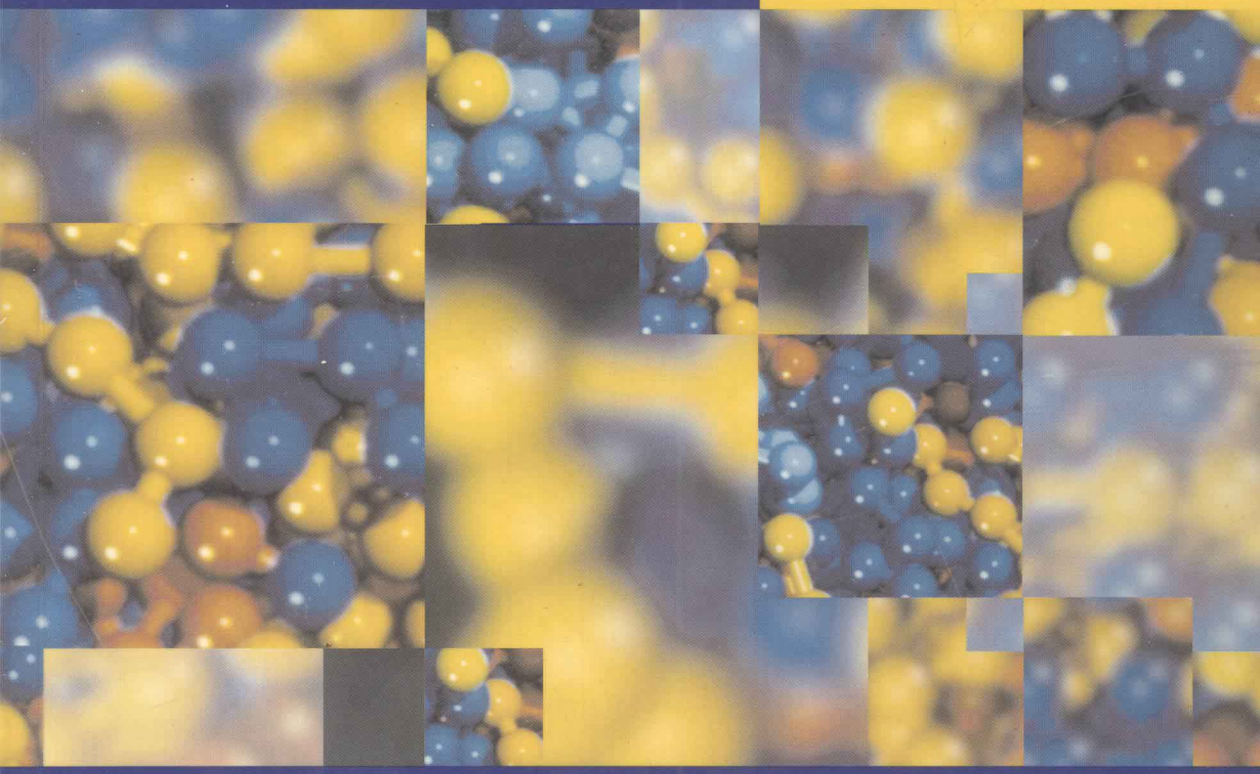
A Guide to Monte Carlo Simulations in Statistical Physics

David P. **Landau** &
Kurt **Binder**



A Guide to
Monte Carlo Simulations in Statistical Physics

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A Guide to Monte Carlo Simulations in Statistical Physics

This book deals with all aspects of Monte Carlo simulation of complex physical systems encountered in condensed-matter physics and statistical mechanics as well as in related fields, for example polymer science and lattice gauge theory.

After briefly recalling essential background in statistical mechanics and probability theory, the authors give a succinct overview of simple sampling methods. The next several chapters develop the importance sampling method, both for lattice models and for systems in continuum space. The concepts behind the various simulation algorithms are explained in a comprehensive fashion, as are the techniques for efficient evaluation of system configurations generated by simulation (histogram extrapolation, multicanonical sampling, thermodynamic integration and so forth). The fact that simulations deal with small systems is emphasized, and the text incorporates various finite size scaling concepts to show how a careful analysis of finite size effects can be a useful tool for the analysis of simulation results. Other chapters also provide introductions to quantum Monte Carlo methods, aspects of simulations of growth phenomena and other systems far from equilibrium, and the Monte Carlo renormalization group approach to critical phenomena. Throughout the book there are many applications, examples, and exercises to help the reader in a thorough study of this book; furthermore, many up-to-date references to more specialized literature are also provided.

This book will be bought by graduate students who have to deal with computer simulations in their research, as well as by postdoctoral researchers, in both physics and physical chemistry. It can be used as a textbook for graduate courses on computer simulations in physics and related disciplines.

DAVID P. LANDAU was born on June 22, 1941 in St. Louis, MO, USA. He received a B.A. in Physics from Princeton University in 1963 and a Ph.D. in Physics from Yale University in 1967. His Ph.D. research involved experimental studies of magnetic phase transitions as did his postdoctoral research at the CNRS in Grenoble, France. After teaching at Yale for a year he moved to the University of Georgia and initiated a research program of Monte Carlo studies in statistical physics. He is currently the Research Professor of Physics and founding Director of the Center for Simulational Physics at the University of Georgia. He has been teaching graduate courses in computer simulations since 1982. David Landau has authored/co-authored almost 300 research publications and is editor/co-editor of more than a dozen books. The University of Georgia awarded him a Creative Research Medal in 1981 and named him a Senior Teaching Fellow in 1993. In 1998 he also became an Adjunct Professor at the Helsinki University of Technology. He is a Fellow of the American Physical Society and a past Chair of the Division of Computational Physics of the APS. He received the Jesse W. Beams award from SESAPS in 1987, and a Humboldt Fellowship and Humboldt Senior U.S. Scientist award in 1975 and 1988 respectively. In 1999 he was named a Fellow of the Japan Society for the Promotion of Science. He is currently a Principal Editor for the journal *Computer Physics Communications.*

KURT BINDER was born on February 10, 1944 in Korneuburg, Austria and then lived in Vienna, where he received his Ph.D. in 1969 at the Technical University of Vienna. Even then his thesis dealt with Monte Carlo simulations of Ising and Heisenberg magnets, and since then he has pioneered the development of Monte Carlo simulation methods in statistical physics. From 1969 until 1974 Kurt Binder worked at the Technical University in Munich, where he defended his Habilitation thesis in 1973 after a stay as IBM postdoctoral fellow in Zurich in 1972/73. Further key times in his career were spent at Bell Laboratories, Murray Hill, NJ (1974) and a first appointment as Professor of Theoretical Physics at the University of Saarbrücken back in Germany (1974–1977), followed by a joint appointment as full professor at the University of Cologne and the position as one of the directors of the Institute of Solid State Research at Jülich (1977–1983). He has held his present position as Professor of Theoretical Physics at the University of Mainz, Germany since 1983, and since 1989 he has also been an external member of the Max-Planck-Institut for Polymer Research at Mainz. Kurt Binder has written more than 600 research publications and edited five books dealing with computer simulation. His book (with Dieter W. Hermann) *Monte Carlo Simulation in Statistical Physics: An Introduction*, first published in 1988, is in its 3rd edition. Kurt Binder has been a corresponding member of the Austrian Academy of Sciences in Vienna since 1992 and received the Max Planck Medal of the German Physical Society in 1993. He also acts as Editorial Board member of several journals and presently serves as chairman of the IUPAP Commission on Statistical Physics.

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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 a 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. 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 15 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.

Contents

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1 Introduction

1.1 WHAT IS A MONTE CARLO SIMULATION?

In a Monte Carlo simulation we attempt to follow the 'time dependence' of a model for which change, or growth, does not proceed in some rigorously predefined fashion (e.g. according to Newton's equations of motion) but rather in a stochastic manner which depends on a sequence of random numbers which is generated during the simulation. With a second, different sequence of random numbers the simulation will not give identical results but will yield values which agree with those obtained from the first sequence to within some 'statistical error'. A very large number of different problems fall into this category: in percolation an empty lattice is gradually filled with particles by placing a particle on the lattice randomly with each 'tick of the clock'. Lots of questions may then be asked about the resulting 'clusters' which are formed of neighboring occupied sites. Particular attention has been paid to the determination of the 'percolation threshold', i.e. the critical concentration of occupied sites for which an 'infinite percolating cluster' first appears. A percolating cluster is one which reaches from one boundary of a (macroscopic) system to the opposite one. The properties of such objects are of interest in the context of diverse physical problems such as conductivity of random mixtures, flow through porous rocks, behavior of dilute magnets, etc. Another example is diffusion limited aggregation (DLA) where a particle executes a random walk in space, taking one step at each time interval, until it encounters a 'seed' mass and sticks to it. The growth of this mass may then be studied as many random walkers are turned loose. The 'fractal' properties of the resulting object are of real interest, and while there is no accepted analytical theory of DLA to date, computer simulation is the method of choice. In fact, the phenomenon of DLA was first discovered by Monte Carlo simulation!

Considering problems of statistical mechanics, we may be attempting to sample a region of phase space in order to estimate certain properties of the model, although we may not be moving in phase space along the same path which an exact solution to the time dependence of the model would yield. Remember that the task of equilibrium statistical mechanics is to calculate thermal averages of (interacting) many-particle systems: Monte Carlo simulations can do that, taking proper account of statistical fluctuations and their

effects in such systems. Many of these models will be discussed in more detail in later chapters so we shall not provide further details here. Since the accuracy of a Monte Carlo estimate depends upon the thoroughness with which phase space is probed, improvement may be obtained by simply running the calculation a little longer to increase the number of samples. Unlike in the application of many analytic techniques (e.g. perturbation theory for which the extension to higher order may be prohibitively difficult), the improvement of the accuracy of Monte Carlo results is possible not just in principle but also in practice!

1.2. WHAT PROBLEMS CAN WE SOLVE WITH IT?

The range of different physical phenomena which can be explored using Monte Carlo methods is exceedingly broad. Models which either naturally or through approximation can be discretized can be considered. The motion of individual atoms may be examined directly; e.g. in a binary (AB) metallic alloy where one is interested in interdiffusion or unmixing kinetics (if the alloy was prepared in a thermodynamically unstable state) the random hopping of atoms to neighboring sites can be modeled directly. This problem is complicated because the jump rates of the different atoms depend on the locally differing environment. Of course, in this description the quantum mechanics of atoms with potential barriers in the eV range is not explicitly considered, and the sole effect of phonons (lattice vibrations) is to provide a 'heat bath' which provides the excitation energy for the jump events. Because of a separation of time scales (the characteristic times between jumps are orders of magnitude larger than atomic vibration periods) this approach provides very good approximation. The same kind of arguments hold true for growth phenomena involving macroscopic objects, such as DLA growth of colloidal particles; since their masses are orders of magnitude larger than atomic masses, the motion of colloidal particles in fluids is well described by classical, random Brownian motion. These systems are hence well suited to study by Monte Carlo simulations which use random numbers to realize random walks. The motion of a fluid may be studied by considering 'blocks' of fluid as individual particles, but these blocks will be far larger than individual molecules. As an example, we consider 'micelle formation' in lattice models of microemulsions (water–oil–surfactant fluid mixtures) in which each surfactant molecule may be modeled by two 'dimers' on the lattice (two occupied nearest neighbor sites on the lattice). Different effective interactions allow one dimer to mimic the hydrophilic group and the other dimer the hydrophobic group of the surfactant molecule. This model then allows the study of the size and shape of the aggregates of surfactant molecules (the micelles) as well as the kinetic aspects of their formation. In reality, this process is quite slow so that a deterministic molecular dynamics simulation (i.e. numerical integration of Newton's second law) is not feasible. This example shows that part of the 'art' of simulation is the appropriate choice

(or invention!) of a suitable (coarse-grained) model. Large collections of interacting classical particles are directly amenable to Monte Carlo simulation, and the behavior of interacting quantized particles is being studied either by transforming the system into a pseudo-classical model or by considering permutation properties directly. These considerations will be discussed in more detail in later chapters. Equilibrium properties of systems of interacting atoms have been extensively studied as have a wide range of models for simple and complex fluids, magnetic materials, metallic alloys, adsorbed surface layers, etc. More recently polymer models have been studied with increasing frequency; note that the simplest model of a flexible polymer is a random walk, an object which is well suited for Monte Carlo simulation. Furthermore, some of the most significant advances in understanding the theory of elementary particles have been made using Monte Carlo simulations of lattice gauge models.

1.3 WHAT DIFFICULTIES WILL WE ENCOUNTER?

1.3.1 Limited computer time and memory

Because of limits on computer speed there are some problems which are inherently not suited to computer simulation, at this time. A simulation which requires years of cpu time on whatever machine is available is simply impractical. Similarly a calculation which requires memory which far exceeds that which is available can be carried out only by using very sophisticated programming techniques which slow down running speeds and greatly increase the probability of errors. It is therefore important that the user first consider the requirements of both memory and cpu time *before* embarking on a project to ascertain whether or not there is a realistic possibility of obtaining the resources to simulate a problem properly. Of course, with the rapid advances being made by the computer industry, it may be necessary to wait only a few years for computer facilities to catch up to your needs. Sometimes the tractability of a problem may require the invention of a new, more efficient simulation algorithm. Of course, developing new strategies to overcome such difficulties constitutes an exciting field of research by itself.

1.3.2 Statistical and other errors

Assuming that the project can be done, there are still potential sources of error which must be considered. These difficulties will arise in many different situations with different algorithms so we wish to mention them briefly at this time without reference to any specific simulation approach. All computers operate with limited word length and hence limited precision for numerical values of any variable. Truncation and round-off errors may in some cases lead to serious problems. In addition there are statistical errors which arise as

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