

CONTENTS

| | |
|--|-----------|
| Preface | x |
| 1 Introduction | 1 |
| 2 Python programming for physicists | 9 |
| 2.1 Getting started | 9 |
| 2.2 Basic programming | 12 |
| 2.2.1 Variables and assignments | 12 |
| 2.2.2 Variable types | 14 |
| 2.2.3 Output and input statements | 18 |
| 2.2.4 Arithmetic | 23 |
| 2.2.5 Functions, packages, and modules | 31 |
| 2.2.6 Built-in functions | 35 |
| 2.2.7 Comment statements | 37 |
| 2.3 Controlling programs with “if” and “while” | 39 |
| 2.3.1 The if statement | 39 |
| 2.3.2 The while statement | 42 |
| 2.3.3 Break and continue | 43 |
| 2.4 Lists and arrays | 46 |
| 2.4.1 Lists | 47 |
| 2.4.2 Arrays | 53 |
| 2.4.3 Reading an array from a file | 57 |
| 2.4.4 Arithmetic with arrays | 58 |
| 2.4.5 Slicing | 66 |
| 2.5 “For” loops | 67 |
| 2.6 User-defined functions | 75 |
| 2.7 Good programming style | 84 |
| 3 Graphics and visualization | 88 |
| 3.1 Graphs | 88 |

CONTENTS

| | | |
|----------|--|------------|
| 3.2 | Scatter plots | 99 |
| 3.3 | Density plots | 102 |
| 3.4 | 3D graphics | 111 |
| 3.5 | Animation | 117 |
| 4 | Accuracy and speed | 126 |
| 4.1 | Variables and ranges | 126 |
| 4.2 | Numerical error | 128 |
| 4.3 | Program speed | 134 |
| 5 | Integrals and derivatives | 140 |
| 5.1 | Fundamental methods for evaluating integrals | 140 |
| 5.1.1 | The trapezoidal rule | 141 |
| 5.1.2 | Simpson's rule | 144 |
| 5.2 | Errors on integrals | 149 |
| 5.2.1 | Practical estimation of errors | 153 |
| 5.3 | Choosing the number of steps | 155 |
| 5.4 | Romberg integration | 159 |
| 5.5 | Higher-order integration methods | 163 |
| 5.6 | Gaussian quadrature | 165 |
| 5.6.1 | Nonuniform sample points | 165 |
| 5.6.2 | Sample points for Gaussian quadrature | 168 |
| 5.6.3 | Errors on Gaussian quadrature | 175 |
| 5.7 | Choosing an integration method | 177 |
| 5.8 | Integrals over infinite ranges | 179 |
| 5.9 | Multiple integrals | 182 |
| 5.10 | Derivatives | 188 |
| 5.10.1 | Forward and backward differences | 188 |
| 5.10.2 | Errors | 189 |
| 5.10.3 | Central differences | 191 |
| 5.10.4 | Higher-order approximations for derivatives | 194 |
| 5.10.5 | Second derivatives | 197 |
| 5.10.6 | Partial derivatives | 198 |
| 5.10.7 | Derivatives of noisy data | 199 |
| 5.11 | Interpolation | 202 |
| 6 | Solution of linear and nonlinear equations | 214 |
| 6.1 | Simultaneous linear equations | 214 |
| 6.1.1 | Gaussian elimination | 215 |

| | | |
|----------|--|------------|
| 6.1.2 | Backsubstitution | 217 |
| 6.1.3 | Pivoting | 221 |
| 6.1.4 | LU decomposition | 222 |
| 6.1.5 | Calculating the inverse of a matrix | 231 |
| 6.1.6 | Tridiagonal and banded matrices | 232 |
| 6.2 | Eigenvalues and eigenvectors | 241 |
| 6.3 | Nonlinear equations | 250 |
| 6.3.1 | The relaxation method | 250 |
| 6.3.2 | Rate of convergence of the relaxation method | 255 |
| 6.3.3 | Relaxation method for two or more variables | 261 |
| 6.3.4 | Binary search | 263 |
| 6.3.5 | Newton's method | 268 |
| 6.3.6 | The secant method | 273 |
| 6.3.7 | Newton's method for two or more variables | 275 |
| 6.4 | Maxima and minima of functions | 278 |
| 6.4.1 | Golden ratio search | 279 |
| 6.4.2 | The Gauss–Newton method and gradient descent | 286 |
| 7 | Fourier transforms | 289 |
| 7.1 | Fourier series | 289 |
| 7.2 | The discrete Fourier transform | 292 |
| 7.2.1 | Positions of the sample points | 297 |
| 7.2.2 | Two-dimensional Fourier transforms | 299 |
| 7.2.3 | Physical interpretation of the Fourier transform | 300 |
| 7.3 | Discrete cosine and sine transforms | 304 |
| 7.3.1 | Technological applications of cosine transforms | 308 |
| 7.4 | Fast Fourier transforms | 310 |
| 7.4.1 | Formulas for the FFT | 313 |
| 7.4.2 | Standard functions for fast Fourier transforms | 315 |
| 7.4.3 | Fast cosine and sine transforms | 318 |
| 8 | Ordinary differential equations | 327 |
| 8.1 | First-order differential equations with one variable | 327 |
| 8.1.1 | Euler's method | 328 |
| 8.1.2 | The Runge–Kutta method | 331 |
| 8.1.3 | The fourth-order Runge–Kutta method | 336 |
| 8.1.4 | Solutions over infinite ranges | 340 |
| 8.2 | Differential equations with more than one variable | 343 |

CONTENTS

| | | |
|-----------|---|------------|
| 8.3 | Second-order differential equations | 347 |
| 8.4 | Varying the step size | 355 |
| 8.5 | Other methods for differential equations | 364 |
| 8.5.1 | The leapfrog method | 364 |
| 8.5.2 | Time reversal and energy conservation | 367 |
| 8.5.3 | The Verlet method | 371 |
| 8.5.4 | The modified midpoint method | 374 |
| 8.5.5 | The Bulirsch–Stoer method | 377 |
| 8.5.6 | Interval size for the Bulirsch–Stoer method | 387 |
| 8.6 | Boundary value problems | 388 |
| 8.6.1 | The shooting method | 388 |
| 8.6.2 | The relaxation method | 392 |
| 8.6.3 | Eigenvalue problems | 392 |
| 9 | Partial differential equations | 404 |
| 9.1 | Boundary value problems and the relaxation method | 406 |
| 9.2 | Faster methods for boundary value problems | 414 |
| 9.2.1 | Overrelaxation | 414 |
| 9.2.2 | The Gauss–Seidel method | 415 |
| 9.3 | Initial value problems | 418 |
| 9.3.1 | The FTCS method | 419 |
| 9.3.2 | Numerical stability | 425 |
| 9.3.3 | The implicit and Crank–Nicolson methods | 432 |
| 9.3.4 | Spectral methods | 435 |
| 10 | Random processes and Monte Carlo methods | 444 |
| 10.1 | Random numbers | 444 |
| 10.1.1 | Random number generators | 445 |
| 10.1.2 | Random number seeds | 449 |
| 10.1.3 | Random numbers and secret codes | 450 |
| 10.1.4 | Probabilities and biased coins | 453 |
| 10.1.5 | Nonuniform random numbers | 457 |
| 10.1.6 | Gaussian random numbers | 460 |
| 10.2 | Monte Carlo integration | 464 |
| 10.2.1 | The mean value method | 468 |
| 10.2.2 | Integrals in many dimensions | 470 |
| 10.2.3 | Importance sampling | 472 |
| 10.3 | Monte Carlo simulation | 476 |

| | | |
|--------------------|---|------------|
| 10.3.1 | Importance sampling and statistical mechanics | 476 |
| 10.3.2 | The Markov chain method | 479 |
| 10.4 | Simulated annealing | 490 |
| 11 | Using what you have learned | 502 |
| Appendices: | | |
| A | Installing Python | 508 |
| B | Differences between Python versions | 510 |
| C | Gaussian quadrature | 514 |
| D | Convergence of Markov chain Monte Carlo calculations | 520 |
| E | Useful programs | 523 |
| Index | | 532 |