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K. Binder
D. W. Heermann

Monte Carlo Simulation in Statistical Physics

An Introduction

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With 34 Figures

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Preface

When learning very formal material one comes to a stage where one thinks one has understood the material. Confronted with a "real life" problem, the passivity of this understanding sometimes becomes painfully clear. To be able to solve the problem, ideas, methods, etc. need to be ready at hand. They must be mastered (become active knowledge) in order to employ them successfully. Starting from this idea, the leitmotif, or aim, of this book has been to close this gap as much as possible.

How can this be done? The material presented here was born out of a series of lectures at the Summer School held at Figueira da Foz (Portugal) in 1987. The series of lectures was split into two concurrent parts. In one part the "formal material" was presented. Since the background of those attending varied widely, the presentation of the formal material was kept as pedagogic as possible.

In the formal part the general ideas behind the Monte Carlo method were developed. The Monte Carlo method has now found widespread application in many branches of science such as physics, chemistry, and biology. Because of this, the scope of the lectures had to be narrowed down. We could not give a complete account and restricted the treatment to the application of the Monte Carlo method to the physics of phase transitions. Here particular emphasis is placed on finite-size effects.

The more "informal" part of the lectures concentrated on the practical side. In a step-by-step fashion, those who attended the lectures were led from "easy" applications to more advanced algorithms. In this part we truly tried to give life to the ideas and concepts. We hope that in this book we have captured the spirit of the Summer School. There, the gap mentioned before narrowed, because many actively participated in both parts.

From the above it is clear that the material on the Monte Carlo method presented in this book can be of use to many scientists. It can be used for an advanced undergraduate or graduate course. In fact, a draft of this book has been used for a course held at the University of Mainz. Not only do we present the algorithms in great depth, we also encourage the reader to actively participate by setting many problems to be worked out by the reader.

Also for researchers and scientists using the Monte Carlo method this book contains material which may be of importance for their research. We

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treat, for example, the problem of statistical errors of a Monte Carlo estimate of a quantity. Consideration is also given to the problem of self-averaging.

We would like to thank first of all K. Kremer and D.P. Landau. Without their continuing collaboration and constructive criticism this book would not have its present form. Thanks are also due to the students of the condensed matter theory group at the University of Mainz for their participation and critical reading of the manuscript. Special thanks go to M. DeMeo for running some of the programs.

Mainz, May 1988

Kurt Binder
Dieter W. Heermann

Contents

1. Introduction: Purpose and Scope of this Volume, and Some General Comments

In recent years the method of "computer simulation" has started something like a revolution of science: the old division of physics (as well as chemistry, biology, etc.) into "experimental" and "theoretical" branches is no longer really complete. Rather, "computer simulation" has become a *third branch* complementary to the first two traditional approaches.

What, then, is the specific significance of computer simulation or "computer experiments"? The answer is simply that computer simulation yields *exact* information (apart from statistical errors, but these can be made as small as desired, at least in principle) on *model* systems which are precisely characterized. (For problems in statistical physics this means that parameters describing the Hamiltonian are known explicitly and exhaustively.)

In contrast, the information provided by analytic theory is exact only in rather rare cases, while in most other cases uncontrolled approximations are required. For example, statistical physics problems which are solvable for a three-dimensional geometry are idealized limiting cases such as ideal gases or ideal solutions, coupled harmonic oscillators, etc. The statistical mechanics of even very simple models, such as the three-dimensional Ising model, cannot be solved exactly, and much less is known about models with realistic potentials between the atomic degrees of freedom. Thus computer simulations are often designed to check the accuracy of some approximation made in the analytical treatment of a model.

Similarly, the information provided by experiment is almost never precisely characterized in the sense that the effective Hamiltonian of a given experimental sample is precisely known. Sometimes it is even controversial whether some experimentally observed phenomenon is "intrinsic" or due to some unknown impurity effects – remember that the chemical constitution of an experimental sample is known only approximately anyway. These are just a few examples from which it is clear that the comparison between analytic theory and experiment does not always lead to conclusive answers, and simulations are needed to bridge this gap. Thus, a direct comparison between a simulation of a model and experiment is not hampered by inaccurate approximations, as are often inevitable in analytic theory, and hence may indicate more conclusively whether the model faithfully represents the real system or not.

Of course, this is by no means the only reason why computer simulations are attractive. It should be noted that simulations provide information on model systems which is arbitrarily detailed, and whatever quantity the researcher may consider useful he may attempt to "sample" from the simulation. For example, scattering techniques applied to real systems usually yield information on two-particle correlation functions, but it is very difficult to obtain direct experimental information on triplet correlations or even higher-order correlations. In contrast, simulations can yield such higher-order correlations readily, at least in principle. And while the experimenter may change the temperature and pressure of his sample, he cannot as easily assess the effect of varying the interatomic potential. But arbitrary variations of interatomic potentials do not constitute a major difficulty for a computer simulation in any way. It is now quite clear that the method of computer simulation is of interest in its own right; it is a valid scientific approach to understanding the laws of nature, instructive to its practitioners in a way that is complementary to theory or experiment.

In this situation, it is no surprise that there is a true explosion of the literature on the subject. Many researchers who have previously been doing research in theoretical physics (or theoretical chemistry, biology, etc.) start doing simulations, as well as some experimentalists. And, last but not least, many students who do not have any other research experience are attracted to the field of computer simulation immediately.

This great interest, however, encounters a serious difficulty: at this point, there is hardly any teaching of simulation methods at universites, and there is even a lack of systematic textbooks from which the newcomer to the field could easily learn to become an experienced practitioner. Although one of the authors (K.B.) of the present book has edited two books which collect many applications of the Monte Carlo computer simulation method in statistical physics, these books do not have the character of textbooks from which one can easily learn a new field. The other author (D.W.H.) has written a more pedagogic account of computer simulation methods in general; however, due to its generality it cannot go into very great detail as far as the Monte Carlo investigation of phase transitions and related problems (percolation, random walks, polymers, growth phenomena, etc.) is concerned. Similar reservations apply to other techniques (such as the "molecular dynamics" method) or the techniques have other limitations. Thus the "art" of Monte Carlo simulation so far is predominantly being learned and spread in two ways, namely, either by the tedious comparative study of many original papers dating back over several decades, or by private communications from experienced practitioners.

The purpose of the present book is to fill this gap, at least partially. Thus from the outset we restrict the scope of the book to *one* method of computer simulation, the Monte Carlo method, rather than trying to cover the whole field. This restriction in scope has several motivations: first of all,

the expertise of the authors is mostly connected with this field: second, by this restriction it is realistic to use this book as a textbook for a two hour per week university course on computer simulation during one university term. Alternatively, it is suitable for use as a text for a two-week workshop on computer simulation, where the student may practice every day during this two-week period, and thus learn the Monte Carlo method in a compact intensive course. Finally, for a student or researcher who tries to work through this book just by himself, the task still seems manageable!

Unlike previous literature on Monte Carlo simulation, the present book gives *equal weight* to the *theoretical foundations* of the method (including the analysis of the results) and to *practical work* with the method. Performing "computer experiments" must be learned, just as the experimentalist learns to plan and set up experiments with real systems and evaluate the data gained from them by attending practical courses. This need for practical work in order to learn to carry out such computer experiments has been encountered again and again both by the authors of this book and by many of their colleagues. In fact, preliminary unpublished notes for the present book have been used rather successfully for a workshop on computer simulation held at Figueira da Foz, Portugal, in September 1987, and at various courses held at the University of Mainz. Thus practical experience in teaching Monte Carlo methods to students was a major factor in determining the content of this book. It has been our experience that background knowledge of a programming language such as PASCAL can always be assumed, as well as some knowledge of statistical mechanics, including the basic principle of phase transitions. If the reader is not yet familiar with concepts such as "critical exponents" and the "scaling relations" among them and models such as the Ising model, percolation, etc., he can easily find various texts where these concepts are described clearly (we refer to some of these in this book). Thus there is no need to repeat these basic concepts.

However, in using the present book it is crucial to use the theoretical part (Chap. 2 in this book) together with the "guide to practical work" (Chap. 3). These chapters both deal with the same subjects (simple sampling, random and self-avoiding walks, percolation, the Ising model, etc.) but from somewhat different points of view. In the first part, concepts for the numerical treatment of these problems were introduced and justified. In the second part, these concepts are applied to problems, and *active participation* by the reader (e.g., by working on these problems on a personal computer) is required in order to understand the concepts more deeply.

A particularly suitable way of doing so is the form of a "workshop" where this text is used as the instruction manual. A solution to a problem is presented and immediately tried out, and the method for solving the problem, the algorithm, is improved upon. Of course, a workshop works best if there is interaction between the students and the teacher and among the students. There is a component of feedback, from which everybody in

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the workshop benefits. In the form of a written text a workshop is somewhat less efficient. Nevertheless, we have structured the text such that *some form of interaction with the text, other than passive reading, is possible and necessary.*

The aim is to present enough matieral so that one can start to develop algorithms for other problems based on the concepts presented here. To achieve this goal it is necessary to work through the entire material. Thus this "workshop" (Chap. 3) is a single unit. A second goal of Chap. 3 is to present methods of data analysis and to enable the reader to become familiar with how they are applied. Again, active participation is requested.

With the concept used for this book with two chapters which are strongly correlated with each other, some redundancy is inevitable and even necessary for the sake of clarity and coherence of presentation. In fact, the scientific background of all the methods discussed in this book has been presented elsewhere in the literature: what is new and radically different from previous work is the introductory character which smoothly leads the student to a lot of practical work and experience with the method. For this pedagogic goal slight redundancies are even desirable. We have deliberately selected very simple problems of statistical physics, such as random and self-avoiding walk, percolation and the Ising model, for which all concepts and methods can be explained and demonstrated comparatively easily, and do not treat more complicated problems such as fluids with realistic potentials, spin glasses and other disordered materials, quantum-mechanical Monte Carlo methods, or problems in lattice gauge theory, in this book. In our opinion, the reader will be able to move on to such problems using the other books which exist already on the Monte Carlo method, after he has worked through the present text. We deal with the characteristic features of thermal averaging for lattice problems with discrete degrees of freedom (Ising model, Potts model, etc.) as well as continuous ones (Heisenberg and XY magnets, ϕ^4 model, etc.) in some depth, while off-lattice problems such as simple fluids, are mentioned only briefly. Particular attention is paid to understanding the limitations of the method (effects due to finite size and boundary conditions, finite observation time effects, the question of self-averaging), and what one does to overcome these limitations: for example, finite-size effects at second-order phase transitions as well as at first-order phase transitions can be used as a valuable tool for studying the bulk properties of the system, if the appropriate finite-size scaling theory is invoked. The dynamic interpretation of the Monte Carlo importance sampling is discussed as well. It is shown that although on the one hand an unwanted slowing down of convergence is implied, particularly near critical points (critical slowing down) or in glassy systems, on the other hand the Monte Carlo method becomes a unique tool for the study of the kinetics of stochastic models.

2. Theoretical Foundations of the Monte Carlo Method and Its Applications in Statistical Physics

In this chapter we first introduce the basic concepts of Monte Carlo sampling, give some details on how Monte Carlo programs need to be organized, and then proceed to the interpretation and analysis of Monte Carlo results.

2.1 Simple Sampling Versus Importance Sampling

2.1.1 Models

Statistical physics deals with systems with many degrees of freedom. A typical problem posed by statistical physics is to compute "average" macroscopic observables of a system for which the Hamiltonian is assumed to be known. For instance, let us consider magnetic systems: if a ferrromagnet has very strong uniaxial anisotropy we may describe it by the Ising model, where N spins S_i interact as

$$\mathcal{H}_{\text{Ising}} = -J \sum_{\langle i,j \rangle} S_i S_j - H \sum_{i=1} S_i \quad , \qquad S_i = \pm 1 \quad , \tag{2.1.1}$$

where the spin S_i at lattice site i can point up or down along the "easy axis", the exchange energy J is restricted in (2.1.1) to nearest neighbors, and H is a magnetic field (the term $-H \sum_i S_i$ describing the Zeeman energy of the system). Other cases occur, however, if the ferromagnet has planar anisotropy (the spin being restricted to lie in the xy plane: XY model) or is fully isotropic (Heisenberg model):

$$\mathcal{H}_{XY} = -J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) - H_x \sum_i S_i^x \quad , \tag{2.1.2}$$

$$(S_i^x)^2 + (S_i^y)^2 = 1 \quad ,$$

$$\mathcal{H}_{\text{Heisenberg}} = -J \sum_{\langle i,j \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) - H_z \sum_i S_i^z \quad , \tag{2.1.3}$$

$$(S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 = 1 \quad .$$

Of course, the large variety of real materials that the experimentalist can

prepare in his laboratory creates interest in many variants of these models: instead of spin quantum number $S = \frac{1}{2}$, implied in (2.1.1), or $S \to \infty$, implied in (2.1.2,3), we may wish to consider general spin quantum numbers; instead of exchange between nearest neighbors only, we may wish to include exchange energies between next nearest neighbors, third nearest neighbors, etc.; instead of the full isotropy in (2.1.3), there may be a need to add a uniaxial or planar anisotropy term to it; instead of uniform exchange J and uniform filed H in (2.1.1), it may be appropriate to work with random exchange constants J_{ij} and random fields H_i, to model some frozen-in random disorder in the system. Thus, magnetic solids already provide us with an incredible wealth of model Hamiltonians, for which (2.1.1–3) just provide prototype examples, and this wealth of models is only a small part of the broad spectrum of applications provided by condensed matter physics.

One task of statistical physics is to compute from the model Hamiltonian $\mathcal{H}$ the desired average properties, e.g. the average energy E or average magnetization M per degree of freedom,

$$E = \langle \mathcal{H} \rangle_T / N \quad , \qquad M = \left\langle \sum_i S_i \right\rangle_T / N \quad . \tag{2.1.4}$$

Here the thermal average of any observable $A(\boldsymbol{x})[A = \mathcal{H}, \sum_i S_i$, etc., and the vector $\boldsymbol{x}$ in phase space stands symbolically for the set of variables describing the considered degree of freedom, e.g. $\boldsymbol{x} = (S_1, S_2, \ldots, S_N)$ for (2.1.1) $\boldsymbol{x} = (S_1, S_2, \ldots, S_N)$ for (2.1.3)] is defined in the canonical ensemble

$$\langle A(\boldsymbol{x}) \rangle_T = \frac{1}{Z} \int d\boldsymbol{x} \exp[-\mathcal{H}(\boldsymbol{x})/k_B T] A(\boldsymbol{x}) \quad , \tag{2.1.5}$$

$$Z = \int d\boldsymbol{x} \exp[-\mathcal{H}(\boldsymbol{x})/k_B T] \quad .$$

It is appropriate to call these classes of problems "statistical physics" because the normalized Boltzmann factor

$$p(\boldsymbol{x}) = \frac{1}{Z} \exp[-\mathcal{H}(\boldsymbol{x})/k_B T] \tag{2.1.6}$$

plays the role of a probability density describing the statistical weight with which the configuration $\boldsymbol{x}$ occurs in thermal equilibrium.

Now although (2.1.6) gives a formally exact description of the probability distribution $p(\boldsymbol{x})$, we are still in trouble: we are neither interested in such detailed information (in our examples $\boldsymbol{x}$ stands for a set containing the N spin degrees of freedom), nor is it possible to carry out the integrations in this high-dimensional space (2.1.4,5) in the general case.

2.1.2 Simple Sampling

The Monte Carlo method in equilibrium statistical mechanics starts from the idea of approximating the exact equation (2.1.5), where one integrates over all states $\{\boldsymbol{x}\}$ with their proper weights $p(\boldsymbol{x})$, by an integration using only a characteristic subset of phase space points $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_M\}$ which are used as a statistical sample. Clearly, if one considers the limit $M \to \infty$, the discrete sum

$$\overline{A(\boldsymbol{x})} = \frac{\sum_{l=1}^{M} \exp[-\mathcal{H}(\boldsymbol{x}_l)/k_B T] A(\boldsymbol{x}_l)}{\sum_{l=1}^{M} \exp[-\mathcal{H}(\boldsymbol{x}_l)/k_B T]} \tag{2.1.7}$$

must approximate (2.1.5), just as in numerical integration routines integrals are replaced by sums [for discrete degrees of freedom, such as the Ising problem, $\int d\boldsymbol{x}$ in (2.1.5) already stands for a discrete summation over all the 2^N states $\boldsymbol{x} = (S_1, \ldots, S_N)$, of course, but in (2.1.7) we then wish to work with a small subset of these states only, $M \ll 2^N$]. But, unlike in standard routines to solve one-dimensional integrals $\int f(x)dx$, where $f(x)$ is a function of one real variable x only, instead of a high-dimensional vector $\boldsymbol{x}$, it makes no sense to choose the points $\boldsymbol{x}_l$ according to a regular grid, rather we have to choose the points $\boldsymbol{x}_l$ at random. In order to appreciate this point in detail, let us consider the XY model defined in (2.1.2) as an example. Because $(S_i^x)^2 + (S_i^y)^2 = 1$ for each site i, it is convenient to write $S_i^x = \cos\varphi_i$, $S_i^y = \sin\varphi_i$ and take the angle $\varphi_i (0 \le \varphi_i < 2\pi)$ as a variable to characterize the degrees of freedom. Then $\int d\boldsymbol{x}$ simply means $\prod \int_0^{2\pi} d\varphi_i$. Let us now introduce a regular grid, defined by $\varphi_i^{\gamma} = (\gamma_i/p)2\pi$, with $\gamma_i = 1, 2, \ldots, p$, where p is some integer characterizing the grid. Obviously the total number of points to be used in this grid is p^N, which is very large for large N, impossible to use in practice even if p is rather small. Apart from this difficulty, even if we were able to work with a reasonably large value for p, we would still have the problem that almost all points were located on the surface of the integration hypercube and almost none in its interior. Since in any lattice direction of the hypercube there are p points of the grid, $p-2$ being in the cube interior, the total fraction of points in the interior is

$$[(p-2)/p]^N = (1-2/p)^N = \exp\left[N \log\left(1 - \frac{2}{p}\right)\right] \underset{p \text{ large}}{\approx} \exp\left[-\frac{2N}{p}\right] \underset{N \to \infty}{\longrightarrow} 0 \quad .$$

A much better, i.e. *uniform*, distribution of grid points is achieved if we choose the points x_l *at random*, utilizing *"pseudo-random numbers"* produced by a *"random number generator"* built into the computer. This use

of random numbers has given this game its name! In fact, the method described thus far by (2.1.7) is indeed a variant of Monte Carlo methods, namely the *simple sampling* Monte Carlo method.

2.1.3 Random Walks and Self-Avoiding Walks

As an example of problems for which the simple sampling technique has actually been and is still used, we mention the study of self-avoiding walks (SAWs) on lattices, see e.g. [2.1]. These self-avoiding walks are used for modelling the large-scale properties of long flexible macromolecules in solution [2.2–4]. Since it is rather instructive to discuss both the advantages and the disadvantages of studying such random-walk-type problems with simple sampling Monte Carlo methods, we give a brief digression on this subject in the following.

Figure 2.1 shows various types of random walks on the square lattice. There are four different types of vectors $\boldsymbol{v}(k)$ connecting a site to its nearest neighbor on the lattice (the lattice spacing is taken to be unity)

$$\boldsymbol{v}(1) = (1,0), \quad \boldsymbol{v}(2) = (0,1), \quad \boldsymbol{v}(3) = (-1,0), \quad \boldsymbol{v}(4) = (0,-1) \quad . \tag{2.1.8}$$

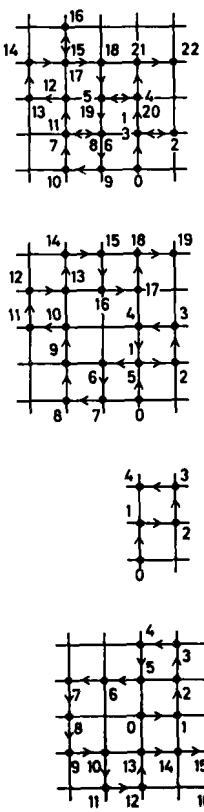

Fig. 2.1. An unrestricted random walk (RW) of 22 steps on the square lattice (**a**), a nonreversal random walk (NRRW) (**b**), and two self-avoiding walks (SAWs) (**c**). Sites are numbered in the order that they are visited. Bonds with arrows are selected consecutively by means of random numbers. The dots on the lattice sites then represent the monomers of the polymer chain

An algorithm which generates simple (unrestricted) random walks of N steps now proceeds as follows:

Algorithm 2.1. Random walks

---

i) $\boldsymbol{r}_0 = 0$ (origin of coordinate system) and put $k = 0$
ii) Choose a random integer ν_k between 1 and 4
iii) Replace k by $k+1$ and put $\boldsymbol{r}_k = \boldsymbol{r}_{k-1} + \boldsymbol{v}(\nu_{k-1})$
iv) If $k = N$ put $\boldsymbol{r}_k = \boldsymbol{R}$ (end to end distance of the walk); else return to step (ii). (2.1.9)

An example of a walk with $N = 22$ generated by this procedure is shown in Fig. 2.1a; the generation of random walks will be studied in more detail in Sect. 3.2.1. At this point we only note that for a lattice of coordination number z the total number Z_N of all such (different) random walks (RWs) is simply

$$Z_N^{\mathrm{RW}} = z^N \quad . \tag{2.1.10}$$

If the random walk is taken as a model for a polymer chain, Z_N is just the polymer partition function. (In the absence of any interactions all chain configurations have exactly the same statistical weight.)

While Algorithm 2.1 my be a reasonable model for hopping conduction in solids or other diffusion processes on ideal lattices, it is not a good model for polymers in solution, not just because of the unrealistic features of using a lattice structure to model the conformations of a macromolecule, but in particular because the excluded volume interaction is ignored. Unlike real polymers, the random walk in Fig. 2.1a intersects itself and folds back on itself. The latter feature is eliminated by defining the nonreversal random walk (NRRW) for which immediate reversals are forbidden. We can define an algorithm for this NRRW by introducing a sort of "periodic" boundary condition for the vectors $\boldsymbol{v}(\nu_k)$ by defining

$$\boldsymbol{v}(\nu \pm 4) = \boldsymbol{v}(\nu) \tag{2.1.11}$$

and modifying step (ii) of (2.1.9) for $k>1$ by introducing a one-step memory:

ii′): Choose a random number out of the triplet
$\{\nu_{k-1} - 1, \nu_{k-1}, \nu_{k-1} + 1\}$ and take it as ν_k. (2.1.12)

An alternative realization of the NRRW would proceed as in (2.1.9) but would throw ν_k away if $\boldsymbol{v}(\nu_k) = \boldsymbol{v}(\nu_k + 2)$, using (2.1.11) if necessary, and iterating step (ii). In this way the same random numbers yielding the RW with $N = 22$ in Fig. 2.1a yield a NRRW with $N = 19$ in Fig. 2.1b. From (2.1.12) we realize that

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