A Guide to Monte Carlo Simulations in Statistical Physics
Third Edition

Dealing with all aspects of Monte Carlo simulation of complex physical systems encountered in condensed-matter physics and statistical mechanics, this book provides an introduction to computer simulations in physics.

This third edition contains extensive new material describing numerous powerful new algorithms that have appeared since the previous edition. It highlights recent technical advances and key applications that these algorithms now make possible. With several new sections and a new chapter on the use of Monte Carlo simulations of biological molecules, this edition expands the discussion of Monte Carlo at the periphery of physics and beyond.

Throughout the book there are many applications, examples, recipes, case studies, and exercises to help the reader understand the material. It is ideal for graduate students and researchers, both in academia and industry, who want to learn techniques which have become a third tool of physical science, complementing experiment and analytical theory.

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Preface

Historically physics was first known as 'natural philosophy' and research was carried out by purely theoretical (or philosophical) investigation. True progress was obviously limited by the lack of real knowledge of whether or not a given theory really applied to nature. Eventually experimental investigation became an accepted form of research although it was always limited by the physicist's ability to prepare a sample for study or to devise techniques to probe for the desired properties. With the advent of computers it became possible to carry out simulations of models which were intractable using 'classical' theoretical techniques. In many cases computers have, for the first time in history, enabled physicists not only to invent new models for various aspects of nature but also to solve those same models without substantial simplification. In recent years computer power has increased quite dramatically, with access to computers becoming both easier and more common (e.g. with personal computers and workstations), and computer simulation methods have also been steadily refined. As a result computer simulations have become another way of doing physics research. They provide another perspective; in some cases simulations provide a theoretical basis for understanding experimental results, and in other instances simulations provide 'experimental' data with which theory may be compared. There are numerous situations in which direct comparison between analytical theory and experiment is inconclusive. For example, the theory of phase transitions in condensed matter must begin with the choice of a Hamiltonian, and it is seldom clear to what extent a particular model actually represents real material on which experiments are done. Since analytical treatments also usually require mathematical approximations whose accuracy is difficult to assess or control, one does not know whether discrepancies between theory and experiment should be attributed to shortcomings of the model, the approximations, or both. The goal of this text is to provide a basic understanding of the methods and philosophy of computer simulations research with an emphasis on problems in statistical thermodynamics as applied to condensed matter physics or materials science. There exist many other simulational problems in physics (e.g. simulating the spectral intensity reaching a detector in a scattering experiment) which are more straightforward and which will only occasionally be mentioned. We shall use many specific examples and, in some cases, give explicit computer programs, but

we wish to emphasize that these methods are applicable to a wide variety of systems including those which are not treated here at all. As computer architecture changes, the methods presented here will in some cases require relatively minor reprogramming and in other instances will require new algorithm development in order to be truly efficient. We hope that this material will prepare the reader for studying new and different problems using both existing as well as new computers.

At this juncture we wish to emphasize that it is important that the simulation algorithm and conditions be chosen with the physics problem at hand in mind. The *interpretation* of the resultant output is critical to the success of any simulational project, and we thus include substantial information about various aspects of thermodynamics and statistical physics to help strengthen this connection. We also wish to draw the reader's attention to the rapid development of scientific visualization and the important role that it can play in producing *understanding* of the results of some simulations.

This book is intended to serve as an introduction to Monte Carlo methods for graduate students, and advanced undergraduates, as well as more senior researchers who are not yet experienced in computer simulations. The book is divided up in such a way that it will be useful for courses which only wish to deal with a restricted number of topics. Some of the later chapters may simply be skipped without affecting the understanding of the chapters which follow. Because of the immensity of the subject, as well as the existence of a number of very good monographs and articles on advanced topics which have become quite technical, we will limit our discussion in certain areas, e.g. polymers, to an introductory level. The examples which are given are in FORTRAN, not because it is necessarily the best scientific computer language, but because it is certainly the most widespread. Many existing Monte Carlo programs and related subprograms are in FORTRAN and will be available to the student from libraries, journals, etc. (FORTRAN has also evolved dramatically over its 50 years of existence, and the newest versions are efficient and well suited for operations involving arrays and for parallel algorithms. Object oriented languages, like C++, while useful for writing complex programs, can be far more difficult to learn. Programs written in popular, non-compiler languages, like Java or MATLAB, can be more difficult to debug and run relatively slowly. Nevertheless, all the methods described in this book can be implemented using the reader's 'language of choice'.) A number of sample problems are suggested in the various chapters; these may be assigned by course instructors or worked out by students on their own. Our experience in assigning problems to students taking a graduate course in simulations at the University of Georgia over a 25-year period suggests that for maximum pedagogical benefit, students should be required to prepare cogent reports after completing each assigned simulational problem. Students were required to complete seven 'projects' in the course of the quarter for which they needed to write and debug programs, take and analyze data, and prepare a report. Each report should briefly describe the algorithm used, provide sample data and data analysis, draw

conclusions, and add comments. (A sample program/output should be included.) In this way, the students obtain practice in the summary and presentation of simulational results, a skill which will prove to be valuable later in their careers. For convenience, the case studies that are described have been simply taken from the research of the authors of this book – the reader should be aware that this is by no means meant as a negative statement on the quality of the research of numerous other groups in the field. Similarly, selected references are given to aid the reader in finding more detailed information, but because of length restrictions it is simply not possible to provide a complete list of relevant literature. Many coworkers have been involved in the work which is mentioned here, and it is a pleasure to thank them for their fruitful collaboration. We have also benefited from the stimulating comments of many of our colleagues and we wish to express our thanks to them as well.

The pace of advances in computer simulations continues unabated. This Third Edition of our 'guide' to Monte Carlo simulations updates some of the references and includes numerous additions. New text describes algorithmic developments that appeared too late for the Second Edition or, in some cases, were excluded for fear that the volume would become too thick. Because of advances in computer technology and algorithmic developments, new results often have much higher statistical precision than some of the older examples in the text. Nonetheless, the older work often provides valuable pedagogical information for the student and may also be more readable than more recent, and more compact, papers. An additional advantage is that the reader can easily reproduce some of the older results with only a modest investment of modern computer resources. Of course, newer, higher resolution studies that are cited often permit yet additional information to be extracted from simulational data, so striving for higher precision should not be viewed as 'busy work'. Because of the growth in importance of Monte Carlo simulations in biologically related problems, we have extracted the subsection on 'protein folding' in Chapter 13 of the Second Edition and placed the material into a new chapter (Chapter 14) on biochemical applications. This new chapter is of potential relevance not only to computational biophysicists and biochemists, but also to bioinformaticists who are interested in extending the range of their capabilities. The material in this chapter goes beyond the treatment of 'toy problems' that we retain under the topic of 'biologically inspired physics' in Chapter 13 on 'Monte Carlo simulations at the periphery of physics and beyond'.