

Contents

Dedication *V*

Preface *XIX*

1	Introduction	<i>1</i>
1.1	Computational Physics and Computational Science	<i>1</i>
1.2	This Book's Subjects	<i>3</i>
1.3	This Book's Problems	<i>4</i>
1.4	This Book's Language: The Python Ecosystem	<i>8</i>
1.4.1	Python Packages (Libraries)	<i>9</i>
1.4.2	This Book's Packages	<i>10</i>
1.4.3	The Easy Way: Python Distributions (Package Collections)	<i>12</i>
1.5	Python's Visualization Tools	<i>13</i>
1.5.1	Visual (VPython)'s 2D Plots	<i>14</i>
1.5.2	VPython's Animations	<i>17</i>
1.5.3	Matplotlib's 2D Plots	<i>17</i>
1.5.4	Matplotlib's 3D Surface Plots	<i>22</i>
1.5.5	Matplotlib's Animations	<i>24</i>
1.5.6	Mayavi's Visualizations Beyond Plotting	<i>26</i>
1.6	Plotting Exercises	<i>30</i>
1.7	Python's Algebraic Tools	<i>31</i>
2	Computing Software Basics	<i>33</i>
2.1	Making Computers Obey	<i>33</i>
2.2	Programming Warmup	<i>35</i>
2.2.1	Structured and Reproducible Program Design	<i>36</i>
2.2.2	Shells, Editors, and Execution	<i>37</i>
2.3	Python I/O	<i>39</i>
2.4	Computer Number Representations (Theory)	<i>40</i>
2.4.1	IEEE Floating-Point Numbers	<i>41</i>
2.4.2	Python and the IEEE 754 Standard	<i>47</i>
2.4.3	Over and Underflow Exercises	<i>48</i>
2.4.4	Machine Precision (Model)	<i>49</i>

2.4.5	Experiment: Your Machine's Precision	50
2.5	Problem: Summing Series	51
2.5.1	Numerical Summation (Method)	51
2.5.2	Implementation and Assessment	52
3	Errors and Uncertainties in Computations	53
3.1	Types of Errors (Theory)	53
3.1.1	Model for Disaster: Subtractive Cancelation	55
3.1.2	Subtractive Cancelation Exercises	56
3.1.3	Round-off Errors	57
3.1.4	Round-off Error Accumulation	58
3.2	Error in Bessel Functions (Problem)	58
3.2.1	Numerical Recursion (Method)	59
3.2.2	Implementation and Assessment: Recursion Relations	61
3.3	Experimental Error Investigation	62
3.3.1	Error Assessment	65
4	Monte Carlo: Randomness, Walks, and Decays	69
4.1	Deterministic Randomness	69
4.2	Random Sequences (Theory)	69
4.2.1	Random-Number Generation (Algorithm)	70
4.2.2	Implementation: Random Sequences	72
4.2.3	Assessing Randomness and Uniformity	73
4.3	Random Walks (Problem)	75
4.3.1	Random-Walk Simulation	76
4.3.2	Implementation: Random Walk	77
4.4	Extension: Protein Folding and Self-Avoiding Random Walks	79
4.5	Spontaneous Decay (Problem)	80
4.5.1	Discrete Decay (Model)	81
4.5.2	Continuous Decay (Model)	82
4.5.3	Decay Simulation with Geiger Counter Sound	82
4.6	Decay Implementation and Visualization	84
5	Differentiation and Integration	85
5.1	Differentiation	85
5.2	Forward Difference (Algorithm)	86
5.3	Central Difference (Algorithm)	87
5.4	Extrapolated Difference (Algorithm)	87
5.5	Error Assessment	88
5.6	Second Derivatives (Problem)	90
5.6.1	Second-Derivative Assessment	90
5.7	Integration	91
5.8	Quadrature as Box Counting (Math)	91
5.9	Algorithm: Trapezoid Rule	93
5.10	Algorithm: Simpson's Rule	94

5.11	Integration Error (Assessment)	96
5.12	Algorithm: Gaussian Quadrature	97
5.12.1	Mapping Integration Points	98
5.12.2	Gaussian Points Derivation	99
5.12.3	Integration Error Assessment	100
5.13	Higher Order Rules (Algorithm)	103
5.14	Monte Carlo Integration by Stone Throwing (Problem)	104
5.14.1	Stone Throwing Implementation	104
5.15	Mean Value Integration (Theory and Math)	105
5.16	Integration Exercises	106
5.17	Multidimensional Monte Carlo Integration (Problem)	108
5.17.1	Multi Dimension Integration Error Assessment	109
5.17.2	Implementation: 10D Monte Carlo Integration	110
5.18	Integrating Rapidly Varying Functions (Problem)	110
5.19	Variance Reduction (Method)	110
5.20	Importance Sampling (Method)	111
5.21	von Neumann Rejection (Method)	111
5.21.1	Simple Random Gaussian Distribution	113
5.22	Nonuniform Assessment ⊙	113
5.22.1	Implementation ⊙	114
6	Matrix Computing	117
6.1	Problem 3: N-D Newton–Raphson; Two Masses on a String	117
6.1.1	Theory: Statics	118
6.1.2	Algorithm: Multidimensional Searching	119
6.2	Why Matrix Computing?	122
6.3	Classes of Matrix Problems (Math)	122
6.3.1	Practical Matrix Computing	124
6.4	Python Lists as Arrays	126
6.5	Numerical Python (NumPy) Arrays	127
6.5.1	NumPy's linalg Package	132
6.6	Exercise: Testing Matrix Programs	134
6.6.1	Matrix Solution of the String Problem	137
6.6.2	Explorations	139
7	Trial-and-Error Searching and Data Fitting	141
7.1	Problem 1: A Search for Quantum States in a Box	141
7.2	Algorithm: Trial-and-Error Roots via Bisection	142
7.2.1	Implementation: Bisection Algorithm	144
7.3	Improved Algorithm: Newton–Raphson Searching	145
7.3.1	Newton–Raphson with Backtracking	147
7.3.2	Implementation: Newton–Raphson Algorithm	148
7.4	Problem 2: Temperature Dependence of Magnetization	148
7.4.1	Searching Exercise	150
7.5	Problem 3: Fitting An Experimental Spectrum	150

7.5.1	Lagrange Implementation, Assessment	152
7.5.2	Cubic Spline Interpolation (Method)	153
7.6	Problem 4: Fitting Exponential Decay	156
7.7	Least-Squares Fitting (Theory)	158
7.7.1	Least-Squares Fitting: Theory and Implementation	160
7.8	Exercises: Fitting Exponential Decay, Heat Flow and Hubble's Law	162
7.8.1	Linear Quadratic Fit	164
7.8.2	Problem 5: Nonlinear Fit to a Breit–Wigner	167
8	Solving Differential Equations: Nonlinear Oscillations	171
8.1	Free Nonlinear Oscillations	171
8.2	Nonlinear Oscillators (Models)	171
8.3	Types of Differential Equations (Math)	173
8.4	Dynamic Form for ODEs (Theory)	175
8.5	ODE Algorithms	177
8.5.1	Euler's Rule	177
8.6	Runge–Kutta Rule	178
8.7	Adams–Bashforth–Moulton Predictor–Corrector Rule	183
8.7.1	Assessment: rk2 vs. rk4 vs. rk45	185
8.8	Solution for Nonlinear Oscillations (Assessment)	187
8.8.1	Precision Assessment: Energy Conservation	188
8.9	Extensions: Nonlinear Resonances, Beats, Friction	189
8.9.1	Friction (Model)	189
8.9.2	Resonances and Beats: Model, Implementation	190
8.10	Extension: Time-Dependent Forces	190
9	ODE Applications: Eigenvalues, Scattering, and Projectiles	193
9.1	Problem: Quantum Eigenvalues in Arbitrary Potential	193
9.1.1	Model: Nucleon in a Box	194
9.2	Algorithms: Eigenvalues via ODE Solver + Search	195
9.2.1	Numerov Algorithm for Schrödinger ODE \odot	197
9.2.2	Implementation: Eigenvalues via ODE Solver + Bisection Algorithm	200
9.3	Explorations	203
9.4	Problem: Classical Chaotic Scattering	203
9.4.1	Model and Theory	204
9.4.2	Implementation	206
9.4.3	Assessment	207
9.5	Problem: Balls Falling Out of the Sky	208
9.6	Theory: Projectile Motion with Drag	208
9.6.1	Simultaneous Second-Order ODEs	209
9.6.2	Assessment	210
9.7	Exercises: 2- and 3-Body Planet Orbits and Chaotic Weather	211
10	High-Performance Hardware and Parallel Computers	215
10.1	High-Performance Computers	215

10.2	Memory Hierarchy	216
10.3	The Central Processing Unit	219
10.4	CPU Design: Reduced Instruction Set Processors	220
10.5	CPU Design: Multiple-Core Processors	221
10.6	CPU Design: Vector Processors	222
10.7	Introduction to Parallel Computing	223
10.8	Parallel Semantics (Theory)	224
10.9	Distributed Memory Programming	226
10.10	Parallel Performance	227
10.10.1	Communication Overhead	229
10.11	Parallelization Strategies	230
10.12	Practical Aspects of MIMD Message Passing	231
10.12.1	High-Level View of Message Passing	233
10.12.2	Message Passing Example and Exercise	234
10.13	Scalability	236
10.13.1	Scalability Exercises	238
10.14	Data Parallelism and Domain Decomposition	239
10.14.1	Domain Decomposition Exercises	242
10.15	Example: The IBM Blue Gene Supercomputers	243
10.16	Exascale Computing via Multinode-Multicore GPUs	245
11	Applied HPC: Optimization, Tuning, and GPU Programming	247
11.1	General Program Optimization	247
11.1.1	Programming for Virtual Memory (Method)	248
11.1.2	Optimization Exercises	249
11.2	Optimized Matrix Programming with NumPy	251
11.2.1	NumPy Optimization Exercises	254
11.3	Empirical Performance of Hardware	254
11.3.1	Racing Python vs. Fortran/C	255
11.4	Programming for the Data Cache (Method)	262
11.4.1	Exercise 1: Cache Misses	264
11.4.2	Exercise 2: Cache Flow	264
11.4.3	Exercise 3: Large-Matrix Multiplication	265
11.5	Graphical Processing Units for High Performance Computing	266
11.5.1	The GPU Card	267
11.6	Practical Tips for Multicore and GPU Programming	267
11.6.1	CUDA Memory Usage	270
11.6.2	CUDA Programming	271
12	Fourier Analysis: Signals and Filters	275
12.1	Fourier Analysis of Nonlinear Oscillations	275
12.2	Fourier Series (Math)	276
12.2.1	Examples: Sawtooth and Half-Wave Functions	278
12.3	Exercise: Summation of Fourier Series	279
12.4	Fourier Transforms (Theory)	279

12.5	The Discrete Fourier Transform	281
12.5.1	Aliasing (Assessment)	285
12.5.2	Fourier Series DFT (Example)	287
12.5.3	Assessments	288
12.5.4	Nonperiodic Function DFT (Exploration)	290
12.6	Filtering Noisy Signals	290
12.7	Noise Reduction via Autocorrelation (Theory)	290
12.7.1	Autocorrelation Function Exercises	293
12.8	Filtering with Transforms (Theory)	294
12.8.1	Digital Filters: Windowed Sinc Filters (Exploration) ⊖	296
12.9	The Fast Fourier Transform Algorithm ⊖	299
12.9.1	Bit Reversal	301
12.10	FFT Implementation	303
12.11	FFT Assessment	304
13	Wavelet and Principal Components Analyses: Nonstationary Signals and Data Compression	307
13.1	Problem: Spectral Analysis of Nonstationary Signals	307
13.2	Wavelet Basics	307
13.3	Wave Packets and Uncertainty Principle (Theory)	309
13.3.1	Wave Packet Assessment	311
13.4	Short-Time Fourier Transforms (Math)	311
13.5	The Wavelet Transform	313
13.5.1	Generating Wavelet Basis Functions	313
13.5.2	Continuous Wavelet Transform Implementation	316
13.6	Discrete Wavelet Transforms, Multiresolution Analysis ⊖	317
13.6.1	Pyramid Scheme Implementation ⊖	323
13.6.2	Daubechies Wavelets via Filtering	327
13.6.3	DWT Implementation and Exercise	330
13.7	Principal Components Analysis	332
13.7.1	Demonstration of Principal Component Analysis	334
13.7.2	PCA Exercises	337
14	Nonlinear Population Dynamics	339
14.1	Bug Population Dynamics	339
14.2	The Logistic Map (Model)	339
14.3	Properties of Nonlinear Maps (Theory and Exercise)	341
14.3.1	Fixed Points	342
14.3.2	Period Doubling, Attractors	343
14.4	Mapping Implementation	344
14.5	Bifurcation Diagram (Assessment)	345
14.5.1	Bifurcation Diagram Implementation	346
14.5.2	Visualization Algorithm: Binning	347
14.5.3	Feigenbaum Constants (Exploration)	348
14.6	Logistic Map Random Numbers (Exploration) ⊖	348

14.7	Other Maps (Exploration)	348
14.8	Signals of Chaos: Lyapunov Coefficient and Shannon Entropy ⊖	349
14.9	Coupled Predator–Prey Models	353
14.10	Lotka–Volterra Model	354
14.10.1	Lotka–Volterra Assessment	356
14.11	Predator–Prey Chaos	356
14.11.1	Exercises	359
14.11.2	LVM with Prey Limit	359
14.11.3	LVM with Predation Efficiency	360
14.11.4	LVM Implementation and Assessment	361
14.11.5	Two Predators, One Prey (Exploration)	362
15	Continuous Nonlinear Dynamics	363
15.1	Chaotic Pendulum	363
15.1.1	Free Pendulum Oscillations	364
15.1.2	Solution as Elliptic Integrals	365
15.1.3	Implementation and Test: Free Pendulum	366
15.2	Visualization: Phase-Space Orbits	367
15.2.1	Chaos in Phase Space	368
15.2.2	Assessment in Phase Space	372
15.3	Exploration: Bifurcations of Chaotic Pendulums	374
15.4	Alternate Problem: The Double Pendulum	375
15.5	Assessment: Fourier/Wavelet Analysis of Chaos	377
15.6	Exploration: Alternate Phase-Space Plots	378
15.7	Further Explorations	379
16	Fractals and Statistical Growth Models	383
16.1	Fractional Dimension (Math)	383
16.2	The Sierpiński Gasket (Problem 1)	384
16.2.1	Sierpiński Implementation	384
16.2.2	Assessing Fractal Dimension	385
16.3	Growing Plants (Problem 2)	386
16.3.1	Self-Affine Connection (Theory)	386
16.3.2	Barnsley's Fern Implementation	387
16.3.3	Self-Affinity in Trees Implementation	389
16.4	Ballistic Deposition (Problem 3)	390
16.4.1	Random Deposition Algorithm	390
16.5	Length of British Coastline (Problem 4)	391
16.5.1	Coastlines as Fractals (Model)	392
16.5.2	Box Counting Algorithm	392
16.5.3	Coastline Implementation and Exercise	393
16.6	Correlated Growth, Forests, Films (Problem 5)	395
16.6.1	Correlated Ballistic Deposition Algorithm	395
16.7	Globular Cluster (Problem 6)	396
16.7.1	Diffusion-Limited Aggregation Algorithm	396

16.7.2	Fractal Analysis of DLA or a Pollock	399
16.8	Fractals in Bifurcation Plot (Problem 7)	400
16.9	Fractals from Cellular Automata	400
16.10	Perlin Noise Adds Realism \odot	402
16.10.1	Ray Tracing Algorithms	404
16.11	Exercises	407
17	Thermodynamic Simulations and Feynman Path Integrals	409
17.1	Magnets via Metropolis Algorithm	409
17.2	An Ising Chain (Model)	410
17.3	Statistical Mechanics (Theory)	412
17.3.1	Analytic Solution	413
17.4	Metropolis Algorithm	413
17.4.1	Metropolis Algorithm Implementation	416
17.4.2	Equilibration, Thermodynamic Properties (Assessment)	417
17.4.3	Beyond Nearest Neighbors, 1D (Exploration)	419
17.5	Magnets via Wang–Landau Sampling \odot	420
17.6	Wang–Landau Algorithm	423
17.6.1	WLS Ising Model Implementation	425
17.6.2	WLS Ising Model Assessment	428
17.7	Feynman Path Integral Quantum Mechanics \odot	429
17.8	Feynman’s Space–Time Propagation (Theory)	429
17.8.1	Bound-State Wave Function (Theory)	431
17.8.2	Lattice Path Integration (Algorithm)	432
17.8.3	Lattice Implementation	437
17.8.4	Assessment and Exploration	440
17.9	Exploration: Quantum Bouncer’s Paths \odot	440
18	Molecular Dynamics Simulations	445
18.1	Molecular Dynamics (Theory)	445
18.1.1	Connection to Thermodynamic Variables	449
18.1.2	Setting Initial Velocities	449
18.1.3	Periodic Boundary Conditions and Potential Cutoff	450
18.2	Verlet and Velocity–Verlet Algorithms	451
18.3	1D Implementation and Exercise	453
18.4	Analysis	456
19	PDE Review and Electrostatics via Finite Differences and Electrostatics via Finite Differences	461
19.1	PDE Generalities	461
19.2	Electrostatic Potentials	463
19.2.1	Laplace’s Elliptic PDE (Theory)	463
19.3	Fourier Series Solution of a PDE	464
19.3.1	Polynomial Expansion as an Algorithm	466
19.4	Finite-Difference Algorithm	467

19.4.1	Relaxation and Over-relaxation	469
19.4.2	Lattice PDE Implementation	470
19.5	Assessment via Surface Plot	471
19.6	Alternate Capacitor Problems	471
19.7	Implementation and Assessment	474
19.8	Electric Field Visualization (Exploration)	475
19.9	Review Exercise	476
20	Heat Flow via Time Stepping	477
20.1	Heat Flow via Time-Stepping (Leapfrog)	477
20.2	The Parabolic Heat Equation (Theory)	478
20.2.1	Solution: Analytic Expansion	478
20.2.2	Solution: Time Stepping	479
20.2.3	von Neumann Stability Assessment	481
20.2.4	Heat Equation Implementation	483
20.3	Assessment and Visualization	483
20.4	Improved Heat Flow: Crank–Nicolson Method	484
20.4.1	Solution of Tridiagonal Matrix Equations ⊖	487
20.4.2	Crank–Nicolson Implementation, Assessment	490
21	Wave Equations I: Strings and Membranes	491
21.1	A Vibrating String	491
21.2	The Hyperbolic Wave Equation (Theory)	491
21.2.1	Solution via Normal-Mode Expansion	493
21.2.2	Algorithm: Time Stepping	494
21.2.3	Wave Equation Implementation	496
21.2.4	Assessment, Exploration	497
21.3	Strings with Friction (Extension)	499
21.4	Strings with Variable Tension and Density	500
21.4.1	Waves on Catenary	501
21.4.2	Derivation of Catenary Shape	501
21.4.3	Catenary and Frictional Wave Exercises	503
21.5	Vibrating Membrane (2D Waves)	504
21.6	Analytical Solution	505
21.7	Numerical Solution for 2D Waves	508
22	Wave Equations II: Quantum Packets and Electromagnetic	511
22.1	Quantum Wave Packets	511
22.2	Time-Dependent Schrödinger Equation (Theory)	511
22.2.1	Finite-Difference Algorithm	513
22.2.2	Wave Packet Implementation, Animation	514
22.2.3	Wave Packets in Other Wells (Exploration)	516
22.3	Algorithm for the 2D Schrödinger Equation	517
22.3.1	Exploration: Bound and Diffracted 2D Packet	518
22.4	Wave Packet–Wave Packet Scattering	518

22.4.1	Algorithm	520
22.4.2	Implementation	520
22.4.3	Results and Visualization	522
22.5	E&M Waves via Finite-Difference Time Domain	525
22.6	Maxwell's Equations	525
22.7	FDTD Algorithm	526
22.7.1	Implementation	530
22.7.2	Assessment	530
22.7.3	Extension: Circularly Polarized Waves	531
22.8	Application: Wave Plates	533
22.9	Algorithm	534
22.10	FDTD Exercise and Assessment	535
23	Electrostatics via Finite Elements	537
23.1	Finite-Element Method \odot	537
23.2	Electric Field from Charge Density (Problem)	538
23.3	Analytic Solution	538
23.4	Finite-Element (Not Difference) Methods, 1D	539
23.4.1	Weak Form of PDE	539
23.4.2	Galerkin Spectral Decomposition	540
23.5	1D FEM Implementation and Exercises	544
23.5.1	1D Exploration	547
23.6	Extension to 2D Finite Elements	547
23.6.1	Weak Form of PDE	548
23.6.2	Galerkin's Spectral Decomposition	548
23.6.3	Triangular Elements	549
23.6.4	Solution as Linear Equations	551
23.6.5	Imposing Boundary Conditions	552
23.6.6	FEM 2D Implementation and Exercise	554
23.6.7	FEM 2D Exercises	554
24	Shocks Waves and Solitons	555
24.1	Shocks and Solitons in Shallow Water	555
24.2	Theory: Continuity and Advection Equations	556
24.2.1	Advection Implementation	558
24.3	Theory: Shock Waves via Burgers' Equation	559
24.3.1	Lax–Wendroff Algorithm for Burgers' Equation	560
24.3.2	Implementation and Assessment of Burgers' Shock Equation	561
24.4	Including Dispersion	562
24.5	Shallow-Water Solitons: The KdV Equation	563
24.5.1	Analytic Soliton Solution	563
24.5.2	Algorithm for KdV Solitons	564
24.5.3	Implementation: KdV Solitons	565
24.5.4	Exploration: Solitons in Phase Space, Crossing	567
24.6	Solitons on Pendulum Chain	567

24.6.1	Including Dispersion	568
24.6.2	Continuum Limit, the Sine-Gordon Equation	570
24.6.3	Analytic SGE Solution	571
24.6.4	Numeric Solution: 2D SGE Solitons	571
24.6.5	2D Soliton Implementation	573
24.6.6	SGE Soliton Visualization	574
25	Fluid Dynamics	575
25.1	River Hydrodynamics	575
25.2	Navier–Stokes Equation (Theory)	576
25.2.1	Boundary Conditions for Parallel Plates	578
25.2.2	Finite-Difference Algorithm and Overrelaxation	580
25.2.3	Successive Overrelaxation Implementation	581
25.3	2D Flow over a Beam	581
25.4	Theory: Vorticity Form of Navier–Stokes Equation	582
25.4.1	Finite Differences and the SOR Algorithm	584
25.4.2	Boundary Conditions for a Beam	585
25.4.3	SOR on a Grid	587
25.4.4	Flow Assessment	589
25.4.5	Exploration	590
26	Integral Equations of Quantum Mechanics	591
26.1	Bound States of Nonlocal Potentials	591
26.2	Momentum–Space Schrödinger Equation (Theory)	592
26.2.1	Integral to Matrix Equations	593
26.2.2	Delta-Shell Potential (Model)	595
26.2.3	Binding Energies Solution	595
26.2.4	Wave Function (Exploration)	597
26.3	Scattering States of Nonlocal Potentials ◉	597
26.4	Lippmann–Schwinger Equation (Theory)	598
26.4.1	Singular Integrals (Math)	599
26.4.2	Numerical Principal Values	600
26.4.3	Reducing Integral Equations to Matrix Equations (Method)	600
26.4.4	Solution via Inversion, Elimination	602
26.4.5	Scattering Implementation	603
26.4.6	Scattering Wave Function (Exploration)	604
Appendix A Codes, Applets, and Animations 607		
Bibliography 609		
Index 615		