

Contents

1	Introduction — 1
1.1	Goal, contents, and outline — 1
1.2	The environment required for program development — 5
1.2.1	Operating system — 5
1.2.2	Software packages — 6
1.2.3	Graphics — 6
1.2.4	Program development and a simple script — 6
1.3	A first example – the logistic map — 7
1.3.1	Map — 7
1.3.2	FORTRAN — 9
1.3.3	Problems — 12
	Bibliography — 12
2	Nonlinear maps — 13
2.1	Frenkel–Kotorova model — 13
2.1.1	Classical formulation — 13
2.1.2	Equilibrium solutions — 14
2.1.3	The standard map — 14
2.1.4	Problems — 15
2.2	Chaos and Lyapunov exponents — 16
2.2.1	Stability, butterfly effect, and chaos — 16
2.2.2	Lyapunov exponent of the logistic map — 17
2.2.3	Lyapunov exponents for multidimensional maps — 19
2.3	Affine maps and fractals — 22
2.3.1	Sierpinski triangle — 23
2.3.2	About ferns and other plants — 25
2.3.3	Problems — 26
2.4	Fractal dimension — 26
2.4.1	Box-counting — 26
2.4.2	Application: Sierpinski triangle — 27
2.4.3	Problem — 28
2.5	Neural networks — 29
2.5.1	Perceptron — 29
2.5.2	Self-organized maps: Kohonen’s model — 36
2.5.3	Problems — 40
	Bibliography — 40
3	Dynamical systems — 42
3.1	Quasilinear differential equations — 42
3.1.1	Example: logistic map and logistic ODE — 44

3.1.2	Problems — 45
3.2	Fixed points and instabilities — 45
3.2.1	Fixed points — 45
3.2.2	Stability — 45
3.2.3	Trajectories — 47
3.2.4	Gradient dynamics — 47
3.2.5	Special case $N = 1$ — 48
3.2.6	Special case $N = 2$ — 48
3.2.7	Special case $N = 3$ — 50
3.3	Hamiltonian systems — 53
3.3.1	Hamilton function and canonical equations — 53
3.3.2	Symplectic integrators — 54
3.3.3	Poincaré section — 60
	Bibliography — 62

4	Ordinary differential equations I, initial value problems — 63
4.1	Newton's mechanics — 63
4.1.1	Equations of motion — 63
4.1.2	The mathematical pendulum — 64
4.2	Numerical methods of the lowest order — 65
4.2.1	Euler method — 65
4.2.2	Numerical stability of the Euler method — 67
4.2.3	Implicit and explicit methods — 68
4.3	Higher order methods — 69
4.3.1	Heun's method — 70
4.3.2	Problems — 73
4.3.3	Runge–Kutta method — 73
4.4	RK4 applications: celestial mechanics — 79
4.4.1	Kepler problem: closed orbits — 79
4.4.2	Quasiperiodic orbits and apsidal precession — 82
4.4.3	Multiple planets: is our solar system stable? — 83
4.4.4	The reduced three-body problem — 86
4.4.5	Problems — 92
4.5	Molecular dynamics (MD) — 93
4.5.1	Classical formulation — 93
4.5.2	Boundary conditions — 94
4.5.3	Microcanonical and canonical ensemble — 95
4.5.4	A symplectic algorithm — 96
4.5.5	Evaluation — 97
4.5.6	Problems — 101
4.6	Chaos — 102
4.6.1	Harmonically driven pendulum — 103

4.6.2	Poincaré section and bifurcation diagrams — 105
4.6.3	Lyapunov exponents — 105
4.6.4	Fractal dimension — 115
4.6.5	Reconstruction of attractors — 117
4.7	Differential equations with periodic coefficients — 119
4.7.1	Floquet theorem — 119
4.7.2	Stability of limit cycles — 121
4.7.3	Parametric instability: pendulum with an oscillating support — 121
4.7.4	Mathieu equation — 123
4.7.5	Problems — 125
	Bibliography — 125
5	Ordinary differential equations II, boundary value problems — 127
5.1	Preliminary remarks — 127
5.1.1	Boundary conditions — 127
5.1.2	Example: ballistic flight — 128
5.2	Finite differences — 129
5.2.1	Discretization — 129
5.2.2	Example: Schrödinger equation — 132
5.3	Weighted residual methods — 138
5.3.1	Weight and base functions — 138
5.3.2	Example: Stark effect — 140
5.4	Nonlinear boundary value problems — 142
5.4.1	Nonlinear systems — 143
5.4.2	Newton–Raphson — 144
5.4.3	Example: the nonlinear Schrödinger equation — 145
5.4.4	Example: a moonshot — 148
5.5	Shooting — 151
5.5.1	The method — 151
5.5.2	Example: free fall with quadratic friction — 152
5.5.3	Systems of equations — 154
5.6	Problems — 155
	Bibliography — 155
6	Ordinary differential equations III, memory, delay and noise — 156
6.1	Why memory? Two examples and numerical methods — 156
6.1.1	Logistic equation – the Hutchinson–Wright equation — 157
6.1.2	Pointer method — 159
6.1.3	Mackey–Glass equation — 160
6.2	Linearized memory equations and oscillatory instability — 163
6.2.1	Stability of a fixed point — 163
6.2.2	One equation, one δ -kernel — 164

6.2.3	One equation, one arbitrary kernel — 169
6.3	Chaos and Lyapunov exponents for memory systems — 171
6.3.1	Projection onto a finite dimensional system of ODEs — 171
6.3.2	Determination of the largest Lyapunov exponent — 171
6.3.3	The complete Lyapunov spectrum — 173
6.3.4	Problems — 174
6.4	Epidemic models — 175
6.4.1	Predator-prey systems and SIR model — 175
6.4.2	SIRS model — 180
6.4.3	SIRS model with infection rate control — 183
6.4.4	Delayed infection rate control — 183
6.4.5	Problems — 186
6.5	Noise and stochastic differential equations — 186
6.5.1	Brownian motion — 186
6.5.2	Stochastic differential equation — 189
6.5.3	Stochastic delay differential equation — 191
6.5.4	SIRS model with delayed and noisy infection rate control — 191
6.6	A microscopic traffic flow model — 194
6.6.1	The model — 194
6.6.2	The nondimensional basic system — 196
6.6.3	Stationary solution and linear stability analysis — 196
6.6.4	The fully nonlinear system – numerical solutions — 199
	Bibliography — 201
7	Partial differential equations I, basics — 202
7.1	Classification — 202
7.1.1	PDEs of the first order — 202
7.1.2	PDEs of the second order — 205
7.1.3	Boundary and initial conditions — 207
7.2	Finite differences — 211
7.2.1	Discretization — 211
7.2.2	Elliptic PDEs, example: Poisson equation — 214
7.2.3	Parabolic PDEs, example: heat equation — 220
7.2.4	Hyperbolic PDEs, example: convection equation, wave equation — 226
7.3	Alternative discretization methods — 232
7.3.1	Chebyshev spectral method — 233
7.3.2	Spectral method by Fourier transformation — 238
7.3.3	Finite-element method — 242
7.4	Nonlinear PDEs — 246
7.4.1	Real Ginzburg–Landau equation — 247
7.4.2	Numerical solution, explicit method — 248
7.4.3	Numerical solution, semi-implicit method — 249

7.4.4	Problems — 251
	Bibliography — 253
8	Partial differential equations II, applications — 254
8.1	Quantum mechanics in one dimension — 254
8.1.1	Stationary two-particle equation — 254
8.1.2	Time-dependent Schrödinger equation — 257
8.2	Quantum mechanics in two dimensions — 263
8.2.1	Schrödinger equation — 264
8.2.2	Algorithm — 264
8.2.3	Evaluation — 265
8.3	Fluid mechanics: flow of an incompressible liquid — 266
8.3.1	Hydrodynamic basic equations — 266
8.3.2	Example: driven cavity — 269
8.3.3	Thermal convection: (A) square geometry — 272
8.3.4	Thermal convection: (B) Rayleigh–Bénard convection — 281
8.4	Pattern formation out of equilibrium — 289
8.4.1	Reaction-diffusion systems — 289
8.4.2	Swift–Hohenberg equation — 298
8.4.3	Problems — 303
	Bibliography — 304
9	Monte Carlo methods — 305
9.1	Random numbers and distributions — 305
9.1.1	Random number generator — 305
9.1.2	Distribution function, probability density, mean values — 306
9.1.3	Other distribution functions — 307
9.2	Monte Carlo integration — 311
9.2.1	Integrals in one dimension — 311
9.2.2	Integrals in higher dimensions — 313
9.3	Applications from statistical physics — 315
9.3.1	Two-dimensional classical gas — 316
9.3.2	The Ising model — 322
9.4	Differential equations derived from variational problems — 332
9.4.1	Diffusion equation — 332
9.4.2	Swift–Hohenberg equation — 334
	Bibliography — 335
A	Matrices and systems of linear equations — 337
A.1	Real-valued matrices — 337
A.1.1	Eigenvalues and eigenvectors — 337
A.1.2	Characteristic polynomial — 337

A.1.3	Notations — 338
A.1.4	Normal matrices — 338
A.2	Complex-valued matrices — 339
A.2.1	Notations — 339
A.2.2	Jordan canonical form — 340
A.3	Inhomogeneous systems of linear equations — 341
A.3.1	Regular and singular system matrices — 341
A.3.2	Fredholm alternative — 342
A.3.3	Regular matrices — 343
A.3.4	LU decomposition — 343
A.3.5	Thomas algorithm — 346
A.4	Homogeneous systems of linear equations — 347
A.4.1	Eigenvalue problems — 347
A.4.2	Diagonalization — 347
A.4.3	Application: zeros of a polynomial — 350
	Bibliography — 351

B Program library — 353

B.1	Routines — 353
B.2	Graphics — 354
B.2.1	init — 354
B.2.2	contur — 354
B.2.3	contur1 — 354
B.2.4	ccontu — 355
B.2.5	image — 355
B.2.6	ccircl — 355
B.3	Runge-Kutta — 355
B.3.1	rkg — 355
B.3.2	drkg — 356
B.3.3	drkadt — 356
B.3.4	rkg_del — 356
B.4	Miscellaneous — 356
B.4.1	tridag – Thomas algorithm — 356
B.4.2	ctrida — 357
B.4.3	dlyap_exp – Lyapunov exponents — 357
B.4.4	dlyap_del – Largest Lyapunov exponent of delay-system — 357
B.4.5	dlyap_exp_del – Lyapunov exponents of delay-system — 358
B.4.6	schmid – orthogonalization — 358
B.4.7	FUNCTION volum – volume in n dimensions — 359
B.4.8	FUNCTION deter – determinant — 359
B.4.9	random_init – random numbers — 359

C Solutions of the problems — 361

- C.1 Chapter 1 — 361**
- C.2 Chapter 2 — 362**
- C.3 Chapter 3 — 362**
- C.4 Chapter 4 — 364**
- C.5 Chapter 5 — 374**
- C.6 Chapter 6 — 376**
- C.7 Chapter 7 — 378**
- C.8 Chapter 8 — 382**

D README and a short guide to FE-tools — 387

- D.1 README — 387**
- D.2 Short guide to finite-element tools from Chapter 7 — 390**
- D.2.1 mesh_generator — 390**
- D.2.2 laplace_solver — 391**
- D.2.3 grid_contur — 392**

Index — 393