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Soggetti	Physics Applied mathematics Engineering mathematics Computer science - Mathematics Chemistry, Physical and theoretical Numerical and Computational Physics, Simulation Mathematical and Computational Engineering Computational Mathematics and Numerical Analysis Theoretical and Computational Chemistry
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Nota di contenuto	Some Basic Remarks -- Part I Deterministic Methods -- Numerical Differentiation -- Numerical Integration -- The KEPLER Problem -- Ordinary Differential Equations – Initial Value Problems -- The Double Pendulum -- Molecular Dynamics -- Numerics of Ordinary Differential Equations - Boundary Value Problems -- The One-Dimensional Stationary Heat Equation -- The One-Dimensional Stationary SCHRÖDINGER Equation -- Partial Differential Equations -- Part II Stochastic Methods -- Pseudo Random Number Generators -- Random Sampling Methods -- A Brief Introduction to Monte-Carlo Methods -- The ISING Model -- Some Basics of Stochastic Processes -- The Random Walk and Diffusion Theory -- MARKOV-Chain Monte Carlo and the POTTS Model -- Data Analysis -- Stochastic Optimization -- Appendix: The Two-Body Problem -- Solving Non-Linear Equations. The NEWTON Method -- Numerical Solution of Systems of Equations --

Fast Fourier Transform -- Basics of Probability Theory -- Phase Transitions -- Fractional Integrals and Derivatives in 1D -- Least Squares Fit -- Deterministic Optimization.

Sommario/riassunto

This new edition is a concise introduction to the basic methods of computational physics. Readers will discover the benefits of numerical methods for solving complex mathematical problems and for the direct simulation of physical processes. The book is divided into two main parts: Deterministic methods and stochastic methods in computational physics. Based on concrete problems, the first part discusses numerical differentiation and integration, as well as the treatment of ordinary differential equations. This is extended by a brief introduction to the numerics of partial differential equations. The second part deals with the generation of random numbers, summarizes the basics of stochastics, and subsequently introduces Monte-Carlo (MC) methods. Specific emphasis is on MARKOV chain MC algorithms. The final two chapters discuss data analysis and stochastic optimization. All this is again motivated and augmented by applications from physics. In addition, the book offers a number of appendices to provide the reader with information on topics not discussed in the main text. Numerous problems with worked-out solutions, chapter introductions and summaries, together with a clear and application-oriented style support the reader. Ready to use C++ codes are provided online.