Contents

I The Three Pillars of Computational Physics **1**

1 Finite Differences **7**
1.1 Interpolation Formulae . . . 9
1.1.1 NGF Interpolation . . . 9
1.1.2 NGB Interpolation . . . 10
1.1.3 ST Interpolation . . . 11
1.2 Difference Quotients . . . 12
1.2.1 DNGF Formulae . . . 12
1.2.2 DNGB Formulae . . . 14
1.2.3 DST Formulae . . . 15
1.3 Finite Differences in Two Dimensions . . . 17
1.4 Sample Applications . . . 18
1.4.1 Classical Point Mechanics . . . 18
1.4.2 Diffusion and Thermal Conduction . . . 19

2 Linear Algebra **21**
2.1 Exact Methods . . . 22
2.1.1 Gauss Elimination and Back Substitution . . . 22
2.1.2 Simplifying Matrices: The Householder Transformation . . . 25
2.1.3 LU Decomposition . . . 26
2.1.4 Tridiagonal Matrices: Recursion Method . . . 29
2.2 Iterative Methods . . . 31
2.2.1 Jacobi Relaxation . . . 32
2.2.2 Gauss-Seidel Relaxation (GSR) . . . 34
2.2.3 Successive Over-Relaxation (SOR) . . . 34
2.2.4 Alternating Direction Implicit Method (ADI) . . . 36
2.2.5 Conjugate Gradient Method (CG) . . . 36
2.3 Eigenvalues and Eigenvectors . . . 40
2.3.1 Largest Eigenvalue and Related Eigenvector . . . 40
2.3.2 Arbitrary Eigenvalue/-vector: Inverse Iteration . . . 42
2.4 Sample Applications . . . 43
2.4.1 Diffusion and Thermal Conduction . . . 43
2.4.2 Potential Equation . . . 44
2.4.3 Electronic Orbitals . . . 45

3 Stochastics **47**
3.1 Equidistributed Random Variates 49
3.1.1 Linear Congruential Generators 49
3.1.2 Shift Register Generators 50
3.2 Other Distributions 53
3.2.1 Fundamentals 53
3.2.2 Transformation Method 56
3.2.3 Generalized Transformation Method: 57
3.2.4 Rejection Method 59
3.2.5 Multivariate Gaussian Distribution 62
3.2.6 Equidistribution in Orientation Space 66
3.3 Random Sequences 68
3.3.1 Fundamentals 68
3.3.2 Markov Processes 71
3.3.3 Autoregressive Processes 74
3.3.4 Wiener-Lévy Process 77
3.3.5 Markov Chains and the Monte Carlo method 78
3.4 Stochastic Optimization 80
3.4.1 Simulated Annealing 81
3.4.2 Genetic Algorithms 82

II Everything Flows **85**

4 Ordinary Differential Equations **89**
4.1 Initial Value Problems of First Order 90
4.1.1 Euler-Cauchy Algorithm 90
4.1.2 Stability and Accuracy of Difference Schemes 91
4.1.3 Explicit Methods 94
4.1.4 Implicit Methods 96
4.1.5 Predictor-Corrector Method 98
4.1.6 Runge-Kutta Method 101
4.1.7 Extrapolation Method 104
4.2 Initial Value Problems of Second Order 105
4.2.1 Verlet Method 105
4.2.2 Predictor-Corrector Method 108
4.2.3 Nordsieck Formulation of the PC Method 110
4.2.4 Runge-Kutta Method 112
4.2.5 Symplectic Algorithms 112
4.2.6 Numerov's Method 117
4.3 Boundary Value Problems 119
4.3.1 Shooting Method 120
4.3.2 Relaxation Method 121

5 Partial Differential Equations **125**
5.1 Initial Value Problems I (Hyperbolic) 129
5.1.1 FTCS Scheme; Stability Analysis 129
5.1.2 Lax Scheme 131
5.1.3 Leapfrog Scheme (LF) 133
5.1.4 Lax-Wendroff Scheme (LW) 135
5.1.5 Lax and Lax-Wendroff in Two Dimensions 135
5.2 Initial Value Problems II (Parabolic) 138
5.2.1 FTCS Scheme 138
5.2.2 Implicit Scheme of First Order 140
5.2.3 Crank-Nicholson Scheme (CN) 141
5.2.4 Dufort-Frankel Scheme (DF) 143
5.3 Boundary Value Problems: Elliptic DE 143
5.3.1 Relaxation and Multigrid Techniques 147
5.3.2 ADI Method for the Potential Equation 148
5.3.3 Fourier Transform Method (FT) 150
5.3.4 Cyclic Reduction (CR) 153

III Anchors Aweigh **157**

6 Simulation and Statistical Mechanics **161**
6.1 Model Systems of Statistical Mechanics 164
6.1.1 A Nutshellfull of Fluids and Solids 164
6.1.2 Tricks of the Trade 168
6.2 Monte Carlo Method 171
6.3 Molecular Dynamics Simulation 175
6.3.1 Hard Spheres 175
6.3.2 Continuous Potentials 177
6.3.3 Beyond Basic Molecular Dynamics 178
6.4 Evaluation of Simulation Experiments 181
6.4.1 Pair Correlation Function 182
6.4.2 Autocorrelation Functions 184
6.5 Particles and Fields 185
6.5.1 Ewald summation 186
6.5.2 Particle-Mesh Methods (PM and P3M): 188
6.6 Stochastic Dynamics 191

7 Quantum Mechanical Simulation **195**
7.1 Diffusion Monte Carlo (DMC) 196
7.2 Path Integral Monte Carlo (PIMC) 201
7.3 Wave Packet Dynamics (WPD) 209
7.4 Density Functional Molecular Dynamics (DFMD) 211

8 Hydrodynamics **215**
8.1 Compressible Flow without Viscosity 216
8.1.1 Explicit Eulerian Methods 217
8.1.2 Particle-in-Cell Method (PIC) 218
8.1.3 Smoothed Particle Hydrodynamics (SPH) 220
8.2 Incompressible Flow with Viscosity 226
8.2.1 Vorticity Method 227
8.2.2 Pressure Method 229
8.2.3 Free Surfaces: Marker-and-Cell Method (MAC) 231
8.3 Lattice Gas Models for Hydrodynamics 232
8.3.1 Lattice Gas Cellular Automata 232
8.3.2 The Lattice Boltzmann Method 236
8.4 Direct Simulation Monte Carlo / Bird method 237

Appendixes **239**

A Machine Errors **241**

B Discrete Fourier Transformation **245**
B.1 Fundamentals 245
B.2 Fast Fourier Transform (FFT) 246

Bibliography **249**

Index **257**