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The use of Monte Carlo (MC) methods to study physical systems was introduced by Metropolis *et al.*[1] over 35 years ago. Since that time, MC methods have been used extensively in the study of phase transitions,[2] lattice gauge theories,[3] and chemical and biological systems.[4–6] MC simulations yield estimates for the average values of thermodynamic quantities at particular values of external parameters such as the temperature, magnetic field, and chemical potential. Since we are usually interested in studying the behavior of the system over ranges of the external parameters, it is necessary, using standard MC methods, to perform many simulations for each desired value of the external parameters. The result for each average is a set of discrete points that is usually shown as a continuous line "drawn to guide the eye."

For systems whose behavior depends on more than one external parameter, it is necessary to perform enough simulations to cover a multidimensional region of parameter space. Using standard techniques, a multiparameter scan is extremely time consuming for two parameters and impractical for three or more.

The availability of averages at only particular values of the external parameters is particularly limiting for systems near first- and second-order phase transitions where the system exhibits narrow peaks in various thermodynamic functions. The positions and heights of the peaks provide important information about the nature of the transition but, because standard MC techniques provide only a set of discrete points, the position of these peaks can be determined only approximately.

An additional problem in the study of phase transitions is that the correlation time can become large if the system is near the transition. This problem was discussed by Harvey Gould and Jan Tobochnik in the July/August 1989 issue of *Computers in Physics*.

The approach we discuss here is the use of *histograms* to extract more information from a Monte Carlo simulation. The idea is to use our knowledge of the equilibrium probability distribution at one value of a parameter to determine the probability distribution at another value of the parameter. The application of this idea to MC simulations dates back to 1959. Salsburg *et al.*[7] were the first to discuss how a single histogram of an observable could be used to evaluate any function of that quantity at a neighboring value of the corresponding parameter. However, they used the histogram only at the temperature of the original simulation and did not obtain additional information. Chesnut and Salsburg[8] described the use of histograms to obtain information over a range of continuously varying parameters, but they also did not implement this idea.

To the best of our knowledge, McDonald and Singer[9] were the first workers to use a single histogram method to evaluate thermodynamic functions over a continuous range of temperatures. (They also introduced an alternative to the Metropolis importance sampling method. Their sampling method involves making random changes of the system configuration subject only to an upper limit on the total energy of the system.) They recognized that the range of temperatures for which a single histogram would give reliable results was limited by the width of the measured histogram, although they did not obtain this relationship. They also noticed that the range of temperatures decreased as the system size was increased. From these observations it was concluded, incorrectly as we shall see, that a single histogram was not useful for the study of phase transitions.

In order to understand the single histogram method, we consider a MC simulation of the Ising model. For simplicity, we assume that the external magnetic field is zero so that the only relevant external parameter is the temperature T. Suppose that we do a standard MC run at $T = T_1$ and measure the histogram $H_1(E)$, the number of configurations that have energy E during a run of N_1 MC steps per spin. The probability $P_E(\beta_1)$ that the system has energy E at $\beta_1 = 1/k_B T_1$ is given by

$$P_E(\beta_1) = H_1(E)/N_1 = W(E)\,[e^{-\beta_1 E}/Z(\beta_1)], \quad (1)$$

where $W(E)$ is the density of states at energy E. The partition function $Z(\beta_1)$ is given by

$$Z(\beta_1) = \sum_s e^{-\beta_1 E} = \sum_E W(E) e^{-\beta_1 E}. \quad (2)$$

Since the histogram $H_1(E)$ is proportional to P_E, a MC estimate for $W(E)$ is given by

$$W(E) = a_1 H_1(E) e^{\beta_1 E}, \quad (3)$$

where a_1 is a proportionality constant. Since $W(E)$ is independent of T, the probability that the system has energy E at $\beta = 1/k_B T$ takes the form

$$P_E(\beta) = H_1(E) e^{-(\beta-\beta_1)E} \times \left(\sum_E H_1(E) e^{-(\beta-\beta_1)E}\right)^{-1}. \quad (4)$$

Alan M. Ferrenberg completed the work described here as part of the requirements for the Ph.D. in physics at Carnegie-Mellon University. He is now a post-doctoral research associate at the Center for Simulational Physics, Department of Physics and Astronomy, University of Georgia, Athens, GA 30602. Robert H. Swendsen is a professor of physics at Carnegie-Mellon University, Pittsburgh, PA 15213.

Since β is a continuous variable, we can estimate the temperature dependence of the average value of any function of E, e.g.,

$$\langle A \rangle = \sum_E A(E) P_E(\beta). \tag{5}$$

The form of the histogram at $T = 2/\ln(1+\sqrt{2})$ for a 16×16 square lattice is shown in Fig. 1.

In Ref. 10 we showed that the single histogram method is much more efficient for studying phase transitions than had been previously believed. We were able to demonstrate that the range of validity of a single histogram taken at the critical point scales in the same way as the finite-size scaling region so that information about the transition does not deteriorate with increasing system size. Hence information about a phase transition can usually be obtained with a single simulation without the need for multistage sampling (described below). We also demonstrated that histogram techniques provide the most accurate method for determining the position and height of peaks associated with a phase transition.

An effort to overcome the limitations of the single histogram method and to use *multiple* histograms was made in 1972 by Valleau and Card.[11] They introduced the idea of multistage sampling in which supplemental or *bridging* distributions are used to provide information in the wings of the original distribution. They recognized that the proportionality constant a_1 in (3) cannot be obtained from a run at a single temperature, but a second histogram can be generated at a different temperature T_2. If T_1 and T_2 are not too different, the corresponding histograms $H_1(E)$ and $H_2(E)$ will overlap over a range of values of E and the ratio a_2/a_1 can be determined by integrating over the overlap region. This procedure can be repeated if additional runs are performed and determines the entire set of a_i values to within a multiplicative constant. If enough bridging distributions are generated, overlap with the histogram from an infinite temperature simulation can be attained. In this limit the total number of states available to the system can usually be found exactly and the proportionality constant a_0 can be determined. The determination of a_0 fixes all the other a_i values so that the partition function and the absolute free energy can be obtained.

An important contribution was made in 1976 by Bennett,[12] although the relevance of his work to the problem of linking MC simulations for use in multistage sampling was not immediately recognized. Bennett considered the problem of computing free-energy differences between two different temperatures and derived equations based on optimized contributions to the estimate of the density of states from each simulation *at each value of the energy*. The result has the form of expectation values of Fermi functions, with the free-energy difference playing the role of the chemical potential.

In 1977, Torrie and Valleau[13] introduced the method of "umbrella sampling" in order to generate probability distributions wider than the Boltzmann distribution. The problem is that importance sampling typically generates a narrow distribution centered about the average value. Hence, in order to use multistage sampling, it is necessary either to perform many runs, or to rely on the overlap of the tails of the distributions where the statistics are poor. Umbrella sampling was used[13] in a study of a Lennard-Jones system by simulating only the repulsive part of the interaction. Although the method led to an increased width, the simulation became much less efficient and the results using umbrella sampling showed little improvement over those obtained with simple multistage sampling.

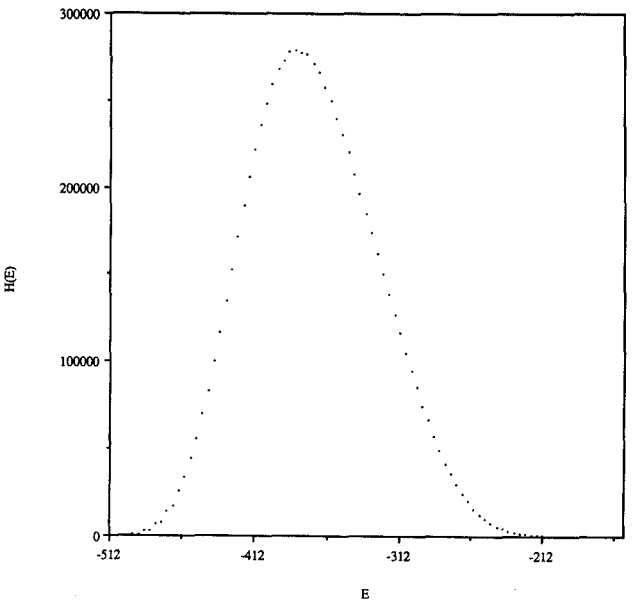

FIG. 1. The energy dependence of the histogram $H(E)$ for the Ising model on a 16×16 square lattice at $T = 2/\ln(1+\sqrt{2})$. A total of 8×10^6 Monte Carlo steps per spin was used.

An important application of histograms for the study of phase transitions was made in 1982 by Falcioni and co-workers[14] and in 1984 by Marinari.[15] These workers used the single histogram method, but extended it to complex temperatures. In this way they were able to compute the zeros of the partition function in the complex temperature plane, and hence obtain additional information about the critical behavior at phase transitions.[16]

Bhanot and co-workers[17–20] wrote a series of papers in 1987 on the application of a combination of MC methods. They used a multistage sampling approach,[11] including the method of matching overlap regions, and a simple sampling method[9] with an upper bound on the total energy. They also introduced a lower bound so that each simulation covered only a narrow range of energies. Karliner *et al.*[21] developed a modification of this approach and maintained a narrow energy range, but reintroduced importance sampling within this range. The use of importance sampling resulted in increased efficiency and lower statistical errors.

Recently, we[22] introduced a new method of optimized multiple histogram data analysis that builds on the

multistage sampling method of Valleau and Card.[11] Our approach is similar to that adopted by Bennett[12] for calculating free-energy differences. In our multiple histogram method, the data from each simulation are combined to form an estimate for the density of states which is optimized for each value of the energy. For simplicity, we will consider only a one-parameter Hamiltonian with T the relevant external parameter. The main result of the method is summarized in (13) and (14).

Suppose that we do R MC simulations. The ith simulation, with N_i MC updates, is performed at $T=T_i$ and yields a histogram $H_i(E)$. The histogram provides an estimate for the equilibrium probability distribution, which we write in the form

$$P(E)=H_i(E)/N_i=W(E)e^{-\beta_i E+f_i}, \tag{6}$$

where f_i is a parameter related to the free energy at T_i by $f_i=\beta_i F(\beta_i)$. (The parameter f_i is related to the unknown values of a_i in the multistage sampling method.[11]) Equation (6) can be inverted to obtain an estimate for the density of states:

$$W(E)=[H_i(E)/N_i]e^{\beta_i E-f_i}. \tag{7}$$

Of course, due to statistical errors, the estimate (7) from one run will be reliable only over some range of E values. Since each of the R simulations will yield a different estimate for $W(E)$, an improved estimate for W can be determined as a weighted sum over each individual estimate for the density of states:

$$W(E)=\sum_{i=1}^{R} p_i(E)H_i(E)N_i^{-1}e^{\beta_i E-f_i}. \tag{8}$$

This estimate for $W(E)$ can be optimized for *each* value of E, by choosing $p_i(E)$ so as to minimize the error in the estimate for W. The uncertainty in the histogram values is given by

$$\delta^2 H_i(E)=g_i\,\overline{H_i(E)}, \tag{9}$$

where the bar indicates the expectation value with respect to all MC simulations of duration N_i. If the successive MC configurations are independent, then $g_i=1$; otherwise, we have[23]

$$g_i=1+2\tau_i, \tag{10}$$

where τ_i is the correlation time.

If we minimize the error in the resultant estimate for $W(E)$, we obtain

$$p_i(E)=N_i g_i^{-1}e^{-\beta_i E+f_i}\left(\sum_{i=1}^{R} N_i g_i^{-1}e^{-\beta_i E+f_i}\right)^{-1}. \tag{11}$$

We define

$$P(E,\beta)=W(E)e^{-\beta E} \tag{12}$$

and write the essential multiple histogram equations as

$$P(E,\beta)=\left[\left(\sum_{i=1}^{R} g_i^{-1}H_i(E)\right)e^{-\beta E}\right]\times\left(\sum_{i=1}^{R} N_i g_i^{-1}e^{-\beta_i E+f_i}\right)^{-1}, \tag{13}$$

where

$$e^{-f_i}=\sum_E P(E,\beta_i). \tag{14}$$

Equations (13) and (14) can be iterated to determine the values of f_i self-consistently. The convergence can be accelerated by making use of derivatives of f values on one iteration with respect to those of the previous iteration. If we extend the histograms to sufficiently low or high T where the free energy can be determined exactly, the absolute free energies can be computed.

(As with other Monte Carlo techniques for calculating free energies, (13) and (14) determine the free energy to within an additive constant. For convenience, we can set $f_1=0$ and then determine the other f values with respect to f_1.)

The statistical error in $P(E,\beta)$ is given by

$$\delta P(E,\beta)=\left(\sum_i g_i^{-1}H_i(E)\right)^{-1/2}P(E,\beta). \tag{15}$$

From (15) we see that the method always reduces the statistical errors when additional MC simulations are added to the analysis. This expression also provides a clear guide for planning a series of simulations. The positions and heights of peaks in the relative error, plotted as a function of E, give a direct quantitative indication of the optimum locations and durations of additional MC simulations.

Once the values of f_i are determined, (13) can be used to calculate the average value of any function of E as a function of β,

$$\langle A\rangle=\sum_E A(E)P(E,\beta)\left(\sum_E P(E,\beta)\right)^{-1}. \tag{16}$$

In particular, the specific heat C is given by

$$VC(T)=(1/k_B T^2)(\langle E^2\rangle-\langle E\rangle^2), \tag{17}$$

where V is the volume of the system. The multiple histogram method has already been applied to several MC studies of phase transitions. For the $d=2$ Ising model the results obtained[22] compared favorably to the exact solution for finite lattices.[24] New results for the three-state antiferromagnetic Potts model, including zero-temperature entropies, were recently obtained by Wang *et al.*[25] using the multiple histogram method. Other recent applications include an SU(2) lattice gauge calculation and calculations for several lattice dimer models.

Since the multiple histogram method is able to combine MC simulation data from different sources to increase the total accuracy of the results, it could be used to combine data from different groups working on large problems, such as those encountered in lattice gauge theories. Because there are no limitations on the method

of simulation, we also expect this method to be useful for simulations in chemistry and biology.

Suggestions for Further Study

1. Use the single histogram method to show that the free-energy difference can be expressed as

$$\beta_2 F(\beta_2) - \beta_1 F(\beta_1) = -\ln \sum_E P(E) e^{-(\beta_2 - \beta_1)E}, \tag{18}$$

where $P(E) = H(E)/N_1$. (The unknown constant a_1 does not appear in the free-energy difference.)

2. Write a program to simulate the $d = 2$ Ising model on a $L \times L$ square lattice at a temperature T in a zero magnetic field. As a check on your program, compare your results for $L = 2$ to the results obtained by an exact enumeration of the 16 possible states. Then choose $L = 4$ and compute $H(E)$ at the critical temperature of the infinite system, $T_c = 2/\ln(1+\sqrt{2}) \approx 2.269$. Use the single histogram method to estimate P_E at various T up to $T = 3.13$. How do your predicted results for P_E compare to the results for P_E when measured directly? What is the approximate range of applicability of the single histogram method? Use the single histogram at $T = T_c$ to estimate C in the critical region. How do your results for $L = 4$ compare with the exact solution?[24] Is the temperature at which C is a maximum above or below T_c? Repeat the above measurements of $H(E)$ at $T = T_c$ for $L = 8$ and $L = 16$ and determine the L dependence of the maximum of C and applicability of the single histogram method.

3. Consider the Gaussian probability distribution

$$P_E = (1/\sigma)(1/\sqrt{2\pi}) e^{-E - \langle E \rangle)^2/2\sigma^2}, \tag{19}$$

where $\sigma^2 = \langle E^2 \rangle - \langle E \rangle^2$. Assume that the histogram has the Gaussian form (19) at $T = T_1$ and show that this form implies that $C(T) = T_1^2/T^2 C(T_1)$.

4. Choose $L = 16$ and compute $H(E)$ at $T = T_c$. Would it be preferable to use a cluster-flip or single-flip algorithm to obtain new configurations? How well can this histogram be fitted by a Gaussian function? Why would a Gaussian yield a better fit away from T_c?

5. Use the multiple histogram equations (13) and (14) to combine the results from runs at different temperatures. The correlation times can be computed as discussed in the July/August issue of *Computers in Physics*.

6. A system of particles interacting via the interparticle potential $V(r) = \epsilon(\sigma/r)^{12}$ can be characterized by a single dimensionless parameter $\Gamma = \beta V(r = a)$, where $4\pi n a^3/3 = 1$ and n is the particle density. Since the energy of the system is a continuous variable, how can the histogram be computed? Use the multiple histogram method to compute the mean energy and other thermodynamic quantities for Γ in the range 0.1–300. Compare your results with the MC results of Ref. 26. Can the multiple histogram method be used to determine the fluid–solid boundary? (Although computer time can be saved by considering only 32 particles, this problem is computer intensive.)

7. Use the multistage sampling method[11] to combine the histograms of two simulations. Compare the results with those obtained using the multiple histogram method. Which method produces better results?

The success of this column depends on reader input. Please send us your results, comments, and suggestions for future columns. Regular columnists Gould and Tobochnik will be back next issue. Messages can be sent via email to hgould@clarku or tobochnik%heyl.dnet@gw.wmich.edu.

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References

1. N. Metropolis, A. W. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
2. K. Binder, J. Comput. Phys. **59**, 1 (1985).
3. K. G. Wilson, Phys. Rev. D **10**, 2445 (1974); *Recent Developments in Gauge Theories*, edited by G. 't Hooft *et al.* (Plenum, New York, 1980).
4. See, for example, the collection of papers in *Simulation of Fluids*, edited by G. Ciccotti, D. Frenkel, and I. McDonald (North-Holland, Amsterdam, 1987).
5. J. A. McCammon and S. C. Harvey, *Dynamics of Proteins and Nucleic Acids* (Cambridge U. P., New York, 1987) and references therein.
6. C. H. Brooks III, M. Karplus, and B. M. Pettitt, "Proteins: A Theoretical Perspective of Dynamics, Structure and Thermodynamics," in *Advances in Chemical Physics*, edited by I. Prigogine and S. Rice (Wiley, New York, 1988), Vol. LXXI.
7. Z. W. Salsburg, J. D. Jackson, W. Fickett, and W. W. Wood, J. Chem. Phys. **30**, 65 (1959).
8. D. A. Chesnut and Z. W. Salsburg, J. Chem. Phys. **38**, 2861 (1963).
9. I. R. McDonald and K. Singer, Discuss. Faraday Soc. **43**, 40 (1967).
10. A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988).
11. J. P. Valleau and D. N. Card, J. Chem. Phys. **57**, 5457 (1972).
12. C. H. Bennett, J. Comput. Phys. **22**, 245 (1976).
13. G. Torrie and J. P. Valleau, Chem. Phys. Lett. **28**, 578 (1974); J. Comput. Phys. **23**, 187 (1977).
14. M. Falcioni, E. Marinari, M. L. Paciello, G. Parisi, and B. Taglienti, Phys. Lett. B **108**, 331 (1982).
15. E. Marinari, Nucl. Phys. B **235** [FS11], 123 (1984).
16. C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952).
17. G. Bhanot, S. Black, P. Carter, and R. Salvador, Phys. Lett. B **183**, 331 (1987).
18. G. Bhanot, K. M. Bitar, S. Black, P. Carter, and R. Salvador, Phys. Lett. B **187**, 381 (1987).
19. G. Bhanot, K. M. Bitar, and R. Salvador, Phys. Lett. B **188**, 246 (1987).
20. G. Bhanot, R. Salvador, S. Black, and R. Toral, Phys. Rev. Lett. **59**, 803 (1987).
21. M. Karliner, R. Sharpe, and Y. F. Chang, Nucl. Phys. B **302**, 204 (1988).
22. A. M. Ferrenberg and R. H. Swendsen, Carnegie–Mellon preprint.
23. H. Müller-Krumbhaar and K. Binder, J. Stat. Phys. **8**, 1 (1973).
24. A. E. Ferdinand and M. E. Fisher, Phys. Rev. **185**, 832 (1969).
25. J. S. Wang, R. H. Swendsen, and R. Kotecký, Phys. Rev. Lett. **63**, 109 (1989).
26. W. G. Hoover, M. Ross, K. W. Johnson, D. Henderson, J. A. Barker, and B. C. Brown, J. Chem. Phys. **52**, 4931 (1970).