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Monte Carlo renormalization group with evolution in the space of parameters

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Using data from a single simulation we obtain Monte Carlo renormalization-group information in a finite region of parameter space by adapting the Ferrenberg-Swendsen histogram method. Several quantities are calculated in the two-dimensional $N=2$ Ashkin-Teller and Ising models to show the feasibility of the method. We show renormalization-group Hamiltonian flows and critical-point location by matching of correlations by doing just two simulations at a single temperature in lattices of different sizes to partially eliminate finite-size effects.

The efficiency of Monte Carlo simulations recently received a boost from the work of Ferrenberg and Swendsen,[1] who have brought to our attention the fact that data from a single simulation can be used to obtain thermodynamic information on a region in parameter space. Applications have been rapidly provided by several groups.[2]

The method rests on the fact that, in a finite volume, probability distributions, of any reasonable spin function of thermodynamic interest, are analytic functions of the coupling constants. These probability distributions depend mainly on a geometrical part which can be thought of as an entropic contribution and an energylike part. The former is quite difficult to calculate analytically. However, since it does not depend on coupling constants, once information about it is obtained in a simulation at a point in parameter space, it can be used to infer the probability distribution in other points in parameter space, since the energylike dependence in the couplings is quite simple.

Once again it is clear that much more than simple averages of the thermodynamic quantities are available from a single Monte Carlo run. Another instance where this fact is readily understood is the Monte Carlo renormalization group (MCRG). Our aim in this Rapid Communication is to show that these two methods can be coupled to give the typical information available from the MCRG study from runs performed at a single temperature.

It could be said that not much is gained from this method because in order to have accuracy in the extrapolations one needs extremely high statistics so that the tails of the distributions contain sufficiently accurate information. This is somewhat true if one is interested in big extrapolations outside the scaling region, but not so much in the context of the renormalization group. We will be looking at the vicinity of a critical point. For temperatures very close but not exactly critical, there already will be quite large effects in renormalized coupling constants.

We will look at the flows, in coupling constant space, of the Hamiltonian, induced by renormalization-group transformations. For simplicity, the method will be tried first in the two-dimensional (2D) Ising model. Normal MCRG flows and exponent determination use as consistency checks systematic increase of the truncation basis. We are not able to do that due to our computational constraints, and thus only a base of two operators for the even sector is used in the calculation. The point we want to make, nevertheless, is that this type of calculation is possible, leaving for future applications a more exhaustive treatment. We then turn to the problem of precisely determining critical couplings by finding the value of the coupling constant at which correlation functions at different renormalization stages are equal, thus signaling a fixed point. In both cases a two lattice method is used to decrease finite-size effects. This means that we really perform, instead of one, two simulations. This is comparable to the amount of work necessary for just a single temperature using the conventional ways. Critical coupling determination is a much simpler job than the Hamiltonian flow, and so we can easily look at more complicated systems. The $N=2$ Ashkin-Teller model will serve as our case study.

Let the Hamiltonian be written, as usual, as a sum of operators

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

where S_α is a sum of the translations of products of spins, and K_α are the coupling constants. We will perform $b\times b$ spin blockings, with a majority rule, and we are interested in how the $K_\alpha^{(n)}$ evolve after n RG transformations. We look at two lattices of size $L\times L$ and $bL\times bL$ which we will refer to as the small and large lattices, respectively. We denote by $\langle S_\alpha^{(n)}\rangle_{S,(L)}$ the expected values of the operator S_α after n renormalizations of the small (large) lattices.

If the temperature is near critical, the evolution of the coupling constants is very slow since the system is near a fixed point. The inverse problem in relation to the MCRG, that is, obtaining the probability distribution given its moments, has received attention from several groups;[3-5] in particular, it can then be solved by looking at the system of first-order equations

$$\langle S_\alpha^{(n+1)}\rangle_L - \langle S_\alpha^{(n)}\rangle_S = \sum_\beta \frac{\partial\langle S_\alpha^{(n)}\rangle}{\partial K_\beta}\delta K_\beta\,, \tag{2}$$

which is solved by inverting the matrix $\partial\langle S_\alpha^{(n)}\rangle/\partial K_\beta$. The idea behind this equation[6] is that differences between expected values of an operator at different stages of renormalization can arise from two sources: (i) due to renormalization effects and (ii) due to different size lattices leading to different finite-size effects. By subtracting expectations from different lattices at different renormalization stages, one compares objects where presumably finite-size effects cancel. Eventual differences are thus thought to be due to renormalization. As usual the derivatives, which are generalized specific heats, are calculated from the fluctuations

$$\frac{\partial\langle S_\alpha\rangle}{\partial K_\beta} = \langle S_\alpha S_\beta\rangle - \langle S_\alpha\rangle\langle S_\beta\rangle\,. \tag{3}$$

Of course we are doing an approximation, and we still have to specify from which system, large or small, the left-hand sides are to be measured. In principle, it would be profitable to make an average of large and small system quantities. We, however, will use the information from the small lattice only, because in practice it will reduce our already very stressed memory requirements. One also has better statistics for the smaller system.

Consider a quantity F as a function of any reasonable combination of spins of the lattice at any stage of renormalization. Any expected value $\langle F^k\rangle$ can be easily obtained from the moments of $P_\beta(E,F)$, that is, the joint probability distribution of the energy of the unrenormalized system and F at a given temperature $T=1/\beta$. By using the histogram method, it is also easy to calculate the moments at another temperature T', since

$$P_{\beta'}(E,F) = \frac{1}{Z'}P_\beta(E,F)e^{(\beta-\beta')E}\,, \tag{4}$$

with Z' ensuring normalization.

This is, up to this point, quite general and we turn to the specific problem of examining the Ising model RG flow. The truncated basis for the Hamiltonian consists of just two operators, the nearest-neighbor and next-nearest-neighbor two-body interactions,

$$S_\alpha = \sum_{\substack{|i-j|=\epsilon \\ \langle i,j\rangle}} \sigma_i\sigma_j\,;\quad \epsilon = \begin{cases} 1 & \text{for } \alpha=1, \\ \sqrt{2} & \text{for } \alpha=2, \end{cases}$$

$$\sigma_i = \pm 1\,.$$

Results will be presented for a simulation of an Ising model in a 32×32 (large) and a 16×16 (small) pair of lattices, a scale factor $b=2$, $n=0,1$ and two renormalizations.

The simulation is performed at $(K_1,K_2)=(0.44;0)$,

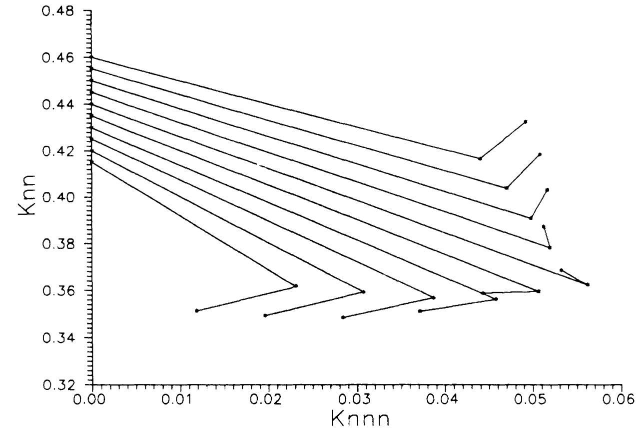

FIG. 1. Renormalization-group Hamiltonian flow from a single simulation, nearest-neighbor vs next-nearest-neighbor couplings.

which is quite near the infinite volume critical couplings. To calculate the coupling constant shifts from the sets of equations (2) and (3), one needs to store the necessary expected values. To calculate the renormalization shifts for an unrenormalized system originally at other values of $(K_1,0)$ one has to store several distributions. Let $E_{L,S}$ indicate the value of the unrenormalized system's energy. We need to store $P(E_L,S_\alpha^{(n)})$ for $\alpha=1,2$ and $n=1,2$, and $P(E_S,S_\alpha^{(n)})$ for $\alpha=1,2$ and $n=0,1$. We can do better than that if we realize that $E_S=S_1^{(0)}$ for the particular case and basis we chose, and so for $n=0$, $\alpha=1$ stores just $P(S_1^{(0)})$. Up to this point we can calculate

$$\langle S_\alpha^{(n+1)}\rangle_L \text{ and } \langle S_\alpha^{(n)}\rangle_S\,,$$

for any initial unrenormalized pure nearest-neighbor interaction system provided, of course, we do not go too far away. We still have to calculate the crossed terms which involve products of S_1 and S_2. We need then to store $P(E_S,S_\alpha^{(n)}S_\beta^{(n)})$ for $n=1$ and $(\alpha,\beta)=(1,1)$, (1,2), and (2,2).

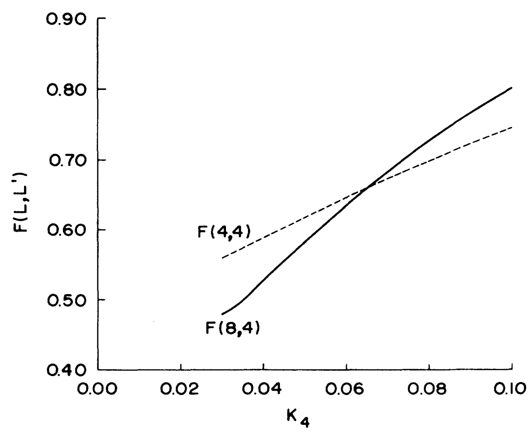

FIG. 2. $F(L,L')$ is the truncated nearest-neighbor correlation function of the Ashkin-Teller model of a system initially of size L renormalized to size L'. $\mathcal{H}=\sum_{\langle i,j\rangle}[K_1(\sigma_i\sigma_j+\mu_i\mu_j)+K_4\sigma_i\sigma_j\mu_i\mu_j]$ from a simulation at $K_1=0.4$ and $K_4=0.03$.

The result of solving the system of Eq. (2) for the evolved (in $K_1^{(0)}$) correlations appears in Fig. 1, where one can clearly use the typical RG Hamiltonian flow trajectories around the fixed point. It can be noticed that this method has the disadvantage of severely straining memory requirements. However, it is, to say the least, interesting to be able to obtain so much information just by sitting at a single temperature.

We now turn to the easier problem of determining the critical coupling of a 2D Ashkin-Teller model. Again look at two lattices of initial size differing by a factor of b. To simplify, we will compare the correlation of the once renormalized big lattice with that of the unrenormalized small lattice. One could, of course, compare the $(n+1)$th and nth renormalization stages, but as it will be clear from the results, one is sufficiently close to the fixed point such that the method can be illustrated.

Let $\mathcal{C}$ be a truncated correlation of the nth renormalization stage

$$\mathcal{C}^n_{L,S} = \sum_{\langle i,j\rangle \in \Lambda_{L,S}} (\langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle) ,$$

where $\Lambda_{L,S}$ is the large or small lattice and σ are the blocked spins.

We show in Fig. 2 the result of evolving $\mathcal{C}^1_L$ and $\mathcal{C}^0_S$. The crossing of the two curves determines, in a first approximation, the value of the four spin coupling constant at which there is a phase transition, with the nearest-neighbor two-body coupling constant fixed at $K_1 = 0.4$. From duality we know exactly the critical value $K_4 = 0.06$, which compares favorably with the matching point $K_4 = 0.065$. This good agreement is found even when the actual simulation is performed at the somewhat distant $K_4 = 0.03$. The agreement seems quite good when compared to the previously published flow diagram by Swendsen.[6]

In summary we have shown the feasibility of joining the very successful MCRG techniques with the histogram method. Whether this can be used in applications, for more interesting and realistic models, in a useful manner, will depend on the ability to keep as small as possible the memory requirements which grow quite rapidly with the increase of the system's complexity.

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[6]See, for a review, R. H. Swendsen, in *Real Space Renormalization,* edited by T. W. Burkhardt and J. M. J. Van Leeuwen, Topics in Current Physics, Vol. 30 (Springer-Verlag, Berlin, 1982).