

Monte Carlo Simulations In Physics Helsingin

Kinetic Monte Carlo (kMC) simulations still represent a quite new area of research, with a rapidly growing number of publications. Broadly speaking, kMC can be applied to any system describable as a set of minima of a potential-energy surface, the evolution of which will then be regarded as hops from one minimum to a neighboring one. The hops in kMC are modeled as stochastic processes and the algorithms use random numbers to determine at which times the hops occur and to which neighboring minimum they go. Sometimes this approach is also called dynamic MC or Stochastic Simulation Algorithm, in particular when it is applied to solving macroscopic rate equations. This book has two objectives. First, it is a primer on the kMC method (predominantly using the lattice-gas model) and thus much of the book will also be useful for applications other than to surface reactions. Second, it is intended to teach the reader what can be learned from kMC simulations of surface reaction kinetics. With these goals in mind, the present text is conceived as a self-contained introduction for students and non-specialist researchers alike who are interested in entering the field and learning about the topic from scratch.

A practical introduction to the use of probability and statistics in experimental physics for graduate students and advanced undergraduates. Intended as a practical guide, and not as a comprehensive text, the emphasis is on applications and understanding, on theorems and techniques that are actually used in experimental physics. Proofs of theorems are generally omitted unless they contribute to the intuition in understanding and applying the theorem. The problems, many with worked solutions, introduce the student to the use of computers; occasional reference is made to some of the Fortran routines available in the CERN library, but other systems, such as Maple, will also be useful.

This monograph reviews the subject of structural disorder in alloys and describes how structural information can be exploited to build sound theoretical descriptions in terms of modified Ising models. Scattering with thermal neutrons and x-rays prove to be complementary approaches to measure the weak diffuse scattering which provides detailed information about the disorder. The authors show how Monte Carlo methods are applied to determine the most realistic effective interactions among the alloying atoms. These results can be used as a benchmark for modern electronic structure calculations. Of more general interest, the limitations of scattering experiments in a determination of an interaction model, and thus also of the structure itself are discussed. Finally, simulations exhibit not only near-surface disordering due to frustration effects but also new possible surface - induced ordering phenomena. Accurate Monte Carlo simulations are used to test existing theories of wetting.

This book provides an introduction to the use of Monte Carlo computer simulation methods suitable for beginning graduate students and beyond. It is suitable for a course text for physics or chemistry departments or for self-teaching.

Deals with the computer simulation of complex physical systems encountered in condensed-matter physics and statistical mechanics as well as in related fields such as metallurgy, polymer research, lattice gauge theory and quantum mechanics.

This book focuses on the state of the art of Monte Carlo methods in radiation physics and particle transport simulation and applications. Special attention is paid to algorithm development for modeling, and the analysis of experiments and measurements in a variety of fields.

Fully updated with the latest developments in the eigenvalue Monte Carlo calculations and automatic variance reduction techniques and containing an entirely new chapter on fission matrix and alternative hybrid techniques. This second edition explores the uses of the Monte Carlo method for real-world applications, explaining its concepts and limitations. Featuring illustrative examples, mathematical derivations, computer algorithms, and homework problems, it is an ideal textbook and practical guide for nuclear engineers and scientists looking into the applications of the Monte Carlo method, in addition to students in physics and engineering, and those engaged in the advancement of the Monte Carlo methods. Describes general and particle-transport-specific automated variance reduction techniques Presents Monte Carlo particle transport eigenvalue issues and methodologies to address these issues Presents detailed derivation of existing and advanced formulations and algorithms with real-world examples from the author's research activities

In the last three decades, there has been a dramatic increase in the use of interacting particle methods as a powerful tool in real-world applications of Monte Carlo simulation in computational physics, population biology, computer sciences, and statistical machine learning. Ideally suited to parallel and distributed computation, these advanced particle algorithms include nonlinear interacting jump diffusions; quantum, diffusion, and resampled Monte Carlo methods; Feynman-Kac particle models; genetic and evolutionary algorithms; sequential Monte Carlo methods; adaptive and interacting Markov chain Monte Carlo models; bootstrapping methods; ensemble Kalman filters; and interacting particle filters. Mean Field Simulation for Monte Carlo Integration presents the first comprehensive and modern mathematical treatment of mean field particle simulation models and interdisciplinary research topics, including interacting jumps and McKean-Vlasov processes, sequential Monte Carlo methodologies, genetic particle algorithms, genealogical tree-based algorithms, and quantum and diffusion Monte Carlo methods. Along with covering refined convergence analysis on nonlinear Markov chain models, the author discusses applications related to parameter estimation in hidden Markov chain models, stochastic optimization, nonlinear filtering and multiple target tracking, stochastic optimization, calibration and uncertainty propagations in numerical codes, rare event simulation, financial mathematics, and free energy and quasi-invariant measures arising in computational physics and population biology. This book shows how mean field particle simulation has revolutionized the field of Monte Carlo integration and stochastic algorithms. It will help theoretical probability researchers, applied statisticians, biologists, statistical physicists, and computer scientists work better across their own disciplinary

boundaries.

This book describes all aspects of Monte Carlo simulation of complex physical systems encountered in condensed-matter physics and statistical mechanics, as well as in related fields, such as polymer science and lattice gauge theory. The authors give a succinct overview of simple sampling methods and develop the importance sampling method. In addition they introduce 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. The book includes many applications, examples, and current references, and exercises to help the reader.

This book is divided into two parts. In the first part we give an elementary introduction to computational physics consisting of 21 simulations which originated from a formal course of lectures and laboratory simulations delivered since 2010 to physics students at Annaba University. The second part is much more advanced and deals with the problem of how to set up working Monte Carlo simulations of matrix field theories which involve finite dimensional matrix regularizations of noncommutative and fuzzy field theories, fuzzy spaces and matrix geometry. The study of matrix field theory in its own right has also become very important to the proper understanding of all noncommutative, fuzzy and matrix phenomena. The second part, which consists of 9 simulations, was delivered informally to doctoral students who were working on various problems in matrix field theory. Sample codes as well as sample key solutions are also provided for convenience and completeness.

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. This fourth edition has been updated and a new chapter on Monte Carlo simulation of quantum-mechanical problems has been added. To help students in their work a special web server has been installed to host programs and discussion groups (<http://wwwcp.tphys.uni-heidelberg.de>). Prof. Binder was the winner of the Berni J. Alder CECAM Award for Computational Physics 2001.

This accessible textbook and supporting web site use Excel (R) to teach introductory econometrics.

Monte Carlo Simulation in Statistical Physics deals with the computer simulation of many-body systems in condensed-matter physics and related fields. The authors provide an excellent introduction to the theory and practice of this method. 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. It also contains a systematic presentation from which newcomers can learn to perform simulations. This fourth edition has been updated and a new chapter on Monte Carlo simulation of quantum-mechanical problems has been added.

The sixth edition of this highly successful textbook provides a detailed introduction to Monte Carlo simulation in statistical physics, which deals with the computer simulation of many-body systems in condensed matter physics and related fields of physics and beyond (traffic flows, stock market fluctuations, etc.). Using random numbers generated by a computer, these powerful simulation methods calculate probability distributions, making it possible to estimate the thermodynamic properties of various systems. The book describes the theoretical background of these methods, enabling newcomers to perform such simulations and to analyse their results. It features a modular structure, with two chapters providing a basic pedagogic introduction plus exercises suitable for university courses; the remaining chapters cover major recent developments in the field. This edition has been updated with two new chapters dealing with recently developed powerful special algorithms and with finite size scaling tools for the study of interfacial phenomena, which are important for nanoscience. Previous editions have been highly praised and widely used by both students and advanced researchers.

This book is based upon a part of the invited and contributing talks at the 25th International Symposium on Ion-Atom Collisions, ISIAAC (biennial), held on July 23-25, 2017 in Palm Cove, Queensland, Australia. To aid the general reader, all the authors tried to present their chapters in the context of the development of the addressed particular themes and the underlying major ideas and intricacies. Some chapters contain new results that have not been previously published elsewhere. Whenever possible, the authors made their attempts to connect the basic research in atomic and molecular collision physics with some important applications in other branches of physics as well as across the physics borders. It is hoped that the material presented in this book will be interesting and useful to the beginners and specialists alike. The contents and expositions are deemed to be helpful to the beginners in assessing the potential overlap of some of the presented material with their own research themes and this might provide motivations for possible further upgrades. Likewise, specialists could take advantage of these reviews to see where the addressed themes were and where they are going, in order to acknowledge the fruits of the efforts made thus far and actively contribute to tailoring the directions of future research. Overall, this book is truly interdisciplinary. It judiciously combines experiments and theories within particle collision physics on atomic and molecular levels. It presents state-of-the-art fundamental research in this field. It addresses the possibilities for significant and versatile applications outside standard atomic and molecular collision physics ranging from astrophysics, surface as well as cluster physics/chemistry, hadron therapy in medicine and to the chemical industry. It is then, as Volume 2, fully in the spirit of the 'Aims and Scope' of this book series by reference to its 'Mission Statement'.

This is a comprehensive overview of fundamental principles and relevant technical issues associated with the behavior of solids exposed to high-energy radiation. These issues are important to the development of materials for existing fission reactors or future fusion and advanced reactors for energy production; to the development of electronic devices such as high-energy detectors; and to the development of novel materials for electronic and photonic applications.

Dealing with all aspects of Monte Carlo simulation of complex physical systems encountered in condensed-matter physics and statistical mechanics, this book provides an introduction to computer simulations in physics. This edition contains extensive new material describing numerous powerful algorithms not covered in previous editions, in some cases representing new developments that have only recently appeared. Older methodologies whose impact was previously unclear or unappreciated are also introduced, in addition to many small revisions that bring the text and cited literature up to date. This edition

also introduces the use of petascale computing facilities in the Monte Carlo arena. Throughout the book there are many applications, examples, recipes, case studies, and exercises to help the reader understand the material.

Featuring detailed explanations of the major algorithms used in quantum Monte Carlo simulations, this is the first textbook of its kind to provide a pedagogical overview of the field and its applications. The book provides a comprehensive introduction to the Monte Carlo method, its use, and its foundations, and examines algorithms for the simulation of quantum many-body lattice problems at finite and zero temperature. These algorithms include continuous-time loop and cluster algorithms for quantum spins, determinant methods for simulating fermions, power methods for computing ground and excited states, and the variational Monte Carlo method. Also discussed are continuous-time algorithms for quantum impurity models and their use within dynamical mean-field theory, along with algorithms for analytically continuing imaginary-time quantum Monte Carlo data. The parallelization of Monte Carlo simulations is also addressed. This is an essential resource for graduate students, teachers, and researchers interested in quantum Monte Carlo techniques.

Computer simulation is an essential tool in studying the chemistry and physics of liquids. Simulations allow us to develop models and to test them against experimental data. This book is an introduction and practical guide to the molecular dynamics and Monte Carlo methods.

Readership: Researchers and graduate students in high energy physics, solid state physics, nuclear physics and computational physics. Keywords:Lattice Gauge Theories;Monte Carlo Simulations;Phase Structures

From first principles to current computer applications, Monte Carlo Calculations in Nuclear Medicine, Second Edition: Applications in Diagnostic Imaging covers the applications of Monte Carlo calculations in nuclear medicine and critically reviews them from a diagnostic perspective. Like the first edition, this book explains the Monte Carlo method and the principles behind SPECT and PET imaging, introduces the reader to some Monte Carlo software currently in use, and gives the reader a detailed idea of some possible applications of Monte Carlo in current research in SPECT and PET. New chapters in this edition cover codes and applications in pre-clinical PET and SPECT. The book explains how Monte Carlo methods and software packages can be applied to evaluate scatter in SPECT and PET imaging, collimation, and image deterioration. A guide for researchers and students developing methods to improve image resolution, it also demonstrates how Monte Carlo techniques can be used to simulate complex imaging systems.

"Dealing with all aspects of Monte Carlo simulation of complex physical systems encountered in condensed-matter physics and statistical mechanics, this book provides an introduction to computer simulations in physics. This fourth edition contains extensive new material describing numerous powerful algorithms not covered in previous editions, in some cases representing new developments that have only recently appeared. Older methodologies whose impact was previously unclear or unappreciated are also introduced, in addition to many small revisions that bring the text and cited literature up to date. This edition also introduces the use of petascale computing facilities in the Monte Carlo arena"--

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++.

This primer is a comprehensive collection of analytical and numerical techniques that can be used to extract the non-perturbative physics of quantum field theories. The intriguing connection between Euclidean Quantum Field Theories (QFTs) and statistical mechanics can be used to apply Markov Chain Monte Carlo (MCMC) methods to investigate strongly coupled QFTs. The overwhelming amount of reliable results coming from the field of lattice quantum chromodynamics stands out as an excellent example of MCMC methods in QFTs in action. MCMC methods have revealed the non-perturbative phase structures, symmetry breaking, and bound states of particles in QFTs. The applications also resulted in new outcomes due to cross-fertilization with research areas such as AdS/CFT correspondence in string theory and condensed matter physics. The book is aimed at advanced undergraduate students and graduate students in physics and applied mathematics, and researchers in MCMC simulations and QFTs. At the end of this book the reader will be able to apply the techniques learned to produce more independent and novel research in the field.

Looking for the real state of play in computational many-particle physics? Look no further. This book presents an overview of state-of-the-art numerical methods for studying interacting classical and quantum many-particle systems. A broad range of techniques and algorithms are covered, and emphasis is placed on their implementation on modern high-performance computers. This excellent book comes complete with online files and updates allowing readers to stay right up to date.

Monte Carlo simulations comprise a substantial part of the new and third major arm of investigation in the physical sciences that has emerged in recent times, to augment the traditional ones of experiment and theory. With the advent of high-speed digital computing, numerical simulations techniques like Monte Carlo have been very successful in extracting real world observations out of seemingly intractable theoretical models.

Monte Carlo methods have been very prominent in computer simulation of various systems in physics, chemistry, biology, and materials science. This book focuses on the discussion and path-integral quantum Monte Carlo methods in many-body physics and provides a concise but complete introduction to the Metropolis algorithm and its applications in these two techniques. To explore the schemes in clarity, several quantum many-body systems are analysed and studied in detail. The book includes exercises to help digest the materials covered. It can be used as a tutorial to learn the discussion and path-integral Monte Carlo or a recipe for developing new research in the reader's own area. Two complete Java programs, one for the discussion Monte Carlo of 4^{He} clusters on a graphite surface and the other for the path-integral Monte Carlo of cold atoms in a potential trap, are ready for download and adoption.

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.

This volume is an eclectic mix of applications of Monte Carlo methods in many fields of research should not be surprising, because of the ubiquitous use of these methods in many fields of human endeavor. In an attempt to focus attention on a manageable set of applications, the main thrust of this book is to emphasize applications of Monte Carlo simulation methods in biology and medicine.

The Monte Carlo method is now widely used and commonly accepted as an important and useful tool in solid state physics and related fields. It is broadly recognized that the technique of "computer simulation" is complementary to both analytical theory and experiment, and can significantly contribute to advancing the understanding of various scientific problems. Widespread applications of the Monte Carlo method to various fields of the statistical mechanics of condensed matter physics have already been reviewed in two previously published books, namely Monte Carlo Methods in Statistical Physics (Topics Current Phys. , Vol. 7, 1st edn. 1979, 2nd edn. 1986) and Applications of the Monte Carlo Method in Statistical Physics (Topics Current Phys. , Vol. 36, 1st edn. 1984, 2nd edn. 1987). Meanwhile the field has continued its rapid growth and expansion, and applications to new fields have appeared that were not treated at all in the above two books (e. g. studies of irreversible growth phenomena, cellular automata, interfaces, and quantum problems on lattices). Also, new methodic aspects have emerged, such as aspects of efficient use of vector computers or parallel computers, more efficient analysis of simulated systems configurations, and methods to reduce critical slowing down at phase transitions. Taken together with the extensive activity in certain traditional areas of research (simulation of classical and quantum fluids, of macromolecular materials, of spin glasses and quadrupolar glasses, etc.

This book covers the techniques of computer simulations of disordered systems. It describes how one performs Monte Carlo simulations in condensed matter physics and deals with spin-glasses, percolating networks and the random field Ising model. Other methods mentioned are molecular dynamics and Brownian dynamics. Use of flow-diagrams enables the reader to grasp both the problem and its solution more readily. The book deals with highly complicated problems at a relatively simple level and will be most useful for advanced undergraduate and other courses in computational modelling.

In the seven years since this volume first appeared, there has been an enormous expansion of the range of problems to which Monte Carlo computer simulation methods have been applied. This fact has already led to the addition of a companion volume ("Applications of the Monte Carlo Method in Statistical Physics", Topics in Current Physics, Vol. 36), edited in 1984, to this book. But the field continues to develop further; rapid progress is being made with respect to the implementation of Monte Carlo algorithms, the construction of special-purpose computers dedicated to execute Monte Carlo programs, and new methods to analyze the "data" generated by these programs. Brief descriptions of these and other developments, together with numerous additional references, are included in a new chapter, "Recent Trends in Monte Carlo Simulations", which has been written for this second edition. Typographical corrections have been made and fuller references given where appropriate, but otherwise the layout and contents of the other chapters are left unchanged. Thus this book, together with its companion volume mentioned above, gives a fairly complete and up-to-date review of the field. It is hoped that the reduced price of this paperback edition will make it accessible to a wide range of scientists and students in the fields to which it is relevant: theoretical physics and physical chemistry, condensed-matter physics and materials science, computational physics and applied mathematics, etc.

In Monte Carlo Methods in Chemical Physics: An Introduction to the Monte Carlo Method for Particle Simulations J. Ilja Siepmann Random Number Generators for Parallel Applications Ashok Srinivasan, David M. Ceperley and Michael Mascagni Between Classical and Quantum Monte Carlo Methods: "Variational" QMC Dario Bressanini and Peter J. Reynolds Monte Carlo Eigenvalue Methods in Quantum Mechanics and Statistical Mechanics M. P. Nightingale and C.J. Umrigar Adaptive Path-Integral Monte Carlo Methods for Accurate Computation of Molecular Thermodynamic Properties Robert Q. Topper Monte Carlo Sampling for Classical Trajectory Simulations Gilles H. Peslherbe Haobin Wang and William L. Hase Monte Carlo Approaches to the Protein Folding Problem Jeffrey Skolnick and Andrzej Kolinski Entropy Sampling Monte Carlo for Polypeptides and Proteins Harold A. Scheraga and Minh-Hong Hao Macrostate Dissection of Thermodynamic Monte Carlo Integrals Bruce W. Church, Alex Ulitsky, and David Shalloway Simulated Annealing-Optimal Histogram Methods David M. Ferguson and David G. Garrett Monte Carlo Methods for Polymeric Systems Juan J. de Pablo and Fernando A. Escobedo Thermodynamic-Scaling Methods in Monte Carlo and Their Application to Phase Equilibria John Valleau Semigrand Canonical Monte Carlo Simulation: Integration Along Coexistence Lines David A. Kofke Monte Carlo Methods for Simulating Phase Equilibria of Complex Fluids J. Ilja Siepmann Reactive Canonical Monte Carlo J. Karl Johnson New Monte Carlo Algorithms for Classical Spin Systems G. T. Barkema and M.E.J. Newman

Thoroughly updated throughout, this second edition of Monte Carlo Techniques in Radiation Therapy: Applications to Dosimetry, Imaging, and Preclinical Radiotherapy, edited by Joao Seco and Frank Verhaegen, explores the use of Monte Carlo methods for modelling various features of internal and external radiation sources. Monte Carlo methods have

been heavily used in the field of radiation therapy in applications such as dosimetry, imaging, radiation chemistry, modelling of small animal irradiation units, etc. The aim of this book is to provide a compendium of the Monte Carlo methods that are commonly used in radiation therapy applications, which will allow students, postdoctoral fellows, and university professors to learn and teach Monte Carlo techniques. This book provides concise but detailed information about many Monte Carlo applications that cannot be found in any other didactic or scientific book. This second edition contains many new chapters on topics such as: Monte Carlo studies of prompt gamma emission Developments in proton imaging Monte Carlo for cone beam CT imaging Monte Carlo modelling of proton beams for small animal irradiation Monte Carlo studies of microbeam radiation therapy Monte Carlo in micro- and nano-dosimetry GPU-based fast Monte Carlo simulations for radiotherapy This book is primarily aimed at students and scientists wishing to learn and improve their knowledge of Monte Carlo methods in radiation therapy.

This revised fourth edition provides an introduction to computer simulations in physics, cutting-edge algorithms, essential techniques, and petascale computing.

Monte Carlo methods have been used for decades in physics, engineering, statistics, and other fields. Monte Carlo Simulation and Finance explains the nuts and bolts of this essential technique used to value derivatives and other securities. Author and educator Don McLeish examines this fundamental process, and discusses important issues, including specialized problems in finance that Monte Carlo and Quasi-Monte Carlo methods can help solve and the different ways Monte Carlo methods can be improved upon. This state-of-the-art book on Monte Carlo simulation methods is ideal for finance professionals and students. Order your copy today.

Dealing with all aspects of Monte Carlo simulation of complex physical systems encountered in condensed-matter physics and statistical mechanics, this book provides an introduction to computer simulations in physics. This edition now contains material describing powerful new algorithms that have appeared since the previous edition was published, and highlights recent technical advances and key applications that these algorithms now make possible. Updates also include several new sections and a chapter on the use of Monte Carlo simulations of biological molecules. Throughout the book there are many applications, examples, recipes, case studies, and exercises to help the reader understand the material. It is ideal for graduate students and researchers, both in academia and industry, who want to learn techniques that have become a third tool of physical science, complementing experiment and analytical theory.

This updated edition deals with the Monte Carlo simulation of complex physical systems encountered in condensed-matter physics, statistical mechanics, and related fields. It contains many applications, examples, and exercises to help the reader. It is an excellent guide for graduate students and researchers who use computer simulations in their research.

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