A Guide to Monte Carlo Simulations in Statistical Physics, Second Edition

This new and updated 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, lattice gauge theory and protein folding.

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, Wang–Landau sampling, thermodynamic integration and so forth). The fact that simulations deal with small systems is emphasized. 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. A brief overview of other methods of computer simulation is given, as is an outlook for the use of Monte Carlo simulations in disciplines outside of physics. Many applications, examples and exercises are provided throughout the book. Furthermore, many new references have been added to highlight both the recent technical advances and the key applications that they now make possible.

This is an excellent guide for graduate students who have to deal with computer simulations in their research, as well as 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 BA 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 Distinguished 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 more than 330 research publications and is editor/co-editor of more than 20 books. 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 US Scientist award in 1975 and 1988 respectively. The University of Georgia named him a Senior Teaching Fellow in 1993. In 1998 he also became an Adjunct Professor at the Helsinki University of Technology. In 1999 he was named a Fellow of the Japan Society for the Promotion of Science. In 2002 he received the Aneesur Rahman Prize for Computational Physics from the APS, and in 2003 the Lamar Dodd Award for Creative Research from the University of Georgia. In 2004 he became the Senior Guangbiao Distringuished Professor (Visiting) at Zhajiang in China. 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 800 research publications and edited 5 books dealing with computer simulation. His book (with Dieter W. Heermann) *Monte Carlo Simulation in Statistical Physics: An Introduction*, first published in 1988, is in its fourth 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 has served as Chairman of the IUPAP Commission on Statistical Physics. In 2001 he was awarded the Berni Alder CECAM prize from the European Physical Society.

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Second Edition

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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 20-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 Second 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 first 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'. We have also added a brief new chapter that provides an overview of some areas outside of physics where traditional Monte Carlo methods have made an impact. Lastly, a few misprints have been corrected, and we thank our colleagues for pointing them out.