

Contents

Part I Numerical Methods

1 Error Analysis	3
1.1 Machine Numbers and Rounding Errors	3
1.2 Numerical Errors of Elementary Floating Point Operations	6
1.2.1 Numerical Extinction	6
1.2.2 Addition	7
1.2.3 Multiplication	8
1.3 Error Propagation	8
1.4 Stability of Iterative Algorithms	11
1.5 Example: Rotation	12
1.6 Truncation Error	13
Problems	13
2 Interpolation	15
2.1 Interpolating Functions	15
2.2 Polynomial Interpolation	16
2.2.1 Lagrange Polynomials	16
2.2.2 Newton's Divided Differences	17
2.2.3 Interpolation Error	18
2.2.4 Neville Method	20
2.3 Spline Interpolation	21
2.4 Multivariate Interpolation	25
Problems	26
3 Numerical Differentiation	29
3.1 Simple Forward Difference	29
3.2 Symmetrical Difference Quotient	30
3.3 Extrapolation Methods	31
3.4 Higher Derivatives	33
3.5 More Dimensions	34
Problems	35

4 Numerical Integration	37
4.1 Equidistant Sample Points	37
4.1.1 Newton–Cotes Rules	38
4.1.2 Newton–Cotes Expressions for an Open Interval	39
4.1.3 Composite Newton–Cotes Formulas	40
4.1.4 Extrapolation Method (Romberg Integration)	40
4.2 Optimized Sample Points	42
4.2.1 Clenshaw–Curtis Expressions	42
4.2.2 Gaussian Integration	43
Problems	45
5 Systems of Inhomogeneous Linear Equations	47
5.1 Gaussian Elimination Method	47
5.1.1 Pivoting	50
5.1.2 Direct LU Decomposition	51
5.2 QR Decomposition	51
5.3 Linear Equations with Tridiagonal Matrix	53
5.4 Cyclic Tridiagonal Systems	55
5.5 Iterative Solution of Inhomogeneous Linear Equations	56
5.5.1 General Treatment	56
5.5.2 Jacobi Method	57
5.5.3 Gauss–Seidel Method	57
5.5.4 Damping and Successive Over-Relaxation	58
5.6 Conjugate Gradients	59
Problems	60
6 Roots and Extremal Points	63
6.1 Root Finding	63
6.1.1 Bisection	63
6.1.2 Regula Falsi Method	64
6.1.3 Newton–Raphson Method	65
6.1.4 Secant Method	66
6.1.5 Roots of Vector Functions	66
6.2 Optimization Without Constraints	67
6.2.1 Steepest Descent Method	68
6.2.2 Conjugate Gradient Method	68
6.2.3 Newton–Raphson Method	69
6.2.4 Quasi-Newton Methods	69
Problems	70
7 Fourier Transformation	73
7.1 Discrete Fourier Transformation	74
7.1.1 Trigonometric Interpolation	75
7.1.2 Real-Valued Functions	77

7.2	Algorithms	78
7.2.1	Goertzel's Algorithm	79
7.2.2	Fast Fourier Transformation	80
	Problems	84
8	Random Numbers and Monte Carlo Methods	87
8.1	Some Basic Statistics	87
8.1.1	Probability Density and Cumulative Probability Distribution	87
8.1.2	Expectation Values and Moments	88
8.1.3	Multivariate Distributions	92
8.1.4	Central Limit Theorem	93
8.1.5	Example: Binomial Distribution	93
8.1.6	Average of Repeated Measurements	94
8.2	Random Numbers	95
8.2.1	The Method by Marsaglia and Zaman	96
8.2.2	Random Numbers with Given Distribution	96
8.2.3	Examples	97
8.3	Monte Carlo Integration	99
8.3.1	Numerical Calculation of π	99
8.3.2	Calculation of an Integral	100
8.3.3	More General Random Numbers	101
8.4	Monte Carlo Method for Thermodynamic Averages	102
8.4.1	Simple (Minded) Sampling	102
8.4.2	Importance Sampling	103
8.4.3	Metropolis Algorithm	104
	Problems	106
9	Eigenvalue Problems	109
9.1	Direct Solution	109
9.2	Jacobi Method	109
9.3	Tridiagonal Matrices	111
9.4	Reduction to a Tridiagonal Matrix	111
9.5	Large Matrices	114
	Problems	115
10	Data Fitting	117
10.1	Least Square Fit	117
10.1.1	Linear Least Square Fit	119
10.1.2	Least Square Fit Using Orthogonalization	120
10.2	Singular Value Decomposition	123
	Problems	127

11 Equations of Motion	129
11.1 State Vector of a Physical System	129
11.2 Time Evolution of the State Vector	130
11.3 Explicit Forward Euler Method	132
11.4 Implicit Backward Euler Method	134
11.5 Improved Euler Methods	135
11.6 Taylor Series Methods	137
11.7 Runge–Kutta Methods	138
11.7.1 Second-Order Runge–Kutta Method	138
11.7.2 Third-Order Runge–Kutta Method	138
11.7.3 Fourth-Order Runge–Kutta Method	139
11.8 Quality Control and Adaptive Step-Size Control	140
11.9 Extrapolation Methods	141
11.10 Multistep Methods	142
11.10.1 Explicit Multistep Methods	142
11.10.2 Implicit Multistep Methods	143
11.10.3 Predictor–Corrector Methods	144
11.11 Verlet Methods	144
11.11.1 Liouville Equation	144
11.11.2 Split Operator Approximation	145
11.11.3 Position Verlet Method	146
11.11.4 Velocity Verlet Method	146
11.11.5 Standard Verlet Method	147
11.11.6 Error Accumulation for the Standard Verlet Method	149
11.11.7 Leap Frog Method	149
Problems	150

Part II Simulation of Classical and Quantum Systems

12 Rotational Motion	157
12.1 Transformation to a Body Fixed Coordinate System	157
12.2 Properties of the Rotation Matrix	158
12.3 Properties of W , Connection with the Vector of Angular Velocity	160
12.4 Transformation Properties of the Angular Velocity	161
12.5 Momentum and Angular Momentum	163
12.6 Equations of Motion of a Rigid Body	163
12.7 Moments of Inertia	164
12.8 Equations of Motion for a Rotor	165
12.9 Explicit Solutions	165
12.10 Loss of Orthogonality	167
12.11 Implicit Method	168
12.12 Example: Free Symmetric Rotor	170
12.13 Kinetic Energy of a Rotor	171
12.14 Parametrization by Euler Angles	172

12.15 Cayley–Klein parameters, Quaternions, Euler Parameters	172
12.16 Solving the Equations of Motion with Quaternions	176
Problems	176
13 Simulation of Thermodynamic Systems	179
13.1 Force Fields for Molecular Dynamics Simulations	179
13.1.1 Intramolecular Forces	179
13.1.2 Intermolecular Forces	180
13.1.3 Approximate Separation of Rotation and Vibrations ..	180
13.2 Simulation of a van der Waals System	181
13.2.1 Integration of the Equations of Motion	181
13.2.2 Boundary Conditions and Average Pressure	182
13.2.3 Initial Conditions and Average Temperature	183
13.2.4 Analysis of the Results	183
13.3 Monte Carlo Simulation	186
13.3.1 One-Dimensional Ising Model	186
13.3.2 Two-Dimensional Ising Model	188
Problems	189
14 Random Walk and Brownian Motion	193
14.1 Random Walk in One Dimension	194
14.1.1 Random Walk with Constant Step Size	195
14.2 The Freely Jointed Chain	196
14.2.1 Basic Statistic Properties	197
14.2.2 Gyration Tensor	199
14.2.3 Hookean Spring Model	200
14.3 Langevin Dynamics	202
Problems	204
15 Electrostatics	207
15.1 Poisson Equation	207
15.1.1 Homogeneous Dielectric Medium	207
15.1.2 Charged Sphere	209
15.1.3 Variable ϵ	210
15.1.4 Discontinuous ϵ	211
15.1.5 Solvation Energy of a Charged Sphere	211
15.1.6 The Shifted Grid Method	213
15.2 Poisson Boltzmann Equation for an Electrolyte	215
15.2.1 Discretization of the Linearized Poisson–Boltzmann Equation	216
15.3 Boundary Element Method for the Poisson Equation	216
15.3.1 Integral Equations for the Potential	217
15.3.2 Calculation of the Boundary Potential	219

15.4	Boundary Element Method for the Linearized Poisson–Boltzmann Equation	222
15.5	Electrostatic Interaction Energy (Onsager Model)	223
15.5.1	Example: Point Charge in a Spherical Cavity	225
	Problems	225
16	Waves	229
16.1	One-Dimensional Waves	229
16.2	Discretization of the Wave Equation	231
16.3	Boundary Values	232
16.4	The Wave Equation as an Eigenvalue Problem	233
16.4.1	Eigenfunction Expansion	233
16.4.2	Application to the Discrete One-Dimensional Wave Equation	234
16.5	Numerical Integration of the Wave Equation	237
16.5.1	Simple Algorithm	237
16.5.2	Stability Analysis	238
16.5.3	Alternative Algorithm with Explicit Velocities	240
16.5.4	Stability Analysis	240
	Problems	242
17	Diffusion	243
17.1	Basic Physics of Diffusion	243
17.2	Boundary Conditions	244
17.3	Numerical Integration of the Diffusion Equation	245
17.3.1	Forward Euler or Explicit Richardson Method	245
17.3.2	Stability Analysis	245
17.3.3	Implicit Backward Euler Algorithm	247
17.3.4	Crank–Nicolson Method	248
17.3.5	Error Order Analysis	249
17.3.6	Practical Considerations	250
17.3.7	Split Operator Method for $d > 1$ Dimensions	250
	Problems	252
18	Nonlinear Systems	253
18.1	Iterated Functions	253
18.1.1	Fixed Points and Stability	254
18.1.2	The Ljapunow Exponent	256
18.1.3	The Logistic Map	257
18.1.4	Fixed Points of the Logistic Map	258
18.1.5	Bifurcation Diagram	259
18.2	Population Dynamics	260
18.2.1	Equilibria and Stability	260
18.2.2	The Continuous Logistic Model	262

18.3	Lotka–Volterra model	262
18.3.1	Stability Analysis	263
18.4	Functional Response	265
18.4.1	Holling–Tanner Model	266
18.5	Reaction–Diffusion Systems	269
18.5.1	General Properties of Reaction–Diffusion Systems	269
18.5.2	Chemical Reactions	270
18.5.3	Diffusive Population Dynamics	270
18.5.4	Stability Analysis	270
18.5.5	Lotka–Volterra Model with Diffusion	272
	Problems	273
19	Simple Quantum Systems	277
19.1	Quantum Particle in a Potential Well	278
19.2	Expansion in a Finite Basis	282
19.3	Time-Independent Problems	284
19.3.1	Simple Two-Level System	285
19.3.2	Three-State Model (Superexchange)	286
19.3.3	Ladder Model for Exponential Decay	290
19.4	Time-Dependent Models	292
19.4.1	Landau–Zener Model	293
19.4.2	Two-State System with Time-Dependent Perturbation	293
19.5	Description of a Two-State System with the Density Matrix Formalism	297
19.5.1	Density Matrix Formalism	297
19.5.2	Analogy to Nuclear Magnetic Resonance	300
19.5.3	Relaxation Processes—Bloch Equations	302
	Problems	307
	Appendix	309
	References	311
	Index	315