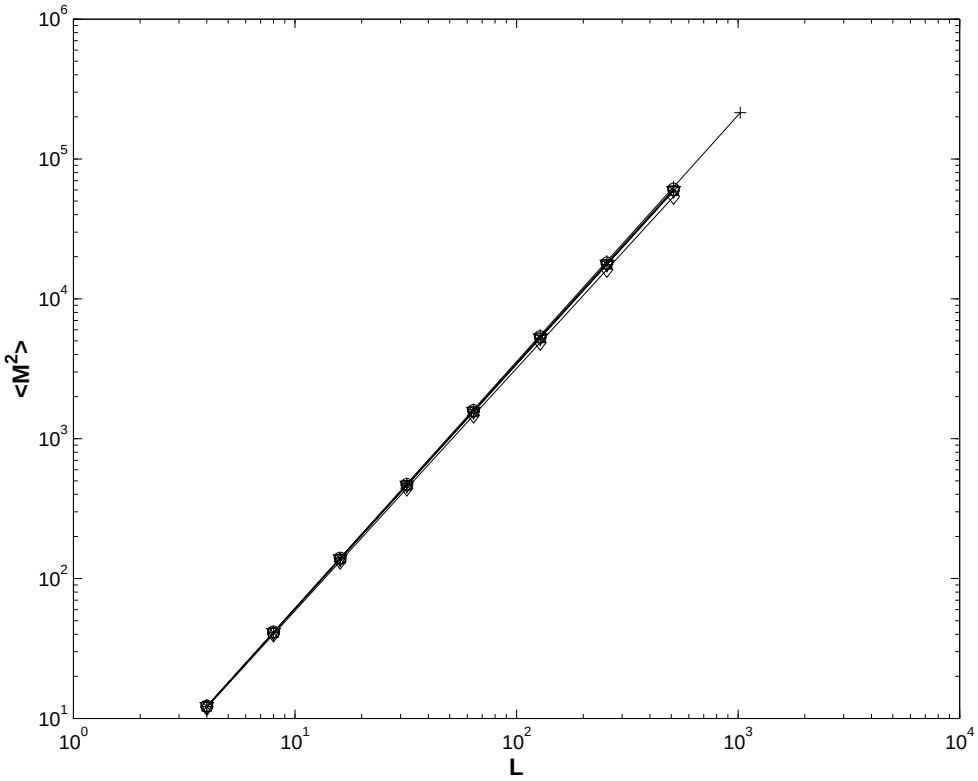

Fig. 1. A log-log plot of the linear size of the lattice L versus the average of the squared magnetization for the two-dimensional Ising model with the majority rule and the six different fixed points introduced in Table 1.

6 Three-dimensional Ising model

For the three-dimensional model, we have neither the exact location of the critical point of the nearest-neighbor model, nor exact values of the critical exponents to compare our results with. However, we do have numerical estimates of the locations of fixed points for a variety of RG transformations. This lets us consider a variety of ways to implement the IRG approach. In all simulations discussed here, we have started from a $4 \times 4 \times 4$ lattice. Larger lattices were obtained by employing 20 CMC sweeps up to a linear size of 128. Each computation generated 5000 independent configurations.

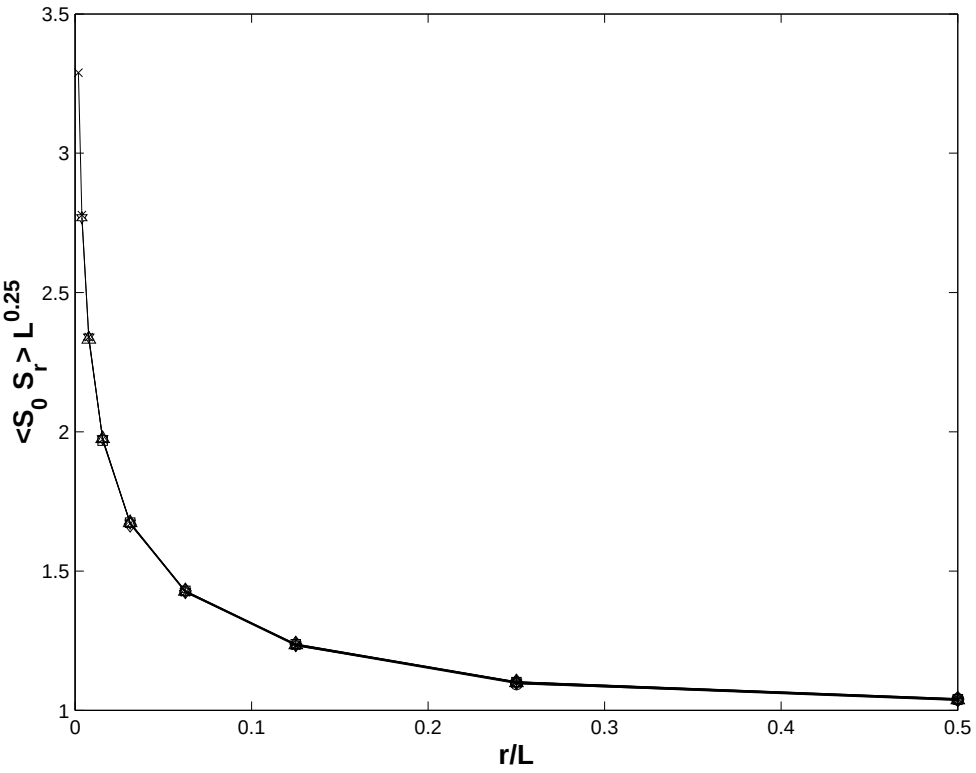

Fig. 2. A log-log plot of the spin-spin correlation function of distance r multiplied by $L^{0.25}$ versus r/L, where $L = 4, 8, ..., 512$ and $r = 1, 2, ..., L/2$, for the approximated FP P_+^{20} of the two-dimensional Ising model with the majority rule RG transformation.

Again, we have first investigated the majority-rule RG transformation using the simple nearest-neighbor Ising model at its critical point. The expected value of the exponent ratio γ/ν is 1.962(2) for the $d = 3$ Ising model[10], and our simple approximation gave $\gamma/\nu = 1.9158(5)$. The deviation from the correct result is about 2.3%, which is considerably larger than for the two-dimensional case. However, it is still rather good for such an obviously bad approximation.

Next, we tried to improve on this result by approximating the FP Hamiltonian for the majority rule RG in the Brandt-Ron representation. The number of P_+'s in three dimensions can be rather large, so we have begun by restricting

our calculation to the first three neighbors of the central spin [(100), (110), (111) and permutations] for a total of 26 spins that form a $3 \times 3 \times 3$ cube around its center. The 12 next nearest neighbors were taken only via their sums, and so were the eight additional spins sitting at locations (111) from the center. The FP estimate was criticalized twice using $\lambda = 3$. The resulting IRG calculation gave $\gamma/\nu = 1.9160(4)$, which is very close to the result obtained for the nearest-neighbor critical Hamiltonian, implying that larger neighborhoods must be considered for better results.

Another estimate of the FP Hamiltonian was made by Swendsen[9], by comparing correlation functions calculated in different methods. His FP estimate, consisting of 17 coupling constants, combined with the majority rule transformation, gave $\gamma/\nu = 1.9507(2)$, which is only about 0.5% from the generally accepted value.

Since the method is not restricted to the majority-rule RG, we tried other possibilities. Blöte et al[10] not only optimized the RG transformation, but also approximated the location of the FP within a space of three coupling constants. Using their transformation and FP location, we found that $\gamma/\nu = 1.9467(4)$, which is about 0.7% off.

As a final example, we tried to find an improved estimate of the FP for Blöte's RG transformation[10], using the Brandt-Ron representation. Again we have used the 26-spin neighborhood described above which contains and thus resembles the use of the three couplings in Blöte's fixed point Hamiltonian. The FP estimate was obtained by the BR perturbative algorithm described in Section 4.1. The result was $\gamma/\nu = 1.9463(4)$, which is essentially the same as the one obtained using the three coupling Hamiltonian. An additional criticaliza-

tion of this FP still results in almost the same estimate for the critical exponent. This calculation provides confirmation of the accuracy of the calculation of Blöte et al[10], as well as confirming the consistency of the criticalization method.

Fig. 3 shows log-log scaling plots for the three-dimensional susceptibility as a function of lattice size. As in the two-dimensional case shown in Fig. 1 , the linearity of the plots is again quite clear. However, the lines no longer lie on top of each other, reflecting the different RG transformations and the different fixed points involved in each calculation: The upper two lines (marked by '$\circ$' and '+') correspond to the majority RG transformation, while the bottom two (marked by 'x' and '$\Box$') are due to Blöte's transformation. (The line marked by '$*$', which has a slightly different slope, is the one obtained with the nearest-neighbor Hamiltonian.) The coefficient for the majority-rule transformation is almost 30% higher than for that of Blöte et al.[10]

Fig. 4 shows data for the spin-spin correlation function as a function of separation for lattices from $4 \times 4 \times 4$ through $128 \times 128 \times 128$. The separation r is again scaled by dividing by L, but the correlation functions are now multiplied by $L^{1.04}$, where the exponent is an approximation for $d - 2 + \eta$. As was the case for the corresponding two-dimensional plot, data from all lattices collapse onto a single curve. Unfortunately, it is very difficult to extract an accurate estimate for the value of η in three dimensions because the exponent in the scaling behavior is dominated by $d-2 = 1$, and η is only a small perturbation.

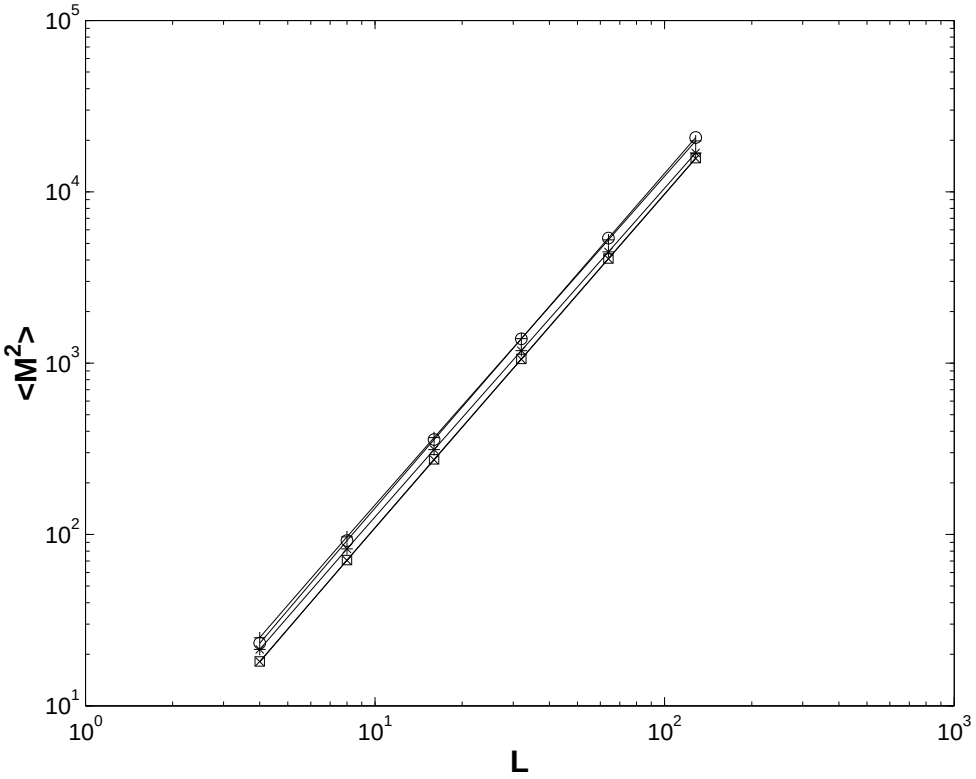

Fig. 3. A log-log plot of the linear size of the lattice L versus the average of the squared magnetization for the three-dimensional Ising model. (The line connecting the '$*$' is obtained by the nearest-neighbor Hamiltonian and the majority-rule RG; the '$\circ$' by the 17-couplings Hamiltonian and the majority-rule RG; the '+' by the BR representation with a neighborhood of 26 followed by 2 FPC; the 'x' by Blöte's Hamiltonian and RG transformation and the '$\Box$' by the BR representation with a 26-spin neighborhood with Blöte's RG transformation).

7 Conclusions and future work

In this paper, we have presented a new approach to the renormalization-group analysis of critical phenomena using Monte Carlo simulations. This method eliminates the problem of critical slowing down completely, for the same reasons that the coarse-to-fine equilibration of Brandt and Ron showed no critical slowing down. However, our approach also eliminates the difficulty that the

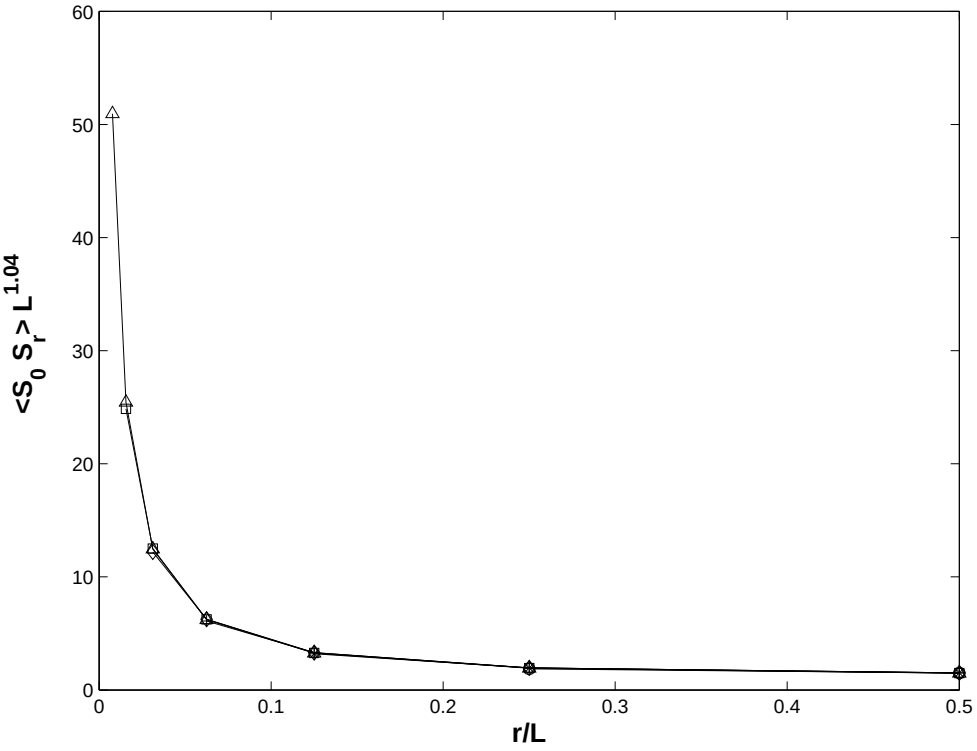

Fig. 4. A log-log plot of the spin-spin correlation function of distance r multiplied by $L^{1.04}$ versus r/L, where $L = 4, 8, ..., 128$ and $r = 1, 2, ..., L/2$, for the approximated FP of the three-dimensional Ising model consisting of 17-coupling constants with the majority rule RG transformation.

coarse-to-fine equilibration method had in calculating appropriate Hamiltonians at every step.

Our results in two dimensions turned out to be better than we could have expected; even the obviously bad approximation of estimating the FP of the majority-rule RG with the nearest-neighbor model produced an error in γ/ν of only 0.7%. With a good estimate of the FP in the Brandt-Ron representation, the error dropped to less than 0.03%. The striking accuracy obtained for the FP approximation using seven couplings is actually greater than the errors in calculating these couplings as reported in [7]. Thus, we suggest that this FP approximation needs to be recalculated either by decreasing the truncation

error, i.e., by adding more couplings, or by reducing the statistical errors, or both.

In three dimensions, the best existing approximation of the FP of the majority-rule RG with the 17 couplings Hamiltonian gives an error of 0.5% in γ/ν. The first few simple attempts in improving this result by using the BR representation were not successful. It is important to emphasize, however, that this is due to the fact that we have used only the *sums* of the next nearest neighbors in our approximations. Further improvement is expected from taking larger neighborhoods and/or including more information from the present neighborhoods.

In future work, we intend to concentrate on developing systematic methods for calculating improved estimations for the fixed point in both representation. We may also return to the question of optimizing the renormalization group transformation itself along with the calculation of the approximated fixed point.

The IRG can also be used to calculate correlations between arbitrarily distant spins on increasingly large lattices. This can be achieved by applying the IRG on some remote *windows* rather than on the entire domain. The desired statistics should then be measured only in the *interior* of each such window (several meshsizes away from its border). In general, one can produce two remote regions of the same equilibrium configuration without calculating (at the fine levels) all the regions in between.

In summary, we have developed a new way of using the renormalization group structure and Monte Carlo simulations to investigate critical behavior without critical slowing down that we hope will open the way to further calculations of

critical properties and insights into the structure of the renormalization group.

8 Acknowledgements

We would like to thank R. Golubev for her helpful programming work. The research has been supported by grants No. 295/01 from the Israel Science Foundation, US Air Force Office Of Scientific Research contract F33615-03-D-5408 and by the Carl F. Gauss Minerva Center for Scientific Computation at the Weizmann Institute of Science.

References

[1] R. H. Swendsen, Phys. Rev. Lett., **42**, 859 (1979).

[2] A. Brandt and D. Ron, J. Stat. Phys, **102**, 231 (2001).

[3] D. Ron and R. H. Swendsen, Phys. Rev. E **63**, 6128 (2001).

[4] D. Ron and R. H. Swendsen, Phys. Rev. E **66**, 6106 (2002).

[5] A. Compagner, A. Hoogland, and H. W. J. Blöte, unpublished.

[6] D. Ron, R. H. Swendsen and A. Brandt, Phys. Rev. Lett., **89**, 5701 (2002).

[7] R. H. Swendsen, Phys. Rev. Lett., **52**, 1165 (1984).

[8] R. H. Swendsen, Phys. Rev. B, **30**, 3866 (1984).

[9] R. H. Swendsen, Phys. Rev. B, **30**, 3875 (1984).

[10] H. W. J. Blöte, J. R. Heringa, A. Hoogland, E. W. Meyer, and T. S. Smit, Phys. Rev. Lett., **76**, 2613 (1996).

[11] R. Gupta and R. Cordery, Phys. Lett. **105A**, 415 (1984).