

Contents

Foreword	vii
1 The Computer	1
1.1 The Operating System	3
1.1.1 Filesystem	3
1.1.2 Commands	11
1.1.3 Looking for Help	14
1.2 Text Processing Tools – Filters	16
1.3 Programming with Emacs	21
1.3.1 Calling Emacs	21
1.3.2 Interacting with Emacs	23
1.3.3 Basic Editing	24
1.3.4 Cut and Paste	27
1.3.5 Windows	29
1.3.6 Files and Buffers	30
1.3.7 Modes	31
1.3.8 Emacs Help	32
1.3.9 Emacs Customization	34
1.4 The Fortran Programming Language	35
1.4.1 The Foundation	35
1.4.2 Details	45
1.4.3 Arrays	50
1.5 Gnuplot	57
1.6 Shell Scripting	62
2 Kinematics	77
2.1 Motion on the Plane	77
2.1.1 Plotting Data	85
2.1.2 More Examples	88
2.2 Motion in Space	99
2.3 Trapped in a Box	107

2.3.1	The One Dimensional Box	108
2.3.2	Errors	114
2.3.3	The Two Dimensional Box	117
2.4	Applications	121
2.5	Problems	140
3	Logistic Map	145
3.1	Introduction	145
3.2	Fixed Points and 2^n Cycles	147
3.3	Bifurcation Diagrams	154
3.4	The Newton-Raphson Method	157
3.5	Calculation of the Bifurcation Points	163
3.6	Liapunov Exponents	167
3.7	Problems	180
4	Motion of a Particle	191
4.1	Numerical Integration of Newton's Equations	191
4.2	Prelude: Euler Methods	192
4.3	Runge–Kutta Methods	204
4.3.1	A Program for the 4th Order Runge–Kutta	208
4.4	Comparison of the Methods	212
4.5	The Forced Damped Oscillator	215
4.6	The Forced Damped Pendulum	222
4.7	Appendix: On the Euler–Verlet Method	229
4.8	Appendix: 2nd order Runge–Kutta Method	233
4.9	Problems	236
5	Planar Motion	241
5.1	Runge–Kutta for Planar Motion	241
5.2	Projectile Motion	246
5.3	Planetary Motion	252
5.4	Scattering	256
5.4.1	Rutherford Scattering	260
5.4.2	More Scattering Potentials	267
5.5	More Particles	270
5.6	Problems	281
6	Motion in Space	285
6.1	Adaptive Stepsize Control for Runge–Kutta Methods	286
6.2	Motion of a Particle in an EM Field	295
6.3	Relativistic Motion	296

6.4	Problems	307
7	Electrostatics	311
7.1	Electrostatic Field of Point Charges	311
7.2	The Program – Appetizer and ... Desert	314
7.3	The Program – Main Dish	323
7.4	The Program - Conclusion	329
7.5	Electrostatic Field in the Vacuum	334
7.6	Results	341
7.7	Poisson Equation	342
7.8	Problems	349
8	Diffusion Equation	353
8.1	Introduction	353
8.2	Heat Conduction in a Thin Rod	355
8.3	Discretization	356
8.4	The Program	358
8.5	Results	361
8.6	Diffusion on the Circle	363
8.7	Analysis	366
8.8	Problems	370
9	The Anharmonic Oscillator	373
9.1	Introduction	373
9.2	Calculation of the Eigenvalues of $H_{nm}(\lambda)$	375
9.3	Results	384
9.4	The Double Well Potential	390
9.5	Problems	398
10	Time Independent Schrödinger Equation	401
10.1	Introduction	401
10.2	The Infinite Potential Well	404
10.3	Bound States	415
10.4	Measurements	424
10.5	The Anharmonic Oscillator - Again...	431
10.6	The Lennard–Jones Potential	435
10.7	Problems	438
11	The Random Walker	443
11.1	(Pseudo)Random Numbers	444
11.2	Using Pseudorandom Number Generators	456

11.3	Random Walks	463
11.4	Problems	471
12	Monte Carlo Simulations	475
12.1	Statistical Physics	476
12.2	Entropy	479
12.3	Fluctuations	483
12.4	Correlation Functions	485
12.5	Sampling	487
	12.5.1 Simple Sampling	488
	12.5.2 Importance Sampling	489
12.6	Markov Processes	490
12.7	Detailed Balance Condition	491
12.8	Problems	493
13	Simulation of the $d = 2$ Ising Model	495
13.1	The Ising Model	495
13.2	Metropolis	501
13.3	Implementation	504
	13.3.1 The Program	509
	13.3.2 Towards a Convenient User Interface	515
13.4	Thermalization	527
13.5	Autocorrelations	529
13.6	Statistical Errors	536
	13.6.1 Errors of Independent Measurements	537
	13.6.2 Jackknife	540
	13.6.3 Bootstrap	542
13.7	Appendix: Autocorrelation Function	543
13.8	Appendix: Error Analysis	551
	13.8.1 The Jackknife Method	551
	13.8.2 The Bootstrap Method	555
	13.8.3 Comparing the Methods	558
13.9	Problems	563
14	Critical Exponents	573
14.1	Critical Slowing Down	575
14.2	Wolff Cluster Algorithm	576
14.3	Implementation	583
	14.3.1 The Program	585
14.4	Production	590
14.5	Data Analysis	593

14.6	Autocorrelation Times	601
14.7	Temperature Scaling	604
14.8	Finite Size Scaling	610
14.9	Calculation of β_c	612
14.10	Studying Scaling with Collapse	617
14.11	Binder Cumulant	627
14.12	Appendix: Scaling	630
14.12.1	Binder Cumulant	630
14.12.2	Scaling	636
14.12.3	Finite Size Scaling	638
14.13	Appendix: Critical Exponents	641
14.13.1	Definitions	641
14.13.2	Hyperscaling Relations	642
14.14	Problems	642
	Bibliography	646
	Index	654