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Nota di contenuto	Preface; Preface to the First Edition; Contents; Glossary of Technical Terms; 1. Time Reversibility, Computer Simulation, Algorithms, Chaos; 1.1 Microscopic Reversibility; Macroscopic Irreversibility; 1.2 Time Reversibility of Irreversible Processes; 1.3 Classical Microscopic and Macroscopic Simulation; 1.4 Continuity, Information, and Bit Reversibility; 1.5 Instability and Chaos; 1.6 Simple Explanations of Complex Phenomena; 1.7 The Paradox: Irreversibility from Reversible Dynamics; 1.8 Algorithm: Fourth-Order Runge-Kutta Integrator; 1.9 Example Problems; 1.9.1 Equilibrium Baker Map 1.9.2 Equilibrium Galton Board 1.9.3 Equilibrium Hookean Pendulum; 1.9.4 Nose-Hoover Oscillator with a Temperature Gradient; 1.10 Summary and Notes; 1.10.1 Notes and References; 2. Time-Reversibility in Physics and Computation; 2.1 Introduction; 2.2 Time Reversibility; 2.3 Levesque and Verlet's Bit-Reversible Algorithm; 2.4 Lagrangian and Hamiltonian Mechanics; 2.5 Liouville's Incompressible Theorem; 2.6 What Is Macroscopic Thermodynamics?; 2.7 First and Second Laws of Thermodynamics; 2.8 Temperature, Zeroth Law, Reservoirs, Thermostats 2.9 Irreversibility from Stochastic Irreversible Equations 2.10 Irreversibility from Time-Reversible Equations?; 2.11 An Algorithm Implementing Bit-Reversible Dynamics; 2.12 Example Problems; 2.12.1

Time-Reversible Dissipative Map; 2.12.2 A Smooth-Potential Galton Board; 2.13 Summary; 2.13.1 Notes and References; 3. Gibbs' Statistical Mechanics; 3.1 Scope and History; 3.2 Formal Structure of Gibbs' Statistical Mechanics; 3.3 Initial Conditions, Boundary Conditions, Ergodicity; 3.4 From Hamiltonian Dynamics to Gibbs' Probability; 3.5 From Gibbs' Probability to Thermodynamics
3.6 Pressure and Energy from Gibbs' Canonical Ensemble
3.7 Gibbs' Entropy versus Boltzmann's Entropy; 3.8 Number-Dependence and Thermodynamic Fluctuations; 3.9 Green and Kubo's Linear-Response Theory; 3.10 An Algorithm for Local Smooth-Particle Averages; 3.11 Example Problems; 3.11.1 Quasiharmonic Thermodynamics; 3.11.2 Hard-Disk and Hard-Sphere Thermodynamics; 3.11.3 Time-Reversible Confined Free Expansion; 3.12 Summary; 3.12.1 Notes and References; 4. Irreversibility in Real Life; 4.1 Introduction; 4.2 Phenomenology - the Linear Dissipative Laws
4.3 Microscopic Basis of the Irreversible Linear Laws
4.4 Solving the Linear Macroscopic Equations; 4.5 Nonequilibrium Entropy Changes; 4.6 Fluctuations and Nonequilibrium States; 4.7 Deviations from the Phenomenological Linear Laws; 4.8 Causes of Irreversibility a la Boltzmann and Lyapunov; 4.9 Rayleigh-Benard Algorithm with Atomistic Flow; 4.10 Rayleigh-Benard Algorithm for a Continuum; 4.11 Three Rayleigh-Benard Example Problems; 4.11.1 Rayleigh-Benard Flow via Lorenz' Attractor; 4.11.2 Rayleigh-Benard Flow with Continuum Mechanics; 4.11.3 Rayleigh-Benard Flow with Molecular Dynamics
4.12 Summary

Sommario/riassunto

A small army of physicists, chemists, mathematicians, and engineers has joined forces to attack a classic problem, the "reversibility paradox", with modern tools. This book describes their work from the perspective of computer simulation, emphasizing the authors' approach to the problem of understanding the compatibility, and even inevitability, of the irreversible second law of thermodynamics with an underlying time-reversible mechanics. Computer simulation has made it possible to probe reversibility from a variety of directions and "chaos theory" or "nonlinear dynamics" has supplied a useful
