Chapter 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 universities, 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 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 material 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 part of the 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.

When the reader has worked through Chaps. 2 and 3, he is invited to move on to read Chap. 4 which describes some more recent methodological advances, which now have become "state of the art". Chapter 5 gives a first introduction to quantum-mechanical problems, a field that has become important recently. Finally, chapter 6 describes recent progress obtained to solve one of the great challenges of Monte Carlo simulations, namely the sampling of free energy landscapes.