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Series Editors

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Florida Atlantic University
Department of Computer and Electrical Engineering and Computer Science
Imaging Science and Technology Center
777 Glades Road SE, Room 456
Boca Raton, FL 33431, USA
E-mail: wrhodes@fau.edu

Professor H. Eugene Stanley
Boston University
Center for Polymer Studies
Department of Physics
590 Commonwealth Avenue, Room 204B
Boston, MA 02215, USA
E-mail: hes@bu.edu

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Kurt Binder
Dieter W. Heermann

Monte Carlo Simulation in Statistical Physics

An Introduction

Fifth Edition

With 54 Figures

Springer

Professor Dr. Kurt Binder
Universität Mainz, Institut für Physik
Staudinger Weg 7, 55099 Mainz, Germany
E-mail: kurt.binder@uni-mainz.de

Professor Dr. Dieter W. Heermann
Ruprecht-Karls-Universität Heidelberg
Fakultät Physik und Astronomie, Institut für Theoretische Physik
Philosophenweg 19, 69120 Heidelberg, Germany
E-mail: heermann@tphys.uni-heidelberg.de

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Preface

The material presented in this book was born out of a series of lectures at a Summer School held at Figueira da Foz (Portugal) in 1987. Since then, the field of computational physics has seen an enormous growth and stormy development.

Many new applications and application areas have been found. In the 1980s, we could not foresee this but hoped that the Monte Carlo method would find such widespread acceptance. We were thus very glad to bring the work forward to a second edition correcting some misprints. Since then and over the years and editions of this book, many chapters have been added accounting for the development of new methods and algorithms. However, the basics have remained stable over the years and still serve as an entry point for researchers who would like to apply the Monte Carlo method and perhaps want to develop new ideas. Appending these basics with chapters on newly developed methods has evolved this book a bit into the direction of a textbook giving an introduction and at the same time covering a very broad spectrum. The first part of the book explains the theoretical foundations of the Monte Carlo method as applied to statistical physics. Chapter 3 guides the reader to practical work by formulating simple exercises and giving hints to solve them. Hence, it is a kind of "primer" for the beginner, who can learn the technique by working through these two chapters in a few weeks of intense study. Alternatively, this material can be used as text for a short course in university teaching covering in one term. The following chapters describe some more sophisticated and advanced techniques, e.g., Chap. 4 describes cluster algorithms and reweighting techniques, Chap. 5 describes the basic aspects of quantum Monte Carlo methods, and Chap. 6 (newly added to the 5th edition) describes recent developments in the last decade, such as "expanded ensemble" methods to sample the energy density of states, e.g., the Wang–Landau algorithm, as well as methods to sample rare events, such as "transition path sampling". These chapters then should be useful even for the more experienced practitioner. However, no attempt is made to cover all existing applications of Monte Carlo methods to statistical physics in an encyclopedic style – such an attempt would make this book almost unreadable and unhandy. While the "classic" applications of Monte Carlo methods in the 1970s and 1980s of the last century now are simple examples that a student can work out on his laptop as an exercise, this is not true for the recent developments described in the last chapter, of course, which often need heavy investment of computer time. Hence, no attempt could as yet be made to enrich the last chapters with exercises as well.

We are very grateful for the many comments, suggestions, and the pointing out of misprints that have been brought to our attention. We would like to thank the many colleagues with whom we had the pleasure to engage with into discussions and that in some way or the other have shaped our thinking and thus have indirectly influenced this work.

Mainz, Heidelberg *Kurt Binder*
July 2010 *Dieter W. Heermann*

Preface to the Fourth Edition

At the beginning of the new millennium, computer simulation is a well established method of doing physics research. By Monte Carlo study of models that are intractable by analytical methods one closes important gaps in our understanding of physical reality. "Computer experiments" can be performed where one switches on interactions at will (or switches them off), and one can "measure" response functions inaccessible by experiment, one can work in reduced dimensionality ($d = 1$, $d = 2$) or one can explore higher-dimensional worlds. These are just a few examples out of many, on how one can get insight by going beyond experiments. A valuable advantage also is the possibility of recognizing important aspects of a problem by visualizing degrees of freedom of a complex many-body system in any desired detail!

These comments should suffice to explain why the simulational approach in physics becomes still more popular, and the number of research papers alone that use it certainly is of the same order as research papers containing experimental work only or current analytical calculations. However, there still is a strange mismatch between the strong role of simulations in physics research, and the relatively small part that is devoted to simulation in the teaching of physics. The present book thus plays a key role, because it contributes significantly to closing this gap. Students with a little background in statistical thermodynamics can use this book to learn how to do simulations, guided using program simulations on classical problems of statistical physics, like the Ising model or other spin models, percolation, the Lennard–Jones fluid, etc. The combination of coherent chapters presenting all the essentials of the techniques of both the generation of simulation "data" and their analysis with a multitude of exercises of widely varying difficulty provides useful material, indispensable for the beginner, but containing facets also useful for the expert.

This concept applied also to previous editions, and has proven successful and useful. Nevertheless, the present edition includes not only significant updates to the chapters contained in the earlier editions, but contains a rich new chapter where an introduction to Quantum Monte Carlo methods is provided. This is a topic which steadily gains more importance, and hence including it should significantly improve the usefulness of the present book.

Again, it is a great pleasure to thank many colleagues for suggestions, as well as our own students for their questions – all these interactions have helped to improve the presentation of material in this book.

Mainz, Heidelberg
May 2002

Kurt Binder
Dieter W. Heermann

Preface to the Third Edition

The last ten years have seen an explosive growth in the computer power available to scientists. Simulations that needed access to big mainframe computers in the past are now feasible on the workstation or powerful personal computer available on everybody's desk. This ease with which physicists (and scientists in neighboring areas such as chemistry, biology, economic science) can carry out simulations of their own, has caused a true scientific revolution, and thus simulational approaches are extremely widespread.

However, teaching simulation methods in physics is still a somewhat neglected field at many universities. Although there is plenty of literature describing advanced applications (the old dream of predicting materials properties from known interactions between atoms or molecules is now reality in many cases!), there is still a lack of textbooks from which the interested student can learn the technique of Monte Carlo simulations and their proper analysis step by step.

Thus the present book still fulfills a need and continues to be useful for students who wish to bridge gaps in their university education in a "do-it-yourself" basis and for university staff who can use it for courses. Also researchers in academia and industry who have recognized the need to catch up with these important developments will find this book invaluable.

This third edition differs from the first in two important respects: printing errors have been eliminated, unclear formulations have been replaced by better ones and so on. We are most indebted to Professor Kecheng Qin (Physics Department, Univ. Beijing) who translated the first edition into Chinese and on that occasion very efficiently helped us to track down all these minor inconsistencies. We have also added an entire new chapter "Some Important Recent Developments of the Monte Carlo Methodology", which describes technical breakthroughs such as cluster algorithms and histogram reweighting, which became established after the first edition was published and are now commonly used by many Monte Carlo practitioners. The many references (far more than 100) in this chapter will make this book useful for the experienced researcher as well as the new student, who is encouraged to apply these techniques when working through the exercises in Chap. 3.

Finally, we wish to thank many colleagues for fruitful interactions, which have helped to improve this book.

Mainz, Heidelberg *Kurt Binder*
June 1997 *Dieter W. Heermann*

Preface to the Earlier Editions

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 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

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