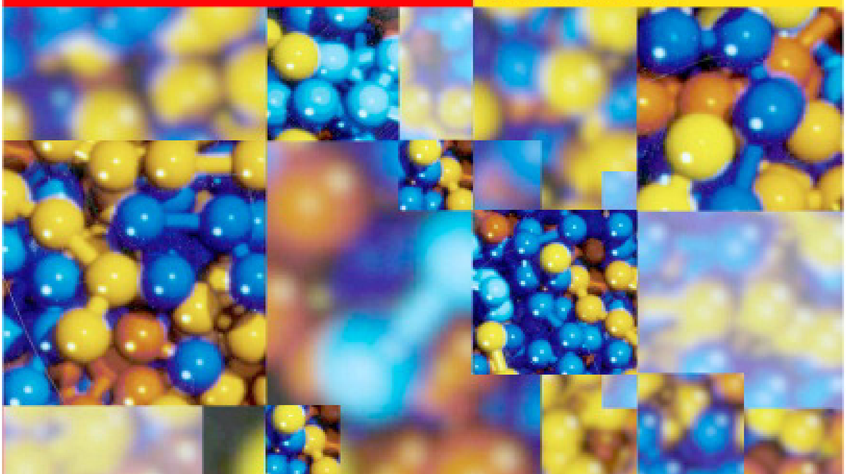
SECOND EDITION

A Guide to Monte Carlo Simulations in Statistical Physics

David P. Landau & Kurt Binder



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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 post-doctoral 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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