

Graduate Texts in Physics

Philipp O.J. Scherer

Computational Physics

Simulation of Classical and Quantum Systems

Second Edition



 Springer

Computational Physics Simulation Of Classical And Quantum Systems Graduate Texts In Physics

Philipp Scherer



Computational Physics Simulation Of Classical And Quantum Systems Graduate Texts In Physics:

Computational Physics Philipp O.J. Scherer,2017 *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 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 **Computational**

Physics II Philipp O. J. Scherer,2025-12-06 This book presents basic numerical methods and applies them to a large variety of physical models in multiple computer experiments Authored by a distinguished expert in the field it combines rigorous theoretical insights with a wealth of practical and easily accessible computational applications This book serves as an ideal

standalone text for computational physics courses at both the graduate and advanced undergraduate levels It offers a detailed and cohesive exploration of the physics of classical and quantum systems electrostatics thermodynamics statistical physics and nonlinear systems integrating foundational principles with advanced simulation techniques The significantly expanded and updated fourth edition comprises two volumes Volume 2 deals with the simulation of classical and quantum systems covering key areas such as rotational motion and molecular mechanics thermodynamic systems Brownian motion and diffusion electrostatics and nonlinear systems It also features a detailed look at simple quantum systems and introduces variational quantum Monte Carlo for calculating ground state energies in quantum systems including the helium atom and hydrogen molecule and time dependent wave functions New in this book are two new chapters on novel and unconventional simulation methods The first focuses on physics informed machine learning methods applying artificial neural networks ANNs to solve and discover differential equations based on a given data set or Hamilton's equations of motion while ensuring energy conservation It presents the idea of a Boltzmann machine which learns and reproduces a given probability distribution and is also useful to provide a trial function for quantum spin systems Neural network quantum states NNQS are explained and optimized by the method of stochastic reconfiguration The second explores the simulation of physical systems using real quantum systems thus redefining the scope of computational physics This includes examples of adiabatic quantum computing AQS and quantum annealing QA with application to quadratic unconstrained binary optimization QUBO and Boolean satisfiability problems SAT Additionally this book introduces tensor networks and path integral methods as mathematical methods to reduce the exponentially growing configuration space to its most relevant parts and efficiently simulate quantum annealing SQA on a classical computer

[Applying Machine Learning in Science Education Research](#)
Peter Wulff, Marcus Kubsch, Christina Krist, 2025-02-28 This open access textbook offers science education researchers a hands on guide for learning critically examining and integrating machine learning ML methods into their science education research projects These methods power many artificial intelligence AI based technologies and are widely adopted in science education research ML can expand the methodological toolkit of science education researchers and provide novel opportunities to gain insights on science related learning and teaching processes however applying ML poses novel challenges and is not suitable for every research context The volume first introduces the theoretical underpinnings of ML methods and their connections to methodological commitments in science education research It then presents exemplar case studies of ML uses in both formal and informal science education settings These case studies include open source data executable programming code and explanations of the methodological criteria and commitments guiding ML use in each case The textbook concludes with a discussion of opportunities and potential future directions for ML in science education This textbook is a valuable resource for science education lecturers researchers under graduate graduate and postgraduate students seeking new ways to apply ML in their work

[Quantum Mechanics](#) Mark Julian Everitt, Kieran Niels

Bjergstrom, Stephen Neil Alexander Duffus, 2023-09-08 **QUANTUM MECHANICS** From classical analytical mechanics to quantum mechanics simulation foundations engineering Quantum mechanics is a fundamental and conceptually challenging area of physics It is usually assumed that students are unfamiliar with Lagrangian and Hamiltonian formulations of classical mechanics and the role played by probability As a result quantum physics is typically introduced using heuristic arguments obscuring synergies with classical mechanics This book takes an alternative approach by leveraging classical analytical mechanics to facilitate a natural transition to quantum physics By doing so a solid foundation for understanding quantum phenomena is provided Key features of this textbook include Mathematics and Classical Analytical Mechanics The necessary mathematical background and classical analytical mechanics are introduced gradually allowing readers to focus on one conceptual challenge at a time Deductive Approach Quantum mechanics is presented on the firm foundation of classical analytical mechanics ensuring a logical progression of concepts Pedagogical Features This book includes helpful notes worked examples problems computational challenges and problem solving approaches to enhance understanding Comprehensive Coverage Including advanced topics such as open quantum systems phase space methods and computational methods for quantum physics including good programming practice and code design Much of the code needed to reproduce figures throughout this book is included Consideration of Foundations The measurement problem and correspondence principle are addressed including an open and critical discussion of their interpretation and consequences Introduction to Quantum Systems Engineering This is the first book to introduce Quantum Systems Engineering approaches for applied quantum technologies development This textbook is suitable for undergraduate students in physics and graduate students in mathematics chemistry engineering and materials science **Applied Computational Physics** Joseph F. Boudreau, Eric Scott Swanson, 2018 A textbook that addresses a wide variety of problems in classical and quantum physics Modern programming techniques are stressed throughout along with the important topics of encapsulation polymorphism and object oriented design Scientific problems are physically motivated solution strategies are developed and explicit code is presented

Elements of Statistical Mechanics Ivo Sachs, Siddhartha Sen, James Sexton, 2006-05-11 This 2006 textbook provides a concise introduction to the key concepts and tools of statistical mechanics It also covers advanced topics such as non relativistic quantum field theory and numerical methods After introducing classical analytical techniques such as cluster expansion and Landau theory the authors present important numerical methods with applications to magnetic systems Lennard Jones fluids and biophysics Quantum statistical mechanics is discussed in detail and applied to Bose Einstein condensation and topics in astrophysics and cosmology In order to describe emergent phenomena in interacting quantum systems canonical non relativistic quantum field theory is introduced and then reformulated in terms of Feynman integrals Combining the authors many years experience of teaching courses in this area this textbook is ideal for advanced undergraduate and graduate students in physics chemistry and mathematics **Computational Multiscale Modeling of**

Fluids and Solids Martin Oliver Steinhauser, 2022-07-28 The expanded 3rd edition of this established textbook offers an updated overview and review of the computational physics techniques used in materials modelling over different length and time scales. It describes in detail the theory and application of some of the most important methods used to simulate materials across the various levels of spatial and temporal resolution. Quantum mechanical methods such as the Hartree Fock approximation for solving the Schrödinger equation at the smallest spatial resolution are discussed as well as the Molecular Dynamics and Monte Carlo methods on the micro and meso scale up to macroscopic methods used predominantly in the Engineering world such as Finite Elements FE or Smoothed Particle Hydrodynamics SPH. Extensively updated throughout this new edition includes additional sections on polymer theory, statistical physics and continuum theory, the latter being the basis of FE methods and SPH. Each chapter now first provides an overview of the key topics covered with a new key points section at the end. The book is aimed at beginning or advanced graduate students who want to enter the field of computational science on multi scales. It provides an in depth overview of the basic physical, mathematical and numerical principles for modelling solids and fluids on the micro, meso and macro scale. With a set of exercises, selected solutions and several case studies, it is a suitable book for students in physics, engineering and materials science and a practical reference resource for those already using materials modelling and computational methods in their research. [Computational Modeling And Simulations Of Biomolecular Systems](#)

Benoit Roux, 2021-08-23 This textbook originated from the course Simulation Modeling and Computations in Biophysics that I have taught at the University of Chicago since 2011. The students typically came from a wide range of backgrounds including biology, physics, chemistry, biochemistry and mathematics and the course was intentionally adapted for senior undergraduate students and graduate students. This is not a highly technical book dedicated to specialists. The objective is to provide a broad survey from the physical description of a complex molecular system at the most fundamental level to the type of phenomenological models commonly used to represent the function of large biological macromolecular machines. The key conceptual elements serving as building blocks in the formulation of different levels of approximations are introduced along the way, aiming to clarify as much as possible how they are interrelated. The only assumption is a basic familiarity with simple mathematics: calculus and integrals, ordinary differential equations, matrix, linear algebra and Fourier Laplace transforms.

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