

Appendix A: Performing the Computer Experiments

The computer experiments are realized as Java programs which can be run on any platform if a Java runtime environment (JRE) is installed. They are written in a C-like fashion which improves the readability for readers who are not so familiar with object oriented programming. The source code can be studied most conveniently with the netbeans environment which is open source and allows quick generation of graphical user interfaces. The screenshot in Fig. A.1 shows an example.

After downloading and unzipping the zipped file from **extras.springer.com** you have two options.

Run a Program Directly

Open the directory CP-examples in your file manager. If the JRE is installed properly you can start any one of the programs by simply clicking onto it. Under Linux, you can alternatively start it in a console window with e.g.

```
java -jar CPexample.jar
```

Figure A.2 shows a screenshot from computer exercise 23.4 (ladder model for exponential decay).

Open a Program with the Netbeans Environment

If you have the netbeans environment installed, you can import any of the programs as a separate project by opening the corresponding folder in the directory CP-examples/NBprojects/. You may have a look at the source code and compile and run it

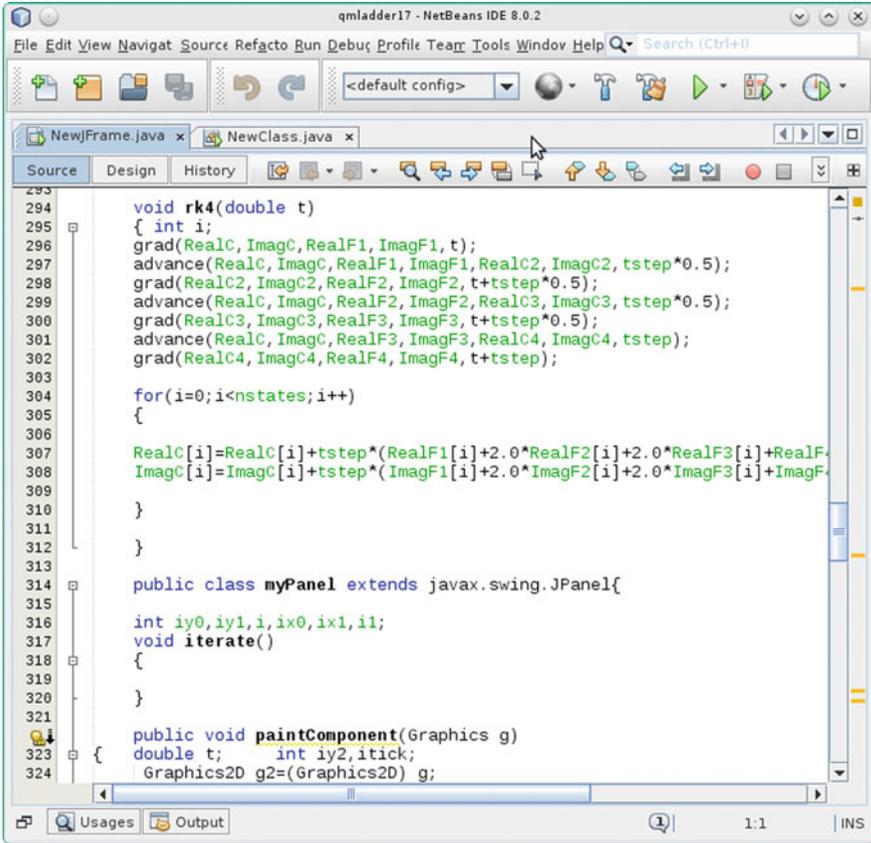


Fig. A.1 Screenshot of the source code

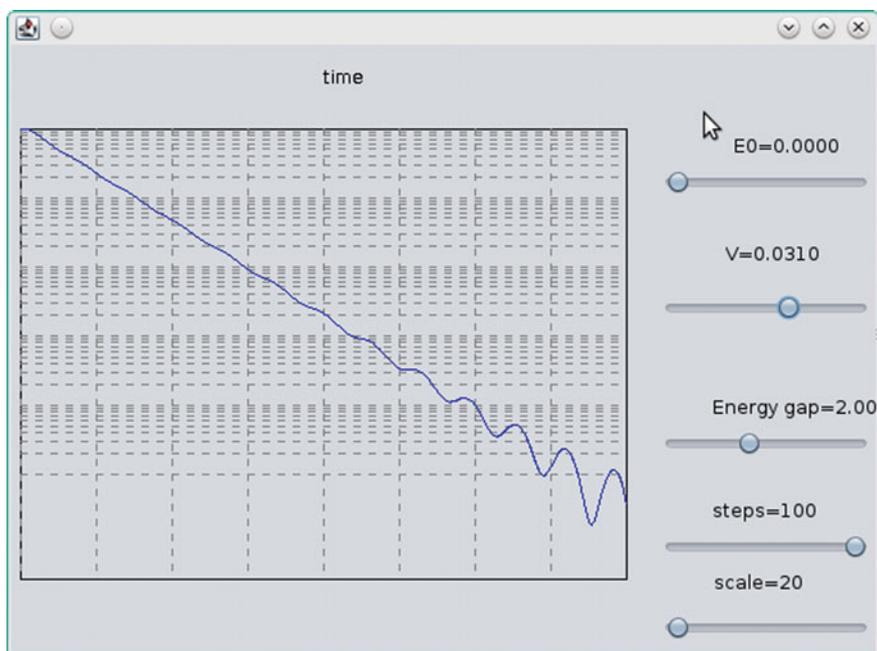


Fig. A.2 Screenshot of computer experiment 23.4

Appendix B: Methods and Algorithms

Purpose	Method	Comments	Pages
Interpolation	Lagrange polynomial	Explicit form, easy to evaluate	19
	Barycentric Lagrange polynomial	For evaluation at many points	19
	Newton's divided differences	New points added easily	21
	Neville method	For evaluation at one point	22
	Spline interpolation	Smoother, less oscillatory	22
	Rational interpolation	Smoother, less oscillatory, often less coefficients necessary	28, 32
	Pade approximation	Often better than Taylor series	29
	Barycentric rational interpolation	Easy to evaluate	30
	Rational interpolation without poles	Alternative to splines, analytical	34
	Multivariate interpolation	Multidimensional	35
	Trigonometric interpolation	Periodic functions	132
Differentiation	One-sided difference quotient	Low error order	39
	Central difference quotient	Higher error order	41
	Extrapolation	High accuracy	41
	Higher derivatives	Finite difference methods	43
	Partial derivatives	Finite difference methods	45

Purpose	Method	Comments	Pages
Integration	Newton-Cotes formulas	Equally spaced points	49
	Trapezoidal rule	Simple, closed interval	49
	Midpoint rule	Simple, open interval	50
	Simpson's rule	More accurate	49
	Composite Newton-Cotes rules	For larger intervals	50
	Extrapolation (Romberg)	High accuracy	51
	Clenshaw-Curtis expressions	Suitable for adaptive and multidimensional quadrature	53
	Gaussian integration	High accuracy if polynomial approximation possible	53
	Monte Carlo integration	High dimensional integrals	202
Linear equations	Gaussian elimination (LU reduction)	Standard method for linear equations and matrix inversion	64
	QR decomposition	Numerically more stable	69
	Iterative solution	Large sparse systems	78
	Richardson iteration	Simplest iterative method	79
	Jacobi relaxation	Iterative matrix-splitting method, converges for diagonally dominant matrices, parallel computation possible	80
	Gauss-Seidel relaxation	Iterative matrix-splitting method, converges for symmetric positive definite or diagonal dominant matrices, no extra storage	81
	Chessboard (black-red)	Two independent subgrids, especially for Poisson equation	402
	Damping and Successive over-relaxation	Speeds up convergence for proper relaxation parameter	81

Purpose	Method	Comments	Pages
	Multigrid method	Fast convergence but more complicated	402
	Conjugate gradients method (CG)	Krylov space method for symmetric positive definite matrices, preconditioning often necessary	86
	General minimum residual method (GMRES)	Krylov space method for nonsymmetric systems	89
	special LU decomposition	Tridiagonal linear equations	75
	Sherman-Morrison formula	Cyclic tridiagonal systems	77
	Root finding	Bisection	Reliable but slow continuous functions
Regula falsi (false position)		Speed and robustness between bisection and interpolation	99
Newton-Raphson		Continuous derivative necessary, converges fast if starting point is close to a root	100
Interpolation (secant)		No derivative necessary, but slower than Newton	101
Inverse interpolation		Mainly used by combined methods	102
Dekker's combined method		Combination of bisection and secant method	106
Brent's combined method		Combination of bisection, secant, and quadratic inverse interpolation methods, very popular	107
Chandrupatla's combined method		Uses quadratic interpolation whenever possible, faster than Brent's method, especially for higher order roots	109
Multidimensional root finding	Newton-Raphson	Needs full Hessian	124
	Quasi-Newton (Broyden)	Hessian not needed, no matrix inversion	125
Function Minimization	Ternary search	No gradient needed, very simple, for unimodal functions	115
	Golden section search (Brent)	Faster than ternary search but more complicated	116

Purpose	Method	Comments	Pages
Multidimensional minimization	Steepest descent	Simple but slow	122
	Conjugate gradients	Faster than steepest descent	124
	Newton-Raphson	Fast, if starting point close to minimum, needs full Hessian	124
	Quasi-Newton (BFGS, DFP)	Hessian not needed, very popular	125
Fourier transformation	Görtzel's algorithm	Efficient if only some Fourier components are needed	136
	Fast Fourier transform	Much faster than direct discrete Fourier transform	138
Time-Frequency Analysis	Short Time Fourier Transform (STFT)	Constant resolution for all frequencies, often used for audio signals	145
	Gabor transform	STFT with Gaussian window represents signal by elementary signals localized in time and frequency	156
	Discrete STFT	Reduced redundancy, still invertible	153
	Continuous Wavelet transform	Constant relative frequency resolution, better time resolution for high frequencies, very time consuming convolution integral	158
	Discrete Wavelet Transform	Uses orthogonal or biorthogonal wavelets, fast scalar product	
	Multiresolution analysis	Represents a signal by a basic approximation and a series of details with increasing resolution	164
	Fast wavelet transform	Recursive filtering, very fast	178
Random numbers	Linear congruent mapping (LC)	Simple pseudo-random number generator	197
	Xorshift	Fast, maximum possible period	197
	Multiply with carry (MWC)	Similar to LC but uses a varying carry	198
	Complementary multiply with carry (CMWC)	Improves MWC, passes many tests	199

Purpose	Method	Comments	Pages
	RN with given distribution	Inverse of cumulative distribution function needed	199
	Random points on unit sphere	Random directions	200
	Gaussian RN (Box-Muller)	Gaussian random numbers	201
Thermodynamic average	Simple sampling	Inefficient	206
	Importance sampling	Samples preferentially important configurations	207
	Metropolis algorithm	Generates configurations according to a canonical distribution	207
Eigenvalue problems	Direct solution	Only for very small dimension	214
	Tridiagonal matrices	Explicit solutions for some special tridiagonal matrices	217
	Jacobi	Simple but not very efficient	214
	Power iteration	Finds dominant eigenvector	225
	QL and QR	Efficient power iteration method for not too large matrices, especially in combination with tridiagonalization by Householder transformations	228
	Lanczos	Iterative method for very large matrices or if only a few eigenvalues are needed	230
	Singular value decomposition (SVD)	Generalization for arbitrary matrices	242
Data fitting	Least square fit	Fit a model function to a set of data	236
	Linear least square fit with normal equations	Simple but less accurate	237
	Linear fit with orthogonalisation	Better numerical stability	239
	Linear fit with SVD	Expensive but more reliable, also for rank deficient matrices	248
	Low rank matrix approximation	Data compression, total linear least squares	245

Purpose	Method	Comments	Pages
Discretization	Method of lines	Continuous time, discretized space	261
	Eigenvector expansion		
	Finite differences	Simplest discretization, uniform grids	259
	Finite volumes	Partial differential equations with a divergence term (conservation laws), flux conservative, allows unstructured meshes and discontinuous material parameters	265
	Finite elements	Very flexible and general discretization method but also more complicated	277
	Spectral methods	Expansion with global basis functions, mostly polynomials and Fourier sums, less expensive than finite elements but not as accurate for discontinuous material parameters and complicated geometries	273
	Dual grid	For finite volumes	265, 409
	Weighted residuals	General method to determine the expansion coefficients	270
	Point collocation	Simplest criterion, often used for nonlinear problems and spectral methods	271
	Sub-domains	More general than finite volumes	271
	Least square	Popular for computational fluid dynamics and electrodynamics	272
	Galerkin	Most widely used criterion, leads often to symmetric matrices	273
	Fourier pseudo-spectral method	Very useful whenever a Laplacian is involved, reduces dispersion	273
Boundary elements	If the Green's function is available	286	

Purpose	Method	Comments	Pages
Time evolution	Explicit forward Euler	Low error order and unstable, mainly used as predictor step	292
	Implicit backward Euler	Low error order but stable, used for stiff problems and as corrector step	295
	Improved Euler (Heun, predictor-corrector)	Higher error order	296
	Nordsieck predictor-corrector	Implicit method, has been used for molecular dynamics	298
	Gear predictor-corrector	Optimized for molecular dynamics	300
	Explicit Runge Kutta (2nd, 3rd, 4th)	General and robust methods, easy step size and quality control	301
	Extrapolation (Gragg-Bulirsch-Stoer)	Very accurate and very slow	305
	Explicit Adams-Bashforth	High error order but not self-starting, for smooth functions, can be used as predictor	306
	Implicit Adams-Moulton	Better stability than explicit method, can be used as corrector	306
	Backward differentiation (Gear)	Implicit, especially for stiff problems	307
	Linear multistep predictor-corrector	General class, includes Adams-Bashforth-Moulton and Gear methods	309
	Verlet integration	Symplectic, time reversible, for molecular dynamics	310
	Position Verlet	Less popular	312
	Velocity Verlet	Often used	313
	Stoermer-Verlet	If velocities are not needed	313
	Beeman's method	Velocities more accurate than for Stoermer-Verlet	315
	Leapfrog	Simple but two different grids	317, 317, 471
	Crank-Nicolson	Implicit, stable, diffusion and Schroedinger equation	486, 474
	FTBS, Lax-Friedrich	simple methods for advection	434, 436
	Lax-Wendroff	Hyperbolic differential equations	472
Taylor-Galerkin	highly accurate for advection	449	
Lax-Wendroff			
Two-step	Differential equation with second order time derivative	464	

Purpose	Method	Comments	Pages
	Reduction to a first order equation	Derivatives treated as additional variables	467
	Two-variable	Transforms wave equation into a system of two first order equations	470
	Split operator	Approximates an operator by a product	490, 311, 533
Unitary time evolution	Rational approximation	Implicit, unitary	526
	Second order differencing	Explicit, not exactly unitary	530
	Split operator Fourier	Low dispersion, needs fast Fourier transformation	533
	Real space product formula	Fast but less accurate, useful for wavepackets in coupled states	534
Rotation	Reorthogonalization	Restore orthogonality of rotation matrix	293
	Quaternions	Optimum parametrization of the rotation matrix	343
	Euler angles	Numerical singularities	343
	Explicit method	Low accuracy, reorthogonalization needed	335
	Implicit method	Higher accuracy, orthogonal transformation	338
Molecular dynamics	Force field gradients	Needed for molecular dynamics	361
	Normal mode analysis	Small amplitude motion around an equilibrium	364
	Behrendsen thermostat	Simple method to control temperature	371
	Langevin dynamics	Brownian motion	395
Many body quantum systems	Variational Quantum Monte-Carlo method (VQMC)	Calculates energy for non separable trial wavefunctions	205, 577

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