

Contents

Frontispiece and Dedication	v
Preface	vii
Chapter 1 Time Reversibility, Computer Simulation, Chaos	1
1.1 Microscopic Time Reversibility and Macroscopic Irreversibility	1
1.2 Time-Reversible Theories of Irreversible Processes	6
1.3 Classical Microscopic and Macroscopic Simulation	8
1.4 Continuity, Information, and Bit Reversibility	9
1.5 Instability and Chaos	11
1.6 Simple Explanations of Complex Phenomena	13
1.7 Reversibility Paradox: Irreversibility from Reversible Dynamics	15
1.8 Example Problems	16
1.8.1 Equilibrium Baker Map	16
1.8.2 Equilibrium Galton Board	21
1.8.3 Equilibrium Hookean Pendulum	25
1.9 Summary	27
Chapter 2 Time-Reversibility in Physics and Computation	29
2.1 Introduction	29
2.2 Time Reversibility	31
2.3 Levesque and Verlet's Bit-Reversible Algorithm	33
2.4 Lagrangian and Hamiltonian Mechanics	36
2.5 Liouville's Incompressible Theorem	38
2.6 What <i>is</i> Macroscopic Thermodynamics?	39
2.7 First and Second Laws of Thermodynamics	41

2.8	Temperature, Zeroth Law, Reservoirs, and Thermostats	43
2.9	Irreversibility from Stochastic Irreversible Equations	47
2.10	Irreversibility from Time-Reversible Equations?	50
2.11	Example Problems	51
	2.11.1 Time-Reversible Dissipative Map	52
	2.11.2 Time-Reversible Smooth Galton Board	57
2.12	Summary	58
Chapter 3 Gibbs' Statistical Mechanics		61
3.1	Introduction	61
3.2	Formal Structure of Statistical Mechanics	63
3.3	Initial Conditions, Boundary Conditions, Ergodicity	66
3.4	From Hamiltonian Dynamics to Gibbs' Probability	69
3.5	From Gibbs' Probability to Thermodynamics	71
3.6	Pressure and Energy from Gibbs' Canonical Ensemble	73
3.7	Gibbs' Entropy <i>versus</i> Boltzmann's Entropy	74
3.8	Number-Dependence and Thermodynamic Fluctuations	77
3.9	Green and Kubo's Linear-Response Theory	77
3.10	Example Problems	79
	3.10.1 Quasiharmonic Thermodynamics	80
	3.10.2 Hard-Sphere Thermodynamics	82
	3.10.3 Time-Reversible Confined Free Expansion	84
3.11	Summary	87
Chapter 4 Irreversibility in Real Life		89
4.1	Introduction	89
4.2	The Phenomenological Linear Laws	92
4.3	Microscopic Basis of Linear Irreversibility	93
4.4	Solving the Linear Macroscopic Equations	95
4.5	Nonequilibrium Entropy Changes	96
4.6	Fluctuations and Nonequilibrium States	99
4.7	Deviations from the Phenomenological Linear Laws	101
4.8	Causes of Irreversibility à la Boltzmann and Lyapunov	102
4.9	Example Problems	104
	4.9.1 Rayleigh-Bénard Flow <i>via</i> Lorenz' Attractor	105
	4.9.2 Rayleigh-Bénard Flow with Atoms	106
4.10	Summary	109

Chapter 5	Microscopic Computer Simulation	111
5.1	Introduction	111
5.2	Integrating the Motion Equations	112
5.3	Interpretation of Results	113
5.4	Control of a Falling Particle	115
5.5	Liouville's Theorems and Nonequilibrium Stability	118
5.6	Second Law of Thermodynamics	123
5.7	Simulating Shear Flow and Heat Flow	123
5.8	Shockwaves	128
5.9	Example Problems	130
5.9.1	Isokinetic Nonequilibrium Galton Board	130
5.9.2	Heat-Conducting One-Dimensional Oscillator	134
5.9.3	Many-Body Heat Flow	137
5.10	Summary	139
Chapter 6	Macroscopic Computer Simulation	141
6.1	Introduction	141
6.2	Continuity and Coordinate Systems	143
6.3	Macroscopic Flow Variables	145
6.4	Finite-Difference Methods	146
6.5	Finite-Element Methods	148
6.6	Smooth Particle Applied Mechanics	150
6.7	Example Problems	153
6.7.1	Rayleigh-Bénard Flow with Finite Differences	154
6.7.2	Rayleigh-Bénard Flow with Smooth Particles	158
6.8	Summary	161
Chapter 7	Chaos, Lyapunov Instability, Fractals	163
7.1	Introduction	163
7.2	Continuum Mathematics	167
7.3	Chaos	168
7.4	Spectrum of Lyapunov Exponents	169
7.5	Fractal Dimensions	175
7.6	A Simple Ergodic Fractal	178
7.7	Fractal Attractor-Repellor Pairs	180
7.8	A Global Second Law from Reversible Chaos	182
7.9	Coarse-Grained and Fine-Grained Entropy	187
7.10	Example Problems	189

7.10.1	Chaotic Double Pendulum	190
7.10.2	Coarse-Grained Galton Board Entropy	191
7.10.3	Heat-Conducting Harmonic Oscillator	193
7.10.4	Color Conductivity	194
7.11	Summary	198
Chapter 8 Resolving the Reversibility Paradox		199
8.1	Introduction	199
8.2	Irreversibility from Boltzmann's Kinetic Theory	200
8.3	Boltzmann's Equation Today	205
8.4	Gibbs' Statistical Mechanics	207
8.5	Jaynes' Information Theory	210
8.6	Green and Kubo's Linear Response Theory	211
8.7	Thermomechanics	213
8.8	Are Initial Conditions Relevant?	215
8.9	Constrained Hamiltonian Ensembles	218
8.10	Anosov Systems and Sinai-Ruelle-Bowen Measures	219
8.11	Trajectories <i>versus</i> Distribution Functions	222
8.12	Are Maps Relevant?	223
8.13	Irreversibility from Time-Reversible Motion Equations	224
8.14	Summary	226
Chapter 9 Afterword—a Research Perspective		229
9.1	Introduction	229
9.2	What do we know?	230
9.3	Why Reversibility is Still a Problem	232
9.4	Change and Innovation	235
9.5	Rôle of Examples	238
9.6	Rôle of Chaos and Fractals	240
9.7	Rôle of Mathematics	240
9.8	Remaining Puzzles	242
9.9	Summary	245
9.10	Acknowledgments	247
Glossary of Technical Terms		249
Alphabetical Bibliography		253
Index		259