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Monte Carlo Renormalization Group

Robert H. Swendsen[1]

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Monte Carlo computer simulations have long been used to obtain information on the behavior of thermodynamic systems. The method has the advantages of being applicable to a very large class of models and of using only systematically improvable approximations (finite size of system, statistical errors, etc.). However, in the critical region, finite-size effects mask the critical singularities, and put severe practical limits onto the accuracy to which the true critical behavior can be determined. By combining Monte Carlo simulations with a real-space renormalization-group analysis, a large increase in efficiency and accuracy can be achieved—without the uncertainties of the usual truncation approximations. The methods are illustrated by explicit calculations on models exhibiting critical and tricritical behavior.

KEY WORDS: Critical phenomena; computer simulations; renormalization groups.

The combination of Monte Carlo (MC) computer simulations[1] with a real-space renormalization-group (RG) analysis[2] was first suggested by Ma[3] in 1976. Since that time, a variety of methods to implement this concept have been suggested which have proven remarkably effective in providing detailed information on the thermodynamic properties of systems at phase transitions. Details of the history of this approach and an extensive bibliography are contained in Ref. 4. I shall describe the advantages of such an approach and give an outline of what can and has been accomplished with a particular realization of the Monte Carlo renormalization group (MCRG)[4,5]

Standard MC simulations produce excellent data on the properties of finite systems, with reliable internal checks.[1] Statistical errors are well

[1] IBM Zurich Research Laboratory, 8803 Rüschlikon, Switzerland.

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understood and easily computed. However, the thermodynamic properties of an infinite system close to the critical temperature exhibit substantial finite-size effects. Since the correlation length diverges as the critical temperature is approached, it eventually becomes greater than the linear dimensions of the system being simulated. The critical singularities are rounded off in finite systems, preventing us from taking much useful data extremely close to T_c.

Real-space RG methods have the advantage of focusing direct onto the critical properties with a simple formalism for calculations. They have been shown to produce excellent agreement with some known results and nontrivial predictions for systems with unknown or partly known properties.[2] The main disadvantage of this approach has been the uncertainty of the usual truncation approximations. It is difficult to judge the accuracy of a calculation, unless a comparison is made with results obtained by other methods.

By combining the two methods, MCRG exploits the advantages of each and avoids some of the disadvantages.

To illustrate the MCRG method, I introduce the following notation. The operator on lattice site i is σ_i. The simplest example is Ising spins, which assume the values $+1$ and -1, but they can more generally assume any values, discrete states, a continuum, or even vectors. The Hamiltonian can be written in the general form

$$H = \sum_{\alpha} K_\alpha S_\alpha \tag{1}$$

where the S_α's are the various possible combinations of the σ_i's that occur in models of interest or are generated by the renormalization-group transformations. A simple example is the operator describing the nearest-neighbor coupling

$$S_{\mathrm{nn}} = \sum_{\langle ij \rangle} \sigma_j \sigma_j \tag{2}$$

The renormalization group transforms the problem so as to focus on the critical properties. Some fraction of the variables associated with short-wavelength fluctuations is integrated out, transforming the original system into a new one with fewer degrees of freedom. Transformations are generally characterized by a local function of the spin variables, assigning a value to each "block spin." These transformations reduce the linear dimensions by a factor b, where b^d is equal to the number of spins in a block. A typical example for the $d = 2$ Ising model is shown in Fig. 1. The square lattice is divided into 3×3 blocks ($b = 3$) and assigned the block spin, σ_j', the value of $+1$ when the sum of the spins is positive and -1 when it is negative. This is known as a "majority-rule" transformation.

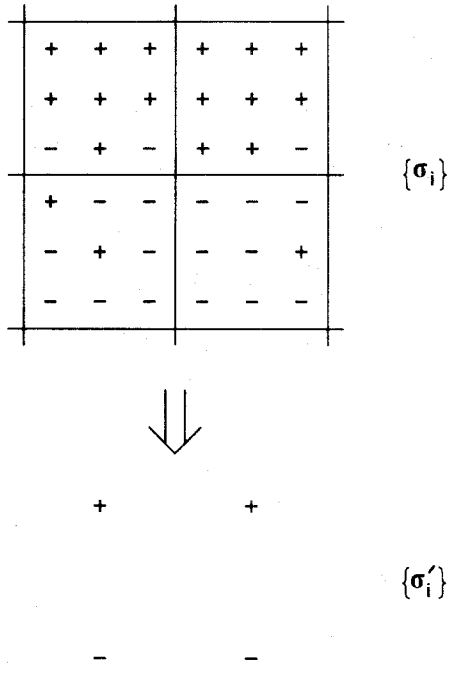

Fig. 1. Diagram of a simple RG block-spin transformation for a $d = 2$ Ising model. The transformation uses a majority rule on 3×3 blocks (scale factor $b = 3$).

The key to MCRG methods is the recognition that such transformations can be implemented directly without approximation on the explicit configurations generated by the MC simulation procedure.

The RG transformation is written in terms of the equilibrium probabilities as

$$P'(\sigma') = \mathrm{Tr}_\sigma T(\sigma', \sigma) P(\sigma) \tag{3}$$

The new probability distribution can then be interpreted in terms of an effective Hamiltonian for the renormalized block spins

$$P'(\sigma') = \exp\left[H'(\sigma') \right] / Z' \tag{4}$$

where the renormalized Hamiltonian is parametrized by a new set of coupling constants $\{K'_\alpha\}$.

However, even for models with only nearest-neighbor interactions and simple RG transformations, the renormalized Hamiltonian contains an infinite number of coupling constants. The RG transformation therefore involves a mapping of an infinite-dimensional space of coupling constants onto itself. The difficulties this creates are essential to the real-space

renormalization-group method, and are treated differently in different formulations of the theory.

Since RG transformations are local, the correlation length is assumed to be unchanged by the transformation, when measured in units of the original lattice constant. This implies that in units of the new lattice constant, the correlation length is reduced by the scale factor b ($b = 3$ for the example used above).

If we start with any Hamiltonian at criticality (infinite correlation length), the renormalized Hamiltonian will also have an infinite correlation length and therefore be a critical point. Further iterations continue to produce Hamiltonians on the critical hypersurface and the sequence of Hamiltonians will converge towards a fixed point.

Figure 2 shows a highly schematic diagram of this process. The vertical axis represents the most important coupling in the original problem (for example, the nearest-neighbor exchange), and the horizontal axis represents

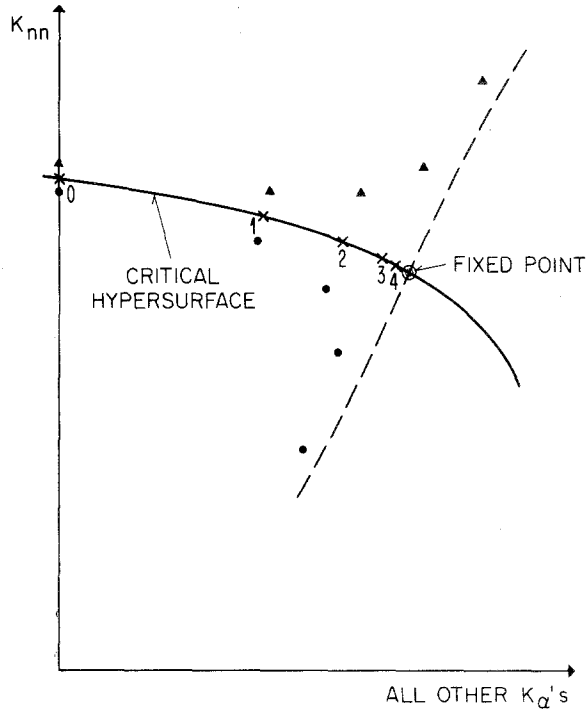

Fig. 2. Schematic diagram of the trajectories in a many-dimensional space of coupling constants under a typical RG transformation. The vertical axis represents the nearest-neighbor coupling constant, and the horizontal axis represents all other coupling constants generated by the RG transformation (after Ref. 5).

all other parameters describing the renormalized Hamiltonians. The RG transformation takes the Hamiltonian successively to the crosses labeled 1, 2, 3, etc. towards the fixed point.

If we start a small distance away from the critical point, the trajectory will first lead towards the fixed point, but eventually, move away from the critical hypersurface and away from the fixed point. The values of the critical exponents are determined by how rapidly the RG transformation brings the renormalized Hamiltonian away from the fixed point.

We can linearize the renormalization-group transformation to obtain

$$\left(K_\alpha^{(n+1)} - K_\alpha^*\right) = \sum_\beta T_{\alpha\beta}\left(K_\beta^{(n)} - K_\beta^*\right) \tag{5}$$

where

$$T_{\alpha\beta} = \partial K_\alpha^{(n+1)} / \partial K_\beta^{(n)} \tag{6}$$

is evaluated at the fixed point. The eigenvalues of this matrix then determine the critical exponents in the usual manner.[2]

Truncation methods of real-space renormalization-group analysis make approximations that eliminate all but a finite number of interactions. In many cases, this has been very successful in reproducing known results. But in addition to approximations that have proven accurate for some models, there are equally plausible approximations that give poor results. A transformation can even be good for one model and poor for another.

In principle, truncation approximations could be improved by including more coupling constants in the calculation. In practice, this is generally impossible because of the rapid increase in the difficulty of computation.[2]

As with other approaches, some sort of truncation must be made using MCRG to reduce the problem to a finite number of parameters. The truncation for MCRG is somewhat complicated in that there are two different ways in which it occurs: Once in the renormalization transformation on the finite lattice and again in the RG analysis. These are distinct and their effects must be considered separately.

The strategy used in MCRG calculations is to start with the Hamiltonian under consideration and use an MC simulation to generate a sequence of configurations characteristic of equilibrium on a finite lattice. The exact RG transformation is applied directly to the configurations. The result is a sequence of configurations for the renormalized spins, characteristic of the renormalized Hamiltonian. No approximation is involved other than the statistical errors implicit in using a finite number of MC steps. The effects of all coupling constants that will fit on the lattice are automatically taken into account correctly.

The effective renormalized Hamiltonian on the finite lattice is used as an approximation to the full renormalized Hamiltonian on an infinite

lattice. This is the first truncation. Only interactions that fit on the finite lattice are included. For the approximation to be valid, the effective range of the renormalized Hamiltonians, especially in the neighborhood of the fixed point, must be small compared with the dimensions of the lattice. This can be checked by repeating the calculation for different-size lattices, providing a simple, self-consistent test of the validity of the finite-lattice truncation.

The MC simulation of the system of interest is performed at its critical temperature. The repeated iterations move the renormalized Hamiltonians towards the fixed point automatically. This gives us a sequence of approximations for the critical exponents, which converges towards the fixed-point values.

The matrix $T_{\alpha\beta}$ is found numerically by solving the set of chain-rule equations

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\beta^{(n)}} = \sum_\alpha \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}} \frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\alpha^{(n+1)}} \tag{7}$$

The derivatives in Eq. (7) are obtained from MC correlation functions,

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\beta^{(n)}} = \langle S_\gamma^{(n+1)} S_\beta^{(n)} \rangle - \langle S_\gamma^{(n+1)} \rangle \langle S_\beta^{(n)} \rangle \tag{8}$$

The set of linear equations (7) is solved numerically for the matrix $T_{\alpha\beta}$, which then provides estimates of the critical exponents.

In principle, the matrix $T_{\alpha\beta}$ has an infinite number of components. We can only calculate part of this matrix, so a truncation is made at this point. The effect of including more interactions can be systematically investigated. Twenty interactions can easily be included in the analysis.

An illustration of a MCRG calculation is shown in Table I for the $d = 2$ Ising model, using a block-spin transformation with scale factor $b = 2$. The renormalized block-spin value was determined by majority rule, with ties being assigned values of $+1$ and -1 with equal probability. Data from lattice sizes of 8×8 to 64×64 are shown, and details of the calculation can be found in Ref. 4.

Table I shows the thermal eigenvalue exponent, y_T, for all lattices used.[4] Each column presents data from a different MC simulation. The data are grouped according to the number (N_r) of RG iterations performed. N_c gives the number of interactions taken into account in the RG analysis, which is also the rank of the part of the matrix $T_{\alpha\beta}$ used for each numerical calculation. The linear dimensions of the lattice are reduced by the scale factor $b = 2$ with each RG iteration. Consequently, the diagonal rows in Table I all refer to the same size lattices. The numbers in parentheses give the approximate statistical uncertainty in the last digit.

Table I. Critical Eigenvalue Exponent Y_T (Exact Value is 1.000) for the $d = 2$ Ising Model as a Function of the Number of RG Iterations (N_r), the Number of Coupling Constants in the RG Analysis (N_c), and the Linear Dimension of the Lattice (L). 2×2 RG block transformation[a]

		Lattice size (L)			
N_r	N_c	64	32	16	8
1	1	0.912(2)	0.904(1)	0.897(3)	0.887(3)
	2	0.967(3)	0.966(2)	0.964(3)	0.965(3)
	3	0.968(3)	0.968(2)	0.966(3)	0.966(3)
	4	0.969(4)	0.968(2)	0.966(3)	0.969(3)
	5	0.969(4)	0.968(3)	0.964(4)	0.964(5)
	6	0.969(3)	0.968(3)	0.965(4)	0.964(5)
	7	0.969(5)	0.967(3)	0.966(4)	0.962(5)
2	1	0.963(4)	0.953(2)	0.937(3)	
	2	0.999(4)	0.998(2)	0.993(3)	
	3	1.001(4)	1.000(2)	0.994(3)	
	4	1.002(5)	0.998(2)	0.984(4)	
	5	1.001(5)	0.997(2)	0.980(5)	
	6	1.001(5)	0.997(2)	0.980(5)	
	7	1.000(5)	0.997(3)	0.980(5)	
3	1	0.957(2)	0.936(3)		
	2	0.998(2)	0.991(3)		
	3	0.999(2)	0.993(3)		
	4	0.999(2)	0.987(4)		
	5	0.997(2)	0.981(7)		
	6	0.997(2)	0.979(7)		
	7	0.997(2)	0.977(9)		
4	1	0.940(7)			
	2	0.993(6)			
	3	0.992(6)			
	4	0.988(5)			
	5	0.990(5)			
	6	0.988(5)			
	7	0.984(4)			

[a] Taken from Ref. 4.

The first column in Table I gives the MCRG estimates for y_T from the 64×64 lattice. There is a difference between using only a single coupling constant (nearest-neighbor) in the analysis and including second-neighbor interactions. However, the third coupling, four-spin interaction, does not have a significant effect. It is typical that only a few couplings are important for the analysis, although this transformation is especially favorable. For the first RG step, the estimate for y_T is about 3% below the exact value of one. By the second RG step, the renormalized Hamiltonian has

moved closer to the fixed point and the estimates of y_T are very close to the exact value. The fourth iteration shows a very small size effect due to the reduction of the renormalized lattice to 4×4.

Comparison with the 32×32 system shows that the first two RG iterations are essentially identical. The third iteration exhibits the same finite-size effect as the fourth iteration of the 64×64 system, exactly as expected, since both systems have been reduced to 4×4 lattices. The same small effect can also be seen in the second iteration from the 16×16 lattice.

The magnetic eigenvalue exponent, y_H, was obtained from the same MC simulations without the necessity of introducing a magnetic field in the initial simulation of the system. The results are actually somewhat better than for the thermal eigenvalue and are shown in Table II. Reference 4 contains a discussion of the details of the calculation, along with the irrelevant eigenvalues and further consistency tests.

It is important to note that the renormalized Hamiltonians are never explicitly calculated. This is an advantage in determining the critical exponents, because numerical errors in determining the fixed point are avoided. However, some knowledge of the renormalized couplings is re-

Table II. Same as Table I for the Critical Eigenvalue Exponent y_H (exact value is 1.875) for the $d = 2$ Ising Model[a]

		Lattice size (L)			
N_r	N_c	64	32	16	8
1	1	1.8810(1)	1.8807(1)	1.8797(2)	1.8769(4)
	2	1.8804(1)	1.8803(1)	1.8800(2)	1.8795(4)
	3	1.8806(1)	1.8806(1)	1.8802(2)	1.8794(4)
	4	1.8808(1)	1.8808(1)	1.8806(2)	1.8799(4)
2	1	1.8757(2)	1.8748(2)	1.8719(2)	
	2	1.8758(2)	1.8757(2)	1.8747(2)	
	3	1.8758(2)	1.8757(2)	1.8745(2)	
	4	1.8759(2)	1.8758(2)	1.8749(2)	
3	1	1.8731(4)	1.8710(5)		
	2	1.8740(4)	1.8742(5)		
	3	1.8740(4)	1.8739(5)		
	4	1.8741(4)	1.8743(5)		
4	1	1.8706(5)			
	2	1.8735(7)			
	3	1.8732(8)			
	4	1.8737(9)			

[a] Taken from Ref. 4.

quired to calculate the critical temperature, and techniques have been developed to treat this problem,[6] based on a method introduced by Wilson[7] for the study of lattice gauge theories.[8]

The size effect can be compensated by performing two simulations on lattices of different sizes. If the two systems differ in size by the scale factor b, one application of the RG transformation to the large system will make it equal in size to the smaller system. This gives us two equal size systems, one of which is described by $H^{(0)}$ and the other by $H^{(1)}$. Since the lattices are now the same size, the size effect will be identical for both.

We can then use the differences in the correlation functions to calculate the differences in the coupling constants. If the differences in the correlation functions are not too large, we can make the linear approximation[6]

$$\langle S_\alpha^{(n)}\rangle_L - \langle S_\alpha^{(n-1)}\rangle_S = \sum_\beta \left[\frac{\partial \langle S_\alpha^{(n)}\rangle_L}{\partial K_\beta^{(n)}} - \frac{\partial \langle S_\alpha^{(n-1)}\rangle_S}{\partial K_\beta^{(n-1)}} \right] \delta K_\beta^{(0)} \tag{9}$$

As the number of RG iterations n increases, the deviations of $H^{(n)}$ from the fixed point [and from $H^{(n-1)}$] in the irrelevant directions decrease. The corresponding differences in the correlation functions also decrease and disappear into the noise.

However, deviations in the relevant directions increase upon repetition of the RG transformation, and the corresponding differences in the correlation functions are amplified. This makes the method extremely sensitive to the location of the critical temperature, since very small changes in the temperature result in large changes in the correlation functions.

Since Eq. (9) can treat several coupling constants in a single calculation, this method can also be used to find multicritical points.[9]

A number of other models are available, for which exact solutions exist. The eight-vertex or Baxter model[10] can be represented by Ising spins on a square lattice with

$$H = K_{\text{nnn}} S_{\text{nnn}} + K_4 S_4 \tag{10}$$

where S_{nnn} is the sum over all next-nearest-neighbor products, and S_4 is the sum over all four-spin products around an elementary plaquette. The critical exponents do not have fixed universal values, but are functions of the coupling constants. This requires a fixed line, instead of a simple fixed point. The MCRG method does not run into difficulties and has reproduced the correct exponents for ν ranging from 0.7 to 1.35.[11]

Since the method described above is sensitive to all relevant operators, it is also effective for multicritical points, as demonstrated for tricritical points in two dimensions.[9] Calculations have been carried out for both the Blume–Capel model and an antiferromagnet in a magnetic field. Although

the models have different symmetries and different RG transformations were used, both calculations produced the same four relevant eigenvalues, with the numerical values expected.

A large number of models has already been successfully treated with MCRG calculations. To save space and still provide an overview of what has been done, I shall just list the models studied. The references to the original papers may be found in the extensive list in Ref. 4.

Ising ferromagnet ($d = 2, 3, 4$)
Baxter model
Ashkin–Teller model
Type-II Ising antiferromagnet ($d = 2$)
Baxter–Wu model
q-state Potts models ($d = 2, 3, 4$)
Tricritical points ($d = 2$)
  Blume–Capel model
  Antiferromagnet in a magnetic field
$d = 3$ XY model
Critical end point
Lattice gauge theories
Percolation

The combination of an RG analysis with MC computer simulations has been demonstrated to provide a powerful tool for the investigation of critical phenomena. There are several directions in which these methods can develop:

1. Calculation of the location of the fixed point to enable improvements in the convergence of the method.
2. Application to systems with quenched random interactions.
3. Fluids.
4. Critical dynamics.
5. Quantum systems.

Work is already going on in all of these areas, and progress can be expected in the near future.

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