

Contents

I	Introduction to Numerical Methods in Physics	1
1	Introduction	3
1.1	Choice of programming language	5
1.2	Designing programs	6
2	Introduction to C++ and Fortran	9
2.1	Introduction	9
2.2	Getting started	9
2.2.1	Scientific hello world	12
2.3	Representation of integer numbers	16
2.3.1	Fortran codes	18
2.3.2	Python codes	19
2.4	Real numbers and numerical precision	20
2.4.1	Representation of real numbers	21
2.4.2	Machine numbers	22
2.5	Programming examples on loss of precision and round-off errors	25
2.5.1	Algorithms for e^{-x}	25
2.5.2	Fortran codes	28
2.5.3	Further examples	31
2.6	Additional features of C++ and Fortran	34
2.6.1	Operators in C++	34
2.6.2	Pointers and arrays in C++.	35
2.6.3	Macros in C++	37
2.6.4	Structures in C++ and TYPE in Fortran	39
2.7	Exercises and projects	40
3	Numerical differentiation	45
3.1	Introduction	45
3.2	Numerical differentiation	45
3.2.1	The second derivative of e^x	49
3.2.2	Error analysis	59
3.3	Exercises and projects	62
4	Linear algebra	63
4.1	Introduction	63
4.2	Mathematical intermezzo	64

4.3	Programming details	67
4.3.1	Declaration of fixed-sized vectors and matrices	68
4.3.2	Runtime declarations of vectors and matrices in C++	69
4.3.3	Matrix operations and C++ and Fortran features of matrix handling	74
4.4	Linear Systems	78
4.4.1	Gaussian elimination	80
4.4.2	LU decomposition of a matrix	83
4.4.3	Solution of linear systems of equations	87
4.4.4	Inverse of a matrix and the determinant	89
4.4.5	Tridiagonal systems of linear equations	94
4.5	Singular value decomposition	96
4.6	Exercises and projects	96
5	Non-linear equations and roots of polynomials	105
5.1	Introduction	105
5.2	Iteration methods	106
5.3	Bisection method	108
5.4	Newton-Raphson's method	110
5.5	The secant method and other methods	113
5.6	Exercises and projects	115
6	Numerical interpolation, extrapolation and fitting of data	117
6.1	Introduction	117
6.2	Interpolation and extrapolation	117
6.2.1	Polynomial interpolation and extrapolation	117
6.3	Richardson's deferred extrapolation method	120
6.4	Qubic spline interpolation	121
7	Numerical integration	125
7.1	Introduction	125
7.2	Newton-Cotes quadrature: equal step methods	125
7.2.1	Romberg integration	131
7.3	Gaussian quadrature	131
7.3.1	Orthogonal polynomials, Legendre	134
7.3.2	Mesh points and weights with orthogonal polynomials	137
7.3.3	Application to the case $N = 2$	138
7.3.4	General integration intervals for Gauss-Legendre	139
7.3.5	Other orthogonal polynomials	140
7.3.6	Applications to selected integrals	141
7.4	Treatment of singular Integrals	144
7.5	Adaptive quadrature methods	146
7.6	Multi-dimensional integrals	146
7.7	Parallel computing	146
7.7.1	Brief survey of supercomputing concepts and terminologies	146
7.7.2	Parallelism	147
7.7.3	MPI with simple examples	149
7.7.4	Numerical integration with MPI	154

8	Outline of the Monte-Carlo strategy	159
8.1	Introduction	159
8.1.1	First illustration of the use of Monte-Carlo methods, crude integration	161
8.1.2	Second illustration, particles in a box	165
8.1.3	Radioactive decay	167
8.1.4	Program example for radioactive decay of one type of nucleus	168
8.1.5	Brief summary	170
8.2	Probability distribution functions	170
8.2.1	Multivariable Expectation Values	173
8.2.2	The central limit theorem	175
8.3	Random numbers	176
8.3.1	Properties of selected random number generators	180
8.4	Improved Monte Carlo integration	181
8.4.1	Change of variables	183
8.4.2	Importance sampling	187
8.4.3	Acceptance-Rejection method	188
8.5	Monte Carlo integration of multidimensional integrals	189
8.5.1	Brute force integration	190
8.5.2	Importance sampling	191
8.6	Exercises and projects	193
9	Random walks and the Metropolis algorithm	197
9.1	Motivation	197
9.2	Diffusion equation and random walks	198
9.2.1	Diffusion equation	198
9.2.2	Random walks	200
9.3	Microscopic derivation of the diffusion equation	204
9.3.1	Discretized diffusion equation and Markov chains	206
9.3.2	Continuous equations	210
9.3.3	Numerical simulation	212
9.4	Entropy and Equilibrium Features	214
9.5	The Metropolis algorithm and detailed balance	217
9.6	Exercises and projects	220
10	Monte Carlo methods in statistical physics	225
10.1	Introduction and motivation	225
10.2	Review of Statistical Physics	227
10.2.1	Microcanonical Ensemble	228
10.2.2	Canonical Ensemble	229
10.2.3	Grand Canonical and Pressure Canonical	230
10.3	Ising model and phase transitions in magnetic systems	231
10.3.1	Theoretical background	231
10.3.2	Phase Transitions	240
10.4	The Metropolis algorithm and the two-dimensional Ising Model	241
10.5	Selected results for the Ising model	248
10.6	Correlation functions and further analysis of the Ising model	251
10.6.1	Thermalization	251

10.6.2	Time-correlation functions	254
10.7	Exercises and projects	257
11	Quantum Monte Carlo methods	261
11.1	Introduction	261
11.2	Postulates of Quantum Mechanics	263
11.2.1	Mathematical Properties of the Wave Functions	263
11.2.2	Important Postulates	264
11.3	First Encounter with the Variational Monte Carlo Method	265
11.4	Variational Monte Carlo for quantum mechanical systems	267
11.4.1	First illustration of variational Monte Carlo methods	269
11.5	Variational Monte Carlo for atoms	271
11.5.1	The Born-Oppenheimer Approximation	272
11.5.2	The hydrogen Atom	273
11.5.3	Metropolis sampling for the hydrogen atom and the harmonic oscillator	278
11.5.4	The helium atom	282
11.5.5	Program example for atomic systems	286
11.5.6	Helium and beyond	291
11.6	The H_2^+ molecule	293
11.7	Exercises and projects	294
12	Eigensystems	299
12.1	Introduction	299
12.2	Eigenvalue problems	299
12.3	Similarity transformations	300
12.4	Jacobi's method	301
12.4.1	Parallel Jacobi algorithm	303
12.5	Diagonalization through the Householder's method for tridiagonalization	303
12.5.1	The Householder's method for tridiagonalization	304
12.5.2	Diagonalization of a tridiagonal matrix	305
12.6	The QR algorithm for finding eigenvalues	307
12.7	Schrödinger's equation through diagonalization	307
12.7.1	Numerical solution of the Schrödinger equation by diagonalization	309
12.7.2	Program example and results for the one-dimensional harmonic oscillator	310
12.8	Discussion of BLAS and LAPACK functionalities	315
12.9	Exercises and projects	315
13	Differential equations	319
13.1	Introduction	319
13.2	Ordinary differential equations	320
13.3	Finite difference methods	321
13.3.1	Improvements to Euler's algorithm, higher-order methods	323
13.3.2	Predictor-Corrector methods	324
13.4	More on finite difference methods, Runge-Kutta methods	325
13.5	Adaptive Runge-Kutta and multistep methods	327
13.6	Physics examples	328
13.6.1	Ideal harmonic oscillations	328

13.6.2	Damping of harmonic oscillations and external forces	333
13.6.3	The pendulum, a nonlinear differential equation	335
13.6.4	Spinning magnet	337
13.7	Physics Project: the pendulum	338
13.7.1	Analytic results for the pendulum	338
13.7.2	The pendulum code	341
13.8	Exercises and projects	346
13.8.1	Equilibrium equations	352
14	Two point boundary value problems	359
14.1	Introduction	359
14.2	Shooting methods	360
14.2.1	Improved approximation to the second derivative, Numerov's method	360
14.2.2	Wave equation with constant acceleration	362
14.2.3	Schrödinger equation for spherical potentials	366
14.3	Numerical procedure, shooting and matching	367
14.3.1	Algorithm for solving Schrödinger's equation	368
14.4	Green's function approach	370
14.5	Projects and exercises	374
15	Partial differential equations	379
15.1	Introduction	379
15.2	Diffusion equation	381
15.2.1	Explicit scheme	382
15.2.2	Implicit scheme	386
15.2.3	Crank-Nicolson scheme	389
15.2.4	Numerical truncation	390
15.2.5	Analytic solution for the one-dimensional diffusion equation	391
15.3	Laplace's and Poisson's equations	393
15.3.1	Jacobi Algorithm for solving Laplace's equation	395
15.3.2	Laplace's equation and the parallel Jacobi algorithm	396
15.3.3	Relaxation methods for boundary value problems with parallel implementation	396
15.4	Wave equation in two dimensions	396
15.4.1	Analytic solution	398
15.5	Exercises and projects	400
II	Advanced topics	403
16	Many-body approaches to studies of atoms and molecules	405
16.1	Introduction	405
16.2	Hartree-Fock theory	407
16.2.1	Derivation of the Hartree-Fock equations	411
16.2.2	Solving the Hartree-Fock Equations	418
16.3	Density functional theory	418
16.4	Variational Monte Carlo studies with importance sampling	419
16.5	Exercises and projects	419

17 Many-body methods for Bose-Einstein condensation	423
17.1 Bose-Einstein condensation in atoms	423
17.2 Exercises and projects	424
18 Modelling Phase Transitions in Statistical Physics	431
19 Quantum Information Theory and Quantum Algorithms	433
III Programs and additional notes on C++, MPI and Fortran 90/95	435
A Additional C++, Python and Fortran programming features	437
A.1 Classes, templates and Blitz++	437
A.1.1 The Complex class	438
A.2 The vector class	446
A.3 Modules in Fortran	452
A.4 Debugging of codes	456
A.5 How to make figures with Gnuplot	457