

Contents

Preface	v
1 Introduction to computer simulation	1
1.1 Physics and computational physics	1
1.2 Choice of programming language	5
1.3 Outfitting your PC for scientific computing	13
1.4 History of computing in a nutshell	17
1.5 Number representation: bits and bytes in computer memory	22
1.5.1 Addition and subtraction of dual integer numbers	24
1.5.2 Basic data types	29
1.6 The role of algorithms in scientific computing	41
1.6.1 Efficient and inefficient calculations	43
1.6.2 Asymptotic analysis of algorithms	51
1.6.3 Merge sort and divide-and-conquer	56
1.7 Theory, modeling and computer simulation	59
1.7.1 What is a theory?	59
1.7.2 What is a model?	67
1.7.3 Model systems: particles or fields?	72
1.7.4 The linear chain as a model system	74
1.7.5 From modeling to computer simulation	78
1.8 Exercises	81
1.8.1 Addition of bit patterns of 1 byte duals	81
1.8.2 Subtracting dual numbers using two's complement	81
1.8.3 Comparison of running times	81
1.8.4 Asymptotic notation	82
1.9 Chapter literature	83
2 Scientific Computing in C	84
2.1 Introduction	84
2.1.1 Basics of a UNIX/Linux programming environment	87
2.2 First steps in C	99
2.2.1 Variables in C	101
2.2.2 Global variables	103

2.2.3	Operators in C	104
2.2.4	Control structures	108
2.2.5	Scientific “Hello world!”	111
2.2.6	Streams – input/output functionality	116
2.2.7	The preprocessor and symbolic constants	119
2.2.8	The function <i>scanf()</i>	122
2.3	Programming examples of rounding errors and loss of precision	125
2.3.1	Algorithms for calculating e^{-x}	130
2.3.2	Algorithm for summing $1/n$	133
2.4	Details on C-Arrays	137
2.4.1	Direct initialization of certain array elements (C99)	141
2.4.2	Arrays with variable length (C99)	141
2.4.3	Arrays as function parameters	142
2.4.4	Pointers	144
2.4.5	Pointers as function parameters	152
2.4.6	Pointers to functions as function parameters	154
2.4.7	Strings	159
2.5	Structures and their representation in computer memory	161
2.5.1	Blending structs and arrays	163
2.6	Numerical differentiation and integration	165
2.6.1	Numerical differentiation	166
2.6.2	Case study: the second derivative of e^x	169
2.6.3	Numerical integration	176
2.7	Remarks on programming and software engineering	181
2.7.1	Good software development practices	181
2.7.2	Reduction of complexity	184
2.7.3	Designing a program	188
2.7.4	Readability of a program	189
2.7.5	Focus your attention by using conventions	190
2.8	Ways to improve your programs	191
2.9	Exercises	193
2.9.1	Questions	193
2.9.2	Errors in programs	194
2.9.3	<i>printf()</i> -statement	197
2.9.4	Assignments	198
2.9.5	Loops	199
2.9.6	Recurrence	199
2.9.7	Macros	200
2.9.8	Strings	200
2.9.9	Structs	201

2.10 Projects	203
2.10.1 Decimal and binary representation	203
2.10.2 Nearest machine number	203
2.10.3 Calculating e^{-x}	203
2.10.4 Loss of precision	204
2.10.5 Summing series	204
2.10.6 Recurrence in orthogonal functions	205
2.10.7 The Towers of Hanoi	205
2.10.8 Spherical harmonics and Legendre polynomials	207
2.10.9 Memory diagram of a battle	208
2.10.10 Computing derivatives numerically	208
2.11 Chapter literature	210
3 Fundamentals of statistical physics	211
3.1 Introduction and basic ideas	212
3.1.1 The macrostate	216
3.1.2 The microstate	218
3.1.3 Information conservation in statistical physics	219
3.1.4 Equations of motion in classical mechanics	225
3.1.5 Statistical physics in phase space	229
3.2 Elementary statistics	235
3.2.1 Random Walk	236
3.2.2 Discrete and continuous probability distributions	241
3.2.3 Reduced probability distributions	242
3.2.4 Important distributions in physics and engineering	244
3.3 Equilibrium distribution	249
3.3.1 The most probable distribution	251
3.3.2 A statistical definition of temperature	253
3.3.3 The Boltzmann distribution and the partition function	255
3.4 The canonical ensemble	258
3.5 Exercises	261
3.5.1 Trajectories of the one-dimensional harmonic oscillator in phase space	261
3.5.2 Important integrals of statistical physics	261
3.5.3 Probability, example from playing cards	261
3.5.4 Rolling dice	262
3.5.5 Problems, using the Poisson density	262
3.5.6 Particle inside a sphere	262

4	Inter- and intramolecular potentials	264
4.1	Introduction	265
4.2	The quantum mechanical origin of particle interactions	266
4.3	The energy hypersurface and classical approximations	270
4.4	Non-bonded interactions	271
4.5	Pair potentials	274
4.5.1	Repulsive Interactions	275
4.5.2	Electric multipoles and multipole expansion	280
4.5.3	Charge-dipole interaction	280
4.5.4	Dipole-dipole interaction	283
4.5.5	Dipole-dipole interaction and temperature	284
4.5.6	Induction energy	285
4.5.7	Dispersion energy	287
4.5.8	Further remarks on pair potentials	288
4.6	Bonded interactions	291
4.7	Chapter literature	292
5	Molecular Dynamics simulations	294
5.1	Introduction	295
5.1.1	Historical notes on MD	299
5.1.2	Limitations of MD	303
5.2	Numerical integration of differential equations	309
5.2.1	Ordinary differential equations	309
5.2.2	Finite Difference methods	310
5.2.3	Improvements to Euler's algorithm	316
5.2.4	Predictor-corrector methods	317
5.2.5	Runge-Kutta methods	318
5.3	Integrating Newton's equation of motion: the Verlet algorithm	320
5.4	The basic MD algorithm	323
5.5	Basic MD: planetary motion	327
5.5.1	Preprocessor statements and basic definitions	327
5.5.2	Organization of the data	328
5.5.3	Function that computes the energy	328
5.5.4	The Verlet velocity algorithm	329
5.5.5	The force calculation	329
5.5.6	The initialization and output functions	332
5.5.7	The <i>main()</i> -function	332
5.6	Planetary motion: suggested project	335

5.7	Periodic boundary conditions	337
5.8	Minimum image convention	338
5.9	Lyapunov instability	338
5.10	Case study: static and dynamic properties of a microcanonical LJ fluid	341
5.10.1	Microcanonical LJ fluid: suggested projects	346
5.11	Chapter literature	356
6	Monte Carlo simulations	357
6.1	Introduction to MC simulation	357
6.1.1	Historical remarks	360
6.2	Simple random numbers	362
6.2.1	The linear congruential method	365
6.2.2	Monte Carlo integration – simple sampling	369
6.3	Case study: MC simulation of harddisks	378
6.3.1	Trial moves	378
6.3.2	Case study: MC simulation of harddisks – suggested exercises	380
6.4	The Metropolis Monte Carlo method	381
6.5	The Ising model	383
6.5.1	Case study: Monte Carlo simulation of the 2D Ising magnet	386
6.6	Case Study: NVT MC of dumbbell molecules in 2D	392
6.7	Exercises	394
6.7.1	The GSL library	394
6.7.2	Calculating π	395
6.7.3	Simple and importance sampling with random walks in 1D	399
6.7.4	Simple sampling and importance sampling with random walks in 1D	399
6.8	Chapter literature	407
7	Advanced topics, and applications in soft matter	408
7.1	Partial differential equations	408
7.1.1	Elliptic PDEs	410
7.1.2	Parabolic PDEs	411
7.1.3	Hyperbolic PDEs	411
7.2	The finite element method (FEM)	412
7.3	Coarse-grained MD for mesoscopic polymer and biomolecular simulations	414
7.3.1	Why coarse-grained simulations?	414
7.4	Scaling properties of polymers	415

7.5	Ideal polymer chains	416
7.6	Single-chain conformations	420
7.7	The ideal (Gaussian) chain model	421
7.8	Scaling of flexible and semiflexible polymer chains	422
7.9	Constant temperature MD	429
7.10	Velocity scaling using the Behrendsen thermostat	430
7.11	Dissipative particle dynamics thermostat	431
7.12	Case study: NVT Metropolis MC simulation of a LJ fluid	434
7.13	Exercise	443
7.13.1	Dumbbell molecules in 3D	443
A	The software development life cycle	444
B	Installation guide to Cygwin	445
C	Introduction to the UNIX/Linux programming environment	448
C.1	Directory structure	448
C.2	Users, rights and privileges	450
C.3	Some basic commands	453
C.4	Processes	455
C.4.1	Ending processes	455
C.4.2	Processes priorities and resources	455
C.5	The Bash	457
C.6	Tips and tricks	458
C.7	Useful programs	458
C.7.1	Remote connection: ssh	459
C.7.2	Gnuplot	459
C.7.3	Text editors: vi, EMACS and others	459
D	Sample program listings	470
D.1	Sample code for file handling	470
E	Reserved keywords in C	473
F	Functions of the standard library <code><string.h></code>	474
G	Elementary combinatorial problems	475
G.1	How many differently ordered sequences of N objects are possible?	475
G.2	In how many ways can N objects be divided into two piles, with n and m objects, respectively?	475

G.3 In how many ways can N objects be arranged in $r + 1$ piles with n_j objects in pile number j with $j \in [0, 1, \dots, r]$?	476
G.4 Stirling's approximation of large numbers	476
H Some useful constants	477
I Installing the GNU Scientific Library, GSL	478
J Standard header files of the <i>ANSI-C</i> library	479
K The central limit theorem	480
Bibliography	481
Acronyms	505
Index	506
Authors	509

The source code of more than two dozen of the program listings is available on the Walter de Gruyter webpage:

<http://www.degruyter.com/staticfiles/pdfs/9783110255904AccompanyingPrograms.zip>