

Computational Physics II

Simulation of Classical and Quantum Systems

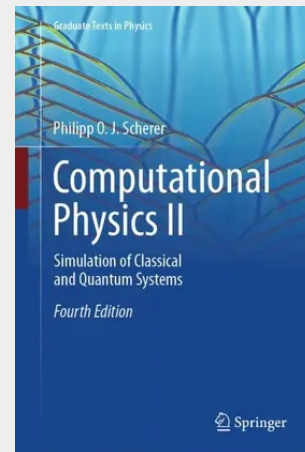
This book presents basic numerical methods and applies them to a large variety of physical models in multiple computer experiments. Authored by a distinguished expert in the field, it combines rigorous theoretical insights with a wealth of practical and easily accessible computational applications. This 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.

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106,99 €
99,99 € (zzgl. MwSt.)

vorbestellbar, Erscheinungstermin ca. August 2026

Artikelnummer: 9783032078513
Medium: Buch
ISBN: 978-3-032-07851-3
Verlag: Springer Nature Switzerland AG
Erscheinungstermin: 17.07.2026
Sprache(n): Englisch
Auflage: Fourth Auflage 2026
Serie: Graduate Texts in Physics
Produktform: Gebunden
Seiten: 419
Format (B x H): 155 x 235 mm

