Dieter W. Heermann

Computer Simulation Methods

in Theoretical Physics

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Computer Simulation Methods In Theoretical Physics

Mauro Ferrario,Giovanni Ciccotti,Kurt Binder

Computer Simulation Methods In Theoretical Physics:

   Computer Simulation Methods in Theoretical Physics Dieter W. Heermann,2012-12-06 Appropriately for a book having the title Computer Simulation Methods in Theoretical Physics this book begins with a disclai mer It does not and cannot give a complete introduction to simu lational physics This exciting field is too new and is expanding too rapidly for even an attempt to be made The intention here is to present a selection of fundamental techniques that are now being widely applied in many areas of physics mathematics chem istry and biology It is worth noting that the methods are not only applicable in physics They have been successfully used in other sciences showing their great flexibility and power This book has two main chapters Chaps 3 and 4 dealing with deterministic and stochastic computer simulation methods Under the heading deterministic are collected methods involving classical dynamics i e classical equations of motion which have become known as the molecular dynamics simulation method The se cond main chapter deals with methods that are partly or entirely of a stochastic nature These include Brownian dynamics and the Monte Carlo method To aid understanding of the material and to develop intuition problems are included at the end of each chapter Upon a first reading the reader is advised to skip Chapter 2 which is a general introduction to computer simUlation methods   *Computer Simulation Methods in Theoretical Physics* Dieter Heermann,2012-03-14 Computational methods pertaining to many branches of science such as physics physical chemistry and biology are presented The text is primarily intended for third year undergraduate or first year graduate students However active researchers wanting to learn about the new techniques of computational science should also benefit from reading the book It treats all major methods including the powerful molecular dynamics method Brownian dynamics and the Monte Carlo method All methods are treated equally from a theroetical point of view In each case the underlying theory is presented and then practical algorithms are displayed giving the reader the opportunity to apply these methods directly For this purpose exercises are included The book also features complete program listings ready for application   **An Introduction to Computer Simulation Methods** Harvey Gould,Jan Tobochnik,1988   **Computer Simulations of Surfaces and Interfaces** Burkhard Dünweg,David P. Landau,Andrey I. Milchev,2003-12-31 Proceedings of the NATO Advanced Study Institute Albena Bulgaria from 9 to 20 September 2002   *An Introduction to Computer Simulation Methods: Appendices* Harvey Gould,1988   Computer Simulations in Condensed Matter Mauro Ferrario,Institut Fur Physik Kurt Binder,Giovanni Ciccotti,2016-04-01 This comprehensive collection of lectures by leading experts in the field introduces and reviews all relevant computer simulation methods and their applications in condensed matter systems Volume 1 is an in depth introduction to a vast spectrum of computational techniques for statistical mechanical systems of condensed matter Volume 2 is a collection of state of the art surveys on numerical experiments carried out for a great number of systems   **Monte Carlo and Molecular Dynamics Simulations in Polymer Science** Kurt Binder,1995 Talks about various computer simulation techniques used for macromolecular materials This book describes how to use simulation to

explain experimental data and gain insight into structure and dynamic properties of polymeric structures Explanations are given on how to overcome challenges posed by large size and slow relaxation polymer coils   Computational Materials Science A.M. Ovrutsky,A. S Prokhoda,M.S. Rasshchupkyna,2013-11-19 Computational Materials Science provides the theoretical basis necessary for understanding atomic surface phenomena and processes of phase transitions especially crystallization is given The most important information concerning computer simulation by different methods and simulation techniques for modeling of physical systems is also presented A number of results are discussed regarding modern studies of surface processes during crystallization There is sufficiently full information on experiments theory and simulations concerning the surface roughening transition kinetic roughening nucleation kinetics stability of crystal shapes thin film formation imperfect structure of small crystals size dependent growth velocity distribution coefficient at growth from alloy melts superstructure ordering in the intermetallic compound Computational experiments described in the last chapter allow visualization of the course of many processes and better understanding of many key problems in Materials Science There is a set of practical steps concerning computational procedures presented Open access to executable files in the book make it possible for everyone to understand better phenomena and processes described in the book Valuable reference book but also helpful as a supplement to courses Computer programs available to supplement examples Presents several new methods of computational materials science and clearly summarizes previous methods and results   *Understanding Molecular Simulation* Daan Frenkel,Berend Smit,2023-07-13 Understanding Molecular Simulation explains molecular simulation from a chemical physics and statistical mechanics perspective It highlights how physical concepts are used to develop better algorithms and expand the range of applicability of simulations Understanding Molecular Simulation is equally relevant for those who develop new code and those who use existing packages Both groups are continuously confronted with the question of which computational technique best suits a given application Understanding Molecular Simulation provides readers with the foundational knowledge they need to learn about select and apply the most appropriate of these tools to their own work The implementation of simulation methods is illustrated in pseudocodes and their practical use is shown via case studies presented throughout the text Since the second edition s publication the simulation world has expanded significantly existing techniques have continued to develop and new ones have emerged opening up novel application areas This new edition aims to describe these new developments without becoming exhaustive examples are included that highlight current uses and several new examples have been added to illustrate recent applications Examples case studies questions and downloadable algorithms are also included to support learning No prior knowledge of computer simulation is assumed Fully updated guide to both the current state and latest developments in the field of molecular simulation including added and expanded information on such topics as molecular dynamics and statistical assessment of simulation results Gives a rounded overview by showing fundamental background information in practice via new examples in a range of key fields Provides online access

to new data algorithms and tutorial slides to support and encourage practice and learning *Computer Meets Theoretical Physics* Giovanni Battimelli,Giovanni Ciccotti,Pietro Greco,2020-06-17 This book provides a vivid account of the early history of molecular simulation a new frontier for our understanding of matter that was opened when the demands of theoretical physicists were met by the availability of the modern computers Since their inception electronic computers have enormously increased their performance thus making possible the unprecedented technological revolution that characterizes our present times This obvious technological advancement has brought with it a silent scientific revolution in the practice of theoretical physics In particular in the physics of matter it has opened up a direct route from the microscopic physical laws to observable phenomena One can now study the time evolution of systems composed of millions of molecules and simulate the behaviour of macroscopic materials and actually predict their properties Molecular simulation has provided a new theoretical and conceptual tool that physicists could only dream of when the foundations of statistical mechanics were laid Molecular simulation has undergone impressive development both in the size of the scientific community involved and in the range and scope of its applications It has become the ubiquitous workhorse for investigating the nature of complex condensed matter systems in physics chemistry materials and the life sciences Yet these developments remain largely unknown outside the inner circles of practitioners and they have so far never been described for a wider public The main objective of this book is therefore to offer a reasonably comprehensive reconstruction of the early history of molecular simulation addressed to an audience of both scientists and interested non scientists describing the scientific and personal trajectories of the main protagonists and discussing the deep conceptual innovations that their work produced **Computational Physics** Philipp Scherer,2013-07-17 This textbook presents basic and advanced computational physics in a very didactic style It contains very well presented and simple mathematical descriptions of many of the most important algorithms used in computational physics The first part of the book discusses the basic numerical methods The second part concentrates on simulation of classical and quantum systems Several classes of integration methods are discussed including not only the standard Euler and Runge Kutta method but also multi step methods and the class of Verlet methods which is introduced by studying the motion in Liouville space A general chapter on the numerical treatment of differential equations provides methods of finite differences finite volumes finite elements and boundary elements together with spectral methods and weighted residual based methods The book gives simple but non trivial examples from a broad range of physical topics trying to give the reader insight into not only the numerical treatment but also simulated problems Different methods are compared with regard to their stability and efficiency The exercises in the book are realised as computer experiments **Computational Multiscale Modeling of Fluids and Solids** Martin Oliver Steinhauser,2016-11-29 The idea of the book is to provide a comprehensive overview of computational physics methods and techniques that are used for materials modeling on different length and time scales Each chapter first provides an overview of the basic physical principles which are the basis for the numerical and

mathematical modeling on the respective length scale The book includes the micro scale the meso scale and the macro scale and the chapters follow this classification The book explains in detail many tricks of the trade of some of the most important methods and techniques that are used to simulate materials on the perspective levels of spatial and temporal resolution Case studies are included to further illustrate some methods or theoretical considerations Example applications for all techniques are provided some of which are from the author s own contributions to some of the research areas The second edition has been expanded by new sections in computational models on meso macroscopic scales for ocean and atmosphere dynamics Numerous applications in environmental physics and geophysics had been added **Encyclopedia of Bioinformatics and Computational Biology** ,2018-08-21 Encyclopedia of Bioinformatics and Computational Biology ABC of Bioinformatics Three Volume Set combines elements of computer science information technology mathematics statistics and biotechnology providing the methodology and in silico solutions to mine biological data and processes The book covers Theory Topics and Applications with a special focus on Integrative omics and Systems Biology The theoretical methodological underpinnings of BCB including phylogeny are covered as are more current areas of focus such as translational bioinformatics cheminformatics and environmental informatics Finally Applications provide guidance for commonly asked questions This major reference work spans basic and cutting edge methodologies authored by leaders in the field providing an invaluable resource for students scientists professionals in research institutes and a broad swath of researchers in biotechnology and the biomedical and pharmaceutical industries Brings together information from computer science information technology mathematics statistics and biotechnology Written and reviewed by leading experts in the field providing a unique and authoritative resource Focuses on the main theoretical and methodological concepts before expanding on specific topics and applications Includes interactive images multimedia tools and crosslinking to further resources and databases

Computational Physics Philipp O.J. Scherer,2017-09-07 This textbook presents basic numerical methods and applies them to a large variety of physical models in multiple computer experiments Classical algorithms and more recent methods are explained Partial differential equations are treated generally comparing important methods and equations of motion are solved by a large number of simple as well as more sophisticated methods Several modern algorithms for quantum wavepacket motion are compared The first part of the book discusses the basic numerical methods while the second part simulates classical and quantum systems Simple but non trivial examples from a broad range of physical topics offer readers insights into the numerical treatment but also the simulated problems Rotational motion is studied in detail as are simple quantum systems A two level system in an external field demonstrates elementary principles from quantum optics and simulation of a quantum bit Principles of molecular dynamics are shown Modern boundary element methods are presented in addition to standard methods and waves and diffusion processes are simulated comparing the stability and efficiency of different methods A large number of computer experiments is provided which can be tried out even by readers with no

programming skills Exercises in the applets complete the pedagogical treatment in the book In the third edition Monte Carlo methods and random number generation have been updated taking recent developments into account Krylov space methods for eigenvalue problems are discussed in much more detail Short time Fourier transformation and wavelet transformation have been included as tools for time frequency analysis Lastly elementary quantum many body problems demonstrate the application of variational and Monte Carlo methods **Monte Carlo Methods in Statistical Physics** Kurt Binder,2012-12-06 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 exe cute Monte Carlo programs and new methods to analyze the data generated by these programs Brief descriptions of these and other developments together with numerous addi tional references are included in a new chapter Recent Trends in Monte Carlo Simulations which has been written for this second edition Typographical correc tions 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 con densed matter physics and materials science computational physics and applied mathematics etc **Monte Carlo Simulation in Statistical Physics** Kurt Binder,Dieter W. Heermann,2019-04-30 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 finitesize 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 **Computer Simulations in Condensed Matter: From Materials to Chemical Biology** Mauro Ferrario,Giovanni Ciccotti,Kurt Binder,2006-11-13 This comprehensive collection of lectures by leading experts in the field introduces and

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Simulation Methods for Polymers Michael Kotelyanskii,Doros N. Theodorou,2004-03-01 *Computer Simulations in Condensed Matter: From Materials to Chemical Biology. Volume 2* Mauro Ferrario,Giovanni Ciccotti,Kurt Binder,2007-04-16 This extensive and comprehensive collection of lectures by world leading experts in the field introduces and reviews all relevant computer simulation methods and their applications in condensed matter systems Volume 2 offers surveys on numerical experiments carried out for a great number of systems ranging from materials sciences to chemical biology including supercooled liquids spin glasses colloids polymers liquid crystals biological membranes and folding proteins

Computational Multiscale Modeling of Fluids and Solids Martin Oliver Steinhauser,2008 The idea of the book is to provide a comprehensive overview of computational physics methods and techniques that are used for materials modeling on different length and time scales Each chapter first provides an overview of the physical basic principles which are the basis for the numerical and mathematical modeling on the respective length scale The book includes the micro scale the meso scale and the macro scale The chapters follow this classification The book will explain in detail many tricks of the trade of some of the most important methods and techniques that are used to simulate materials on the perspective levels of spatial and temporal resolution Case studies are occasionally included to further illustrate some methods or theoretical considerations Example applications for all techniques are provided some of which are from the author s own contributions to some of the research areas Methods are explained if possible on the basis of the original publications but also references to standard text books established in the various fields are mentioned

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