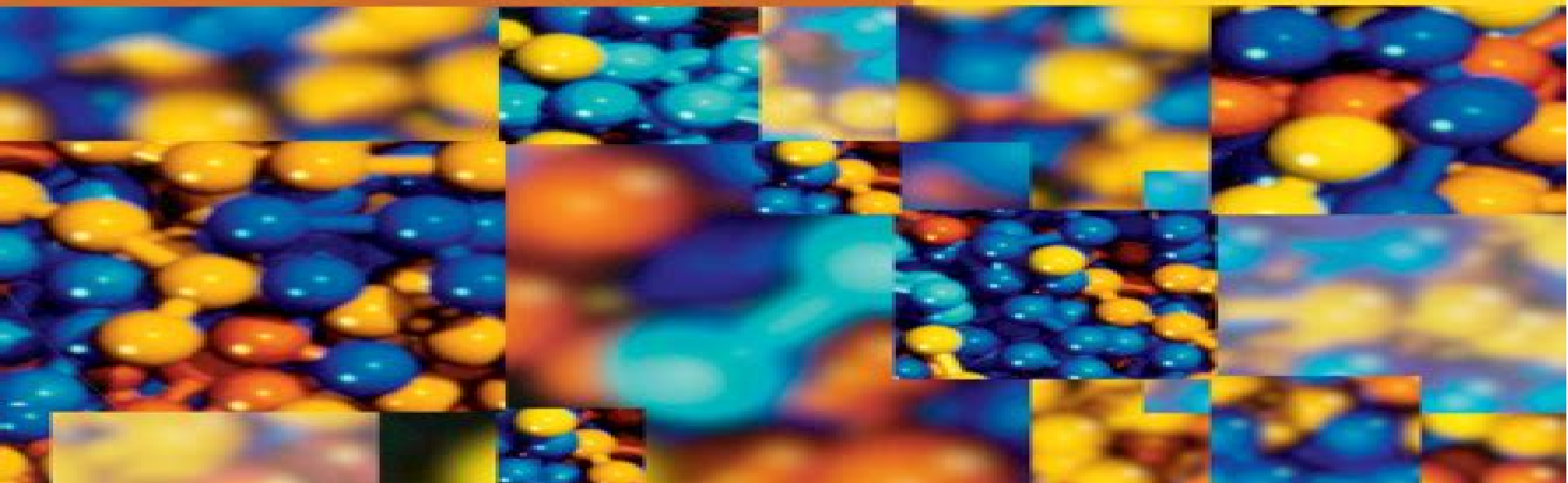


FIFTH EDITION

# A Guide to Monte Carlo Simulations in Statistical Physics

David P. Landau  
Kurt Binder



# 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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plenty of examples and exercises for the student Problems treated by simple sampling random and self avoiding walks percolation clusters etc are included along with such topics as finite size effects and guidelines for the analysis of Monte Carlo simulations The two parts together provide an excellent introduction to the theory and practice of Monte Carlo simulations

**Understanding Molecular Simulation** Daan Frenkel, Berend Smit, 2001-10-19 Understanding Molecular Simulation From Algorithms to Applications explains the physics behind the recipes of molecular simulation for materials science Computer simulators are continuously confronted with questions concerning the choice of a particular technique for a given application A wide variety of tools exist so the choice of technique requires a good understanding of the basic principles More importantly such understanding may greatly improve the efficiency of a simulation program The implementation of simulation methods is illustrated in pseudocodes and their practical use in the case studies used in the text Since the first edition only five years ago the simulation world has changed significantly current techniques have matured and new ones have appeared This new edition deals with these new developments in particular there are sections on Transition path sampling and diffusive barrier crossing to simulate rare events Dissipative particle dynamic as a coarse grained simulation technique Novel schemes to compute the long ranged forces Hamiltonian and non Hamiltonian dynamics in the context constant temperature and constant pressure molecular dynamics simulations Multiple time step algorithms as an alternative for constraints Defects in solids The pruned enriched Rosenbluth sampling recoil growth and concerted rotations for complex molecules Parallel tempering for glassy Hamiltonians Examples are included that highlight current applications and the codes of case studies are available on the World Wide Web Several new examples have been added since the first edition to illustrate recent applications Questions are included in this new edition No prior knowledge of computer simulation is assumed

Monte Carlo Simulation in Statistical Physics Kurt Binder, Dieter W. Heermann, 2010-08-17 Monte Carlo Simulation in Statistical Physics deals with the computer simulation of many body systems in condensed matter physics and related fields of physics chemistry and beyond to traffic flows stock market fluctuations etc Using random numbers generated by a computer probability distributions are calculated allowing the estimation of the thermodynamic properties of various systems This book describes the theoretical background to several variants of these Monte Carlo methods and gives a systematic presentation from which newcomers can learn to perform such simulations and to analyze their results The fifth edition covers Classical as well as Quantum Monte Carlo methods Furthermore a new chapter on the sampling of free energy landscapes has been added To help students in their work a special web server has been installed to host programs and discussion groups <http://www.cp.tphys.uni-heidelberg.de> Prof Binder was the winner of the Berni J Alder CECAM Award for Computational Physics 2001 as well as the Boltzmann Medal in 2007

**Markov Chain Monte Carlo Simulations and Their Statistical Analysis** Bernd A. Berg, 2004 This book teaches modern Markov chain Monte Carlo MC simulation techniques step by step The material should be accessible to advanced undergraduate students and is suitable for a course It

ranges from elementary statistics concepts the theory behind MC simulations through conventional Metropolis and heat bath algorithms autocorrelations and the analysis of the performance of MC algorithms to advanced topics including the multicanonical approach cluster algorithms and parallel computing Therefore it is also of interest to researchers in the field The book relates the theory directly to Web based computer code This allows readers to get quickly started with their own simulations and to verify many numerical examples easily The present code is in Fortran 77 for which compilers are freely available The principles taught are important for users of other programming languages like C or C++

**Monte Carlo Simulations of the Ising Model** Michael Adler, 2016-05 In this book the thermodynamic observables of the classical one and two dimensional ferromagnetic and antiferromagnetic Ising models on a square lattice are simulated especially at the phase transitions if applicable using the classical Monte Carlo algorithm of Metropolis Finite size effects and the influence of an external magnetic field are described The critical temperature of the 2d ferromagnetic Ising model is obtained using finite size scaling Before presenting the Ising model the basic concepts of statistical mechanics are recapped Furthermore the general principles of Monte Carlo methods are explained

**Reviews in Computational Chemistry, Volume 19** Kenny B. Lipkowitz, Raima Larter, Thomas R. Cundari, Donald B. Boyd, 2003-10-07 Auch Band 19 dieser seit Jahren bew hrten und erfolgreichen Reihe f hrt Neueinsteiger in moderne Forschungsgebiete der Computerchemie ein und hilft Fachleuten auf dem Laufenden zu bleiben international renommierte Fachleute diskutieren Themen aus den Bereichen Molecular modeling Quantenchemie computergest tztes Molek ldesign CAMD Molek lmechanik und dynamik sowie QSAR Quantitative Struktur Reaktivit ts Beziehungen ausf hrliche Autoren und Sachregister erleichtern die Orientierung Beitr ge sind allgemein verst ndlich geschrieben und enthalten nur das notwendige Minimum an mathematischen Formalismen dadurch ist die Reihe auch geeignet f r Leser die sich nicht haupts chlich mit den genannten Fachgebieten besch ftigen

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**Thermodynamics and Statistical Mechanics of Macromolecular Systems** Michael Bachmann, 2014-04-24 Reviewing statistical mechanics concepts for analysis of macromolecular structure formation processes for graduate students and researchers in physics and biology

**Single-Ion Solvation** Philippe Hunenberger, Maria Reif, 2015-10-20 Ions are ubiquitous in chemical technological ecological and biological processes Characterizing their role in these processes in the first place requires the evaluation of the thermodynamic parameters associated with the solvation of a given ion However due to the constraint of electroneutrality the involvement of surface effects and the ambiguous connection between microscopic and macroscopic descriptions the determination of single ion solvation properties via both experimental and theoretical approaches has turned out to be a very difficult and highly controversial problem This unique book provides an up to date compact and consistent account of the research field of single ion solvation thermodynamics that has over one hundred years of history and still remains largely unsolved By reviewing the

various approaches employed to date establishing the relevant connections between single ion thermodynamics and electrochemistry resolving conceptual ambiguities and giving an exhaustive data compilation in the context of alkali and halide hydration this book provides a consistent synthesis in depth understanding and clarification of a large and sometimes very confusing research field The book is primarily aimed at researchers professors postgraduates graduates and industrial researchers concerned with processes involving ionic solvation properties these are ubiquitous eg in physical organic analytical chemistry electrochemistry biochemistry pharmacology geology and ecology Because of the concept definitions and data compilations it contains it is also a useful reference book to have in a university library Finally it may be of general interest to anyone wanting to learn more about ions and solvation Key features discusses both experimental and theoretical approaches and establishes the connection between them provides both an account of the past research covering over one hundred years and a discussion of current directions in particular on the theoretical side involves a comprehensive reference list of over 2000 citations employs a very consistent notation including table of symbols and unambiguous definitions of all introduced quantities provides a discussion and clarification of ambiguous concepts ie concepts that have not been defined clearly or have been defined differently by different authors leading to confusion in past literature encompasses an exhaustive data compilation in the restricted context of alkali and halide hydration along with recommended values after critical analysis of this literature data is illustrated by a number of synoptic colour figures that will help the reader to grasp the connections between different concepts in one single picture

*Theory of Simple Liquids* Jean-Pierre Hansen, I.R. McDonald, 2013-08-12 Comprehensive coverage of topics in the theory of classical liquids Widely regarded as the standard text in its field *Theory of Simple Liquids* gives an advanced but self contained account of liquid state theory within the unifying framework provided by classical statistical mechanics The structure of this revised and updated Fourth Edition is similar to that of the previous one but there are significant shifts in emphasis and much new material has been added Major changes and Key Features in content include Expansion of existing sections on simulation methods liquid vapour coexistence the hierarchical reference theory of criticality and the dynamics of super cooled liquids New sections on binary fluid mixtures surface tension wetting the asymptotic decay of pair correlations fluids in porous media the thermodynamics of glasses and fluid flow at solid surfaces An entirely new chapter on applications to soft matter of a combination of liquid state theory and coarse graining strategies with sections on polymer solutions and polymer melts colloidal dispersions colloid polymer mixtures lyotropic liquid crystals colloidal dynamics and on clustering and gelation Expansion of existing sections on simulation methods liquid vapour coexistence the hierarchical reference of criticality and the dynamics of super cooled liquids New sections on binary fluid mixtures surface tension wetting the asymptotic decay of pair correlations fluids in porous media the thermodynamics of glasses and fluid flow at solid surfaces An entirely new chapter on applications to soft matter of a combination of liquid state theory and coarse graining strategies with sections on polymer solutions and polymer

melts colloidal dispersions colloid polymer mixtures lyotropic liquid crystals colloidal dynamics and on clustering and gelation     *Lattice simulations of the  $\phi^4$  theory and related systems* Tadeusz Pudlik, 2009



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