

Computational physics : problem solving with Python

Rubin H. Landau, Manuel J. Páez, Cristian C. Bordeianu

3. compl. rev. ed - ©2015

TABLE OF CONTENTS

Dedication V

Preface XIX

1 Introduction 1

1.1 Computational Physics and Computational Science 1

1.2 This Book's Subjects 3

1.3 This Book's Problems 4

1.4 This Book's Language: The Python Ecosystem 8

1.4.1 Python Packages (Libraries) 9

1.4.2 This Book's Packages 10

1.4.3 The EasyWay: Python Distributions (Package Collections) 12

1.5 Python's Visualization Tools 13

1.5.1 Visual (VPython)'s 2D Plots 14

1.5.2 VPython's Animations 17

1.5.3 Matplotlib's 2D Plots 17

1.5.4 Matplotlib's 3D Surface Plots 22

1.5.5 Matplotlib's Animations 24

1.5.6 Mayavi's Visualizations Beyond Plotting 26

1.6 Plotting Exercises 30

1.7 Python's Algebraic Tools 31

2 Computing Software Basics 33

2.1 Making Computers Obey 33

2.2 ProgrammingWarmup 35

2.2.1 Structured and Reproducible Program Design 36

2.2.2 Shells, Editors, and Execution 37

2.3 Python I/O 39
2.4 Computer Number Representations (Theory) 40
2.4.1 IEEE Floating-Point Numbers 41
2.4.2 Python and the IEEE 754 Standard 47
2.4.3 Over and Underflow Exercises 48
2.4.4 Machine Precision (Model) 49
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 RandomWalks (Problem) 75

- 4.3.1 Random-Walk Simulation 76
 - 4.3.2 Implementation: RandomWalk 77
 - 4.4 Extension: Protein Folding and Self-Avoiding RandomWalks 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: TestingMatrix 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 197
 - 9.2.2 Implementation: Eigenvalues viaODESolver + BisectionAlgorithm 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 Sierpin Gasket (Problem 1) 384
 - 16.2.1 Sierpin 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 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 IsingChain (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 viaWang–Landau Sampling 420
- 17.6 Wang–Landau Algorithm 423
- 17.6.1 WLS IsingModel Implementation 425
- 17.6.2 WLS IsingModel Assessment 428

17.7 Feynman Path Integral Quantum Mechanics 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 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 HyperbolicWave 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 FrictionalWave Exercises 503

21.5 Vibrating Membrane (2DWaves) 504

21.6 Analytical Solution 505

21.7 Numerical Solution for 2DWaves 508

22 Wave Equations II: QuantumPackets 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 OtherWells (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&MWaves 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 PolarizedWaves 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 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 FEMImplementation 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 FEM2D Implementation and Exercise 554
 - 23.6.7 FEM2D Exercises 554
- 24 Shocks Waves and Solitons 555**
 - 24.1 Shocks and Solitons in ShallowWater 555
 - 24.2 Theory: Continuity and Advection Equations 556
 - 24.2.1 Advection Implementation 558
 - 24.3 Theory: ShockWaves 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 toMatrix 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 ScatteringWave Function (Exploration) 604

Appendix A Codes, Applets, and Animations 607

Bibliography 609

Index 615