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Edited by Peter Fulde

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# Monte Carlo Simulation in Statistical Physics

An Introduction

Third Edition  
With 42 Figures



Springer

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# Preface

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 a 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 on 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differs from the first in two important respects: printing errors have been eliminated, unclear formulations have been replaced by better ones and so on.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 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, June 1997  
Heidelberg, June 1997

*Kurt Binder*  
*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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