Contents

Preface *page* xi

1 Introduction 1
- 1.1 Scientific software 1
- 1.2 The plan of this book 4
- 1.3 Can Python compete with compiled languages? 8
- 1.4 Limitations of this book 9
- 1.5 Installing Python and add-ons 9

2 Getting started with *IPython* 11
- 2.1 Generalities 11
- 2.2 Tab completion 12
- 2.3 Introspection 12
- 2.4 History 13
- 2.5 Magic commands 14
- 2.6 The magic `%run` command 15

3 A short Python tutorial 20
- 3.1 Typing Python 20
- 3.2 Objects and identifiers 21
- 3.3 Numbers 23
  - 3.3.1 Integers 23
  - 3.3.2 Real numbers 23
  - 3.3.3 Boolean numbers 24
  - 3.3.4 Complex numbers 25
- 3.4 Namespaces and modules 25
- 3.5 Container objects 27
  - 3.5.1 *Lists* 27
  - 3.5.2 *List* indexing 28
  - 3.5.3 *List* slicing 28
  - 3.5.4 *List* mutability 30
  - 3.5.5 *Tuples* 31
  - 3.5.6 *Strings* 31
  - 3.5.7 *Dictionaries* 32

Published online by Cambridge University Press

3.6 Python *if* statements 32
3.7 Loop constructs 33
3.7.1 The Python *for* loop 34
3.7.2 The Python *continue* statement 35
3.7.3 The Python *break* statement 35
3.7.4 *List* comprehensions 36
3.7.5 Python *while* loops 37
3.8 Functions 37
3.8.1 Syntax and scope 38
3.8.2 Positional arguments 41
3.8.3 Keyword arguments 41
3.8.4 Variable number of positional arguments 41
3.8.5 Variable number of keyword arguments 42
3.8.6 The Python *print* function 42
3.8.7 Anonymous functions 44
3.9 Introduction to Python classes 45
3.10 The structure of Python 47
3.11 Prime numbers: a worked example 48

4 *Numpy* 52
4.1 One-dimensional arrays 54
4.1.1 Ab initio constructors 54
4.1.2 Look alike constructors 55
4.1.3 Arithmetical operations on vectors 56
4.1.4 Ufuncs 58
4.1.5 Logical operations on vectors 59
4.2 Two-dimensional arrays 62
4.2.1 Broadcasting 63
4.2.2 Ab initio constructors 64
4.2.3 Look alike constructors 65
4.2.4 Operations on arrays and ufuncs 66
4.3 Higher-dimensional arrays 66
4.4 Domestic input and output 67
4.4.1 Discursive output and input 67
4.4.2 *Numpy* text output and input 69
4.4.3 *Numpy* binary output and input 69
4.5 Foreign input and output 70
4.5.1 Small amounts of data 70
4.5.2 Large amounts of data 71
4.6 Miscellaneous ufuncs 71
4.6.1 Maxima and minima 71
4.6.2 Sums and products 72
4.6.3 Simple statistics 72
4.7 Polynomials 73

Published online by Cambridge University Press

4.7.1 Converting data to coefficients 73
4.7.2 Converting coefficients to data 73
4.7.3 Manipulating polynomials in coefficient form 74
4.8 Linear algebra 74
4.8.1 Basic operations on matrices 74
4.8.2 More specialized operations on matrices 75
4.8.3 Solving linear systems of equations 75
4.9 More *numpy* and beyond 76
4.9.1 *Scipy* 76
4.9.2 *Scikits* 77

5 Two-dimensional graphics 79
5.1 Introduction 79
5.2 Getting started: simple figures 80
5.2.1 Front-ends 80
5.2.2 Back-ends 80
5.2.3 A simple figure 81
5.2.4 Interactive controls 82
5.3 Cartesian plots 83
5.3.1 The *matplotlib* `plot` function 83
5.3.2 Curve styles 83
5.3.3 Marker styles 84
5.3.4 Axes, grid, labels and title 85
5.3.5 A not-so-simple example: partial sums of Fourier series 86
5.4 Polar plots 87
5.5 Error bars 88
5.6 Text and annotations 89
5.7 Displaying mathematical formulae 90
5.7.1 Non-LaTeX users 90
5.7.2 LaTeX users 91
5.7.3 Alternatives for LaTeX users 92
5.8 Contour plots 92
5.9 Compound figures 95
5.9.1 Multiple figures 95
5.9.2 Multiple plots 96
5.10 Animations 98
5.10.1 In situ animations 99
5.10.2 Movies 100
5.11 Mandelbrot sets: a worked example 102

6 Three-dimensional graphics 107
6.1 Introduction 107
6.1.1 Three-dimensional data sets 107
6.1.2 The reduction to two dimensions 108

Published online by Cambridge University Press

6.2 Visualization software 109
6.3 A three-dimensional curve 110
6.3.1 Visualizing the curve with *mplot3d* 111
6.3.2 Visualizing the curve with *mlab* 112
6.4 A simple surface 114
6.4.1 Visualizing the simple surface with *mplot3d* 114
6.4.2 Visualizing the simple surface with *mlab* 116
6.5 A parametrically defined surface 117
6.5.1 Visualizing Enneper's surface using *mplot3d* 117
6.5.2 Visualizing Enneper's surface using *mlab* 119
6.6 Three-dimensional visualization of a Julia set 120

7 Ordinary differential equations 122
7.1 Initial value problems 122
7.2 Basic concepts 122
7.3 The `odeint` function 125
7.3.1 Theoretical background 125
7.3.2 Practical usage 127
7.4 Two-point boundary value problems 132
7.4.1 Introduction 132
7.4.2 Formulation of the boundary value problem 133
7.4.3 A simple example 135
7.4.4 A linear eigenvalue problem 136
7.4.5 A non-linear boundary value problem 138
7.5 Delay differential equations 142
7.5.1 A model equation 143
7.5.2 More general equations and their numerical solution 144
7.5.3 The logistic equation 145
7.5.4 The Mackey–Glass equation 147
7.6 Stochastic differential equations 150
7.6.1 The Wiener process 150
7.6.2 The Itô calculus 152
7.6.3 Itô and Stratanovich stochastic integrals 155
7.6.4 Numerical solution of stochastic differential equations 156

8 Partial differential equations: a pseudospectral approach 163
8.1 Initial-boundary value problems 163
8.2 Method of lines 164
8.3 Spatial derivatives via finite differencing 164
8.4 Spatial derivatives by spectral techniques for periodic problems 165
8.5 The IVP for spatially periodic problems 167
8.6 Spectral techniques for non-periodic problems 170
8.7 An introduction to `f2py` 172
8.7.1 Simple examples with scalar arguments 172

Published online by Cambridge University Press

8.7.2 Vector arguments 174
8.7.3 A simple example with multi-dimensional arguments 175
8.7.4 Undiscussed features of `f2py` 176
8.8 A real-life `f2py` example 177
8.9 Worked example: Burgers' equation 178
8.9.1 Boundary conditions: the traditional approach 179
8.9.2 Boundary conditions: the penalty approach 179

9 Case study: multigrid 184
9.1 The one-dimensional case 185
9.1.1 Linear elliptic equations 185
9.1.2 Smooth and rough modes 186
9.2 The tools of multigrid 186
9.2.1 Relaxation methods 186
9.2.2 Residual and error 189
9.2.3 Prolongation and restriction 190
9.3 Multigrid schemes 191
9.3.1 The two-grid algorithm 192
9.3.2 The V-cycle scheme 193
9.3.3 The full multigrid scheme (FMG) 194
9.4 A simple Python multigrid implementation 195
9.4.1 Utility functions 196
9.4.2 Smoothing functions 197
9.4.3 Multigrid functions 199

Appendix A Installing a Python environment 205
A.1 Installing Python packages 205
A.2 Communicating with Python 206
A.2.1 Editors for programming 206
A.2.2 The *IPython*-editor interaction 207
A.2.3 The two windows approach 207
A.2.4 Calling the editor from within *IPython* 208
A.2.5 Calling *IPython* from within the editor 208
A.2.6 The *IPython* pager 208
A.3 The Python Package Index 209

Appendix B Fortran77 subroutines for pseudospectral methods 210
References 216
Index 218

Published online by Cambridge University Press

Published online by Cambridge University Press