Contents

Preface **ix**

About the Authors **xii**

1 A First Numerical Problem **1**
1.1 Radioactive Decay . . . 1
1.2 A Numerical Approach . . . 2
1.3 Design and Construction of a Working Program: Codes and Pseudocodes . . . 3
1.4 Testing Your Program . . . 11
1.5 Numerical Considerations . . . 12
1.6 Programming Guidelines and Philosophy . . . 14

2 Realistic Projectile Motion **18**
2.1 Bicycle Racing: The Effect of Air Resistance . . . 18
2.2 Projectile Motion: The Trajectory of a Cannon Shell . . . 25
2.3 Baseball: Motion of a Batted Ball . . . 31
2.4 Throwing a Baseball: The Effects of Spin . . . 36
2.5 Golf . . . 44

3 Oscillatory Motion and Chaos **48**
3.1 Simple Harmonic Motion . . . 48
3.2 Making the Pendulum More Interesting: Adding Dissipation, Nonlinearity, and a Driving Force . . . 54
3.3 Chaos in the Driven Nonlinear Pendulum . . . 58
3.4 Routes to Chaos: Period Doubling . . . 66
3.5 The Logistic Map: Why the Period Doubles . . . 70
3.6 The Lorenz Model . . . 75
3.7 The Billiard Problem . . . 82
3.8 Behavior in the Frequency Domain: Chaos and Noise . . . 88

4 The Solar System **94**
4.1 Kepler's Laws . . . 94
4.2 The Inverse-Square Law and the Stability of Planetary Orbits . . . 101
4.3 Precession of the Perihelion of Mercury . . . 107
4.4 The Three-Body Problem and the Effect of Jupiter on Earth . . . 113
4.5 Resonances in the Solar System: Kirkwood Gaps and Planetary Rings . . . 118
4.6 Chaotic Tumbling of Hyperion . . . 123

5 Potentials and Fields **129**
5.1 Electric Potentials and Fields: Laplace's Equation 129
5.2 Potentials and Fields Near Electric Charges 143
5.3 Magnetic Field Produced by a Current 148
5.4 Magnetic Field of a Solenoid: Inside and Out 151

6 Waves **156**
6.1 Waves: The Ideal Case 156
6.2 Frequency Spectrum of Waves on a String 165
6.3 Motion of a (Somewhat) Realistic String 169
6.4 Waves on a String (Again): Spectral Methods 174

7 Random Systems **181**
7.1 Why Perform Simulations of Random Processes? 181
7.2 Random Walks 183
7.3 Self-Avoiding Walks 188
7.4 Random Walks and Diffusion 195
7.5 Diffusion, Entropy, and the Arrow of Time 201
7.6 Cluster Growth Models 206
7.7 Fractal Dimensionalities of Curves 212
7.8 Percolation 218
7.9 Diffusion on Fractals 229

8 Statistical Mechanics, Phase Transitions, and the Ising Model **235**
8.1 The Ising Model and Statistical Mechanics 235
8.2 Mean Field Theory 239
8.3 The Monte Carlo Method 244
8.4 The Ising Model and Second-Order Phase Transitions 246
8.5 First-Order Phase Transitions 259
8.6 Scaling 264

9 Molecular Dynamics **270**
9.1 Introduction to the Method: Properties of a Dilute Gas 270
9.2 The Melting Transition 285
9.3 Equipartition and the Fermi-Pasta-Ulam Problem 294

10 Quantum Mechanics **303**
10.1 Time-Independent Schrödinger Equation: Some Preliminaries 303
10.2 One Dimension: Shooting and Matching Methods 307
10.3 A Matrix Approach 323
10.4 A Variational Approach 326
10.5 Time-Dependent Schrödinger Equation: Direct Solutions 333
10.6 Time-Dependent Schrödinger Equation in Two Dimensions 345
10.7 Spectral Methods 349

11 Vibrations, Waves, and the Physics of Musical Instruments 357
11.1 Plucking a String: Simulating a Guitar . . . 357
11.2 Striking a String: Pianos and Hammers . . . 362
11.3 Exciting a Vibrating System with Friction: Violins and Bows . . . 367
11.4 Vibrations of a Membrane: Normal Modes and Eigenvalue Problems 372
11.5 Generation of Sound . . . 382

12 Interdisciplinary Topics 389
12.1 Protein Folding . . . 389
12.2 Earthquakes and Self-Organized Criticality . . . 405
12.3 Neural Networks and the Brain . . . 418
12.4 Real Neurons and Action Potentials . . . 436
12.5 Cellular Automata . . . 445

APPENDICES

A Ordinary Differential Equations with Initial Values 456
A.1 First-Order, Ordinary Differential Equations . . . 456
A.2 Second-Order, Ordinary Differential Equations . . . 460
A.3 Centered Difference Methods . . . 464
A.4 Summary . . . 467

B Root Finding and Optimization 469
B.1 Root Finding . . . 469
B.2 Direct Optimization . . . 472
B.3 Stochastic Optimization . . . 473

C The Fourier Transform 479
C.1 Theoretical Background . . . 479
C.2 Discrete Fourier Transform . . . 481
C.3 Fast Fourier Transform (FFT) . . . 483
C.4 Examples: Sampling Interval and Number of Data Points . . . 486
C.5 Examples: Aliasing . . . 488
C.6 Power Spectrum . . . 490

D Fitting Data to a Function 493
D.1 Introduction . . . 493
D.2 Method of Least Squares: Linear Regression for Two Variables . . . 494
D.3 Method of Least Squares: More General Cases . . . 497

E Numerical Integration 500
E.1 Motivation . . . 500
E.2 Newton-Cotes Methods: Using Discrete Panels to Approximate an Integral . . . 500
E.3 Gaussian Quadrature: Beyond Classic Methods of Numerical Integration . . . 504

E.4 Monte Carlo Integration 506

F Generation of Random Numbers **512**
F.1 Linear Congruential Generators 512
F.2 Nonuniform Random Numbers 516

G Statistical Tests of Hypotheses **520**
G.1 Central Limit Theorem and the χ^2 Distribution 521
G.2 χ^2 Test of a Hypothesis 523

H Solving Linear Systems **527**
H.1 Solving $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$, $\mathbf{b} \neq \mathbf{0}$ 528
H.1.1 Gaussian Elimination 528
H.1.2 Gauss-Jordan elimination 530
H.1.3 LU decomposition 531
H.1.4 Relaxational method 533
H.2 Eigenvalues and Eigenfunctions 535
H.2.1 Approximate Solution of Eigensystems 537

Index **541**