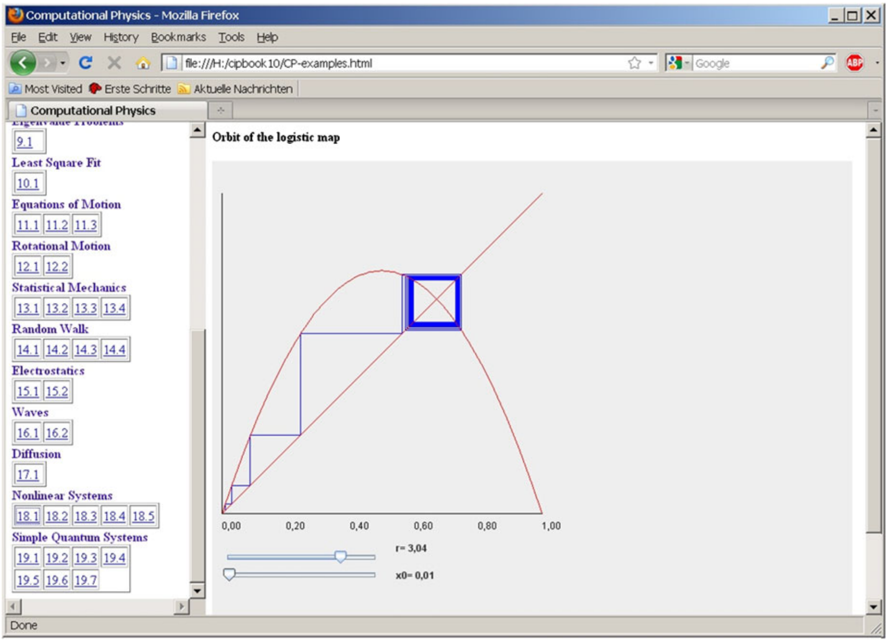
Appendix I
Performing the Computer Experiments



The computer experiments are realized as Java-applets which can be run in any browser that has the Java plug-in installed without installing anything else. 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.

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

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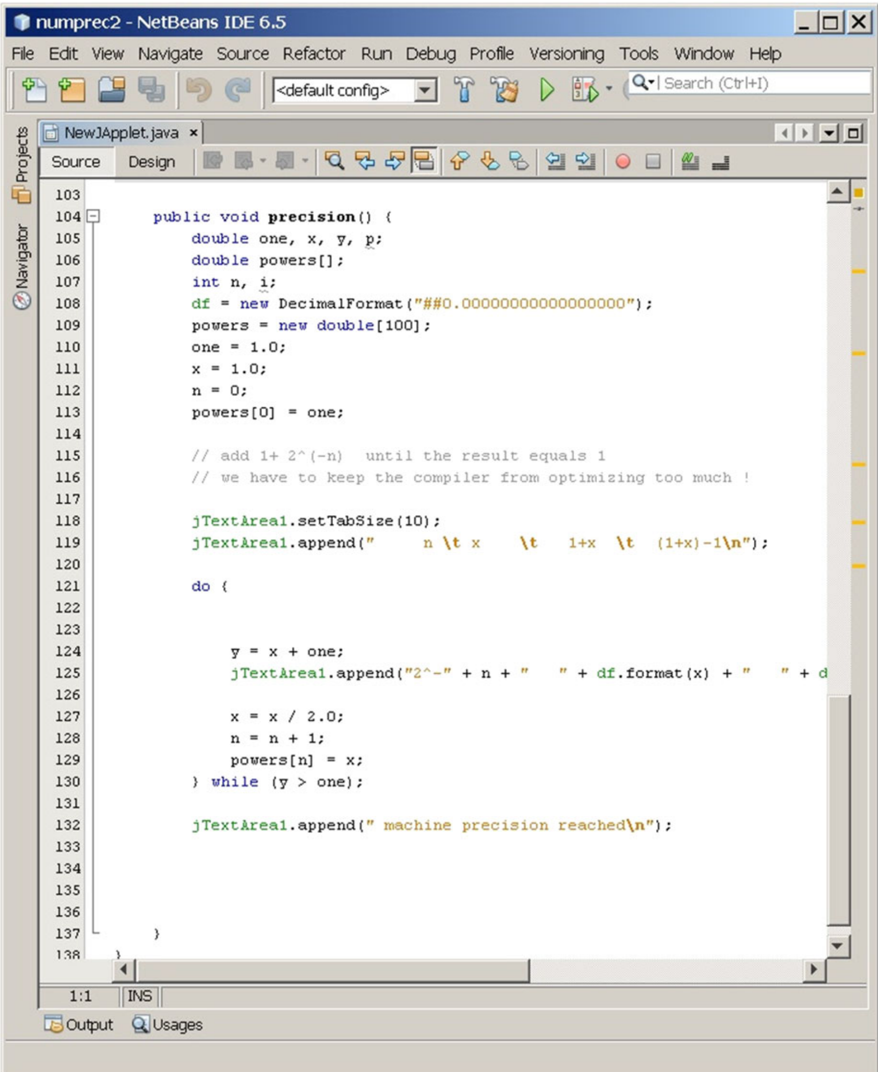
Run a program in your Browser

Open the file CP-examples.html in your browser. If the Java plug-in is installed properly you can start any one of the programs by simply clicking its number in the left hand frame.

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 HTML/code/. You may have a look at the source code and compile and run it



Appendix II
Methods and Algorithms

Purpose	Method	Comments	Pages
Interpolation	Lagrange polynomial	explicit form, easy to evaluate	17
	Barycentric Lagrange polynomial	for evaluation at many points	17
	Newton's divided differences	new points added easily	18
	Neville method	for evaluation at one point	20
	Spline interpolation	smoother, less oscillatory	22
	Rational interpolation	smoother, less oscillatory, often less coefficients necessary	25, 28
	Padé approximation	often better than Taylor series	25
	Barycentric rational interpolation	easy to evaluate	27
	Rational interpolation without poles	alternative to splines, analytical	31
	Multivariate interpolation	multidimensional	32
	Trigonometric interpolation	periodic functions	116
Differentiation	One-sided difference quotient	low error order	37
	Central difference quotient	higher error order	38
	Extrapolation	high accuracy	221
	Higher derivatives	finite difference methods	41
	Partial derivatives	finite difference methods	42

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Purpose	Method	Comments	Pages
Integration	Newton-Cotes formulae	equally spaced points	46
	Trapezoidal rule	simple, closed interval	46
	Midpoint rule	simple, open interval	48
	Simpson's rule	more accurate	46
	Composite Newton-Cotes rules	for larger intervals	48
	Extrapolation (Romberg)	high accuracy	49
	Clenshaw-Curtis expressions	suitable for adaptive and multidimensional quadrature	50
	Gaussian integration	high accuracy if polynomial approximation possible	52
	Monte Carlo integration	high dimensional integrals	139
Linear equations	Gaussian elimination (LU reduction)	standard method for linear equations and matrix inversion	60
	QR decomposition	numerically more stable	64
	Iterative solution	large sparse systems	73
	Jacobi relaxation	converges for diagonally dominant matrices, parallel computation possible	73
	Gauss-Seidel relaxation	converges for symmetric positive definite or diagonal dominant matrices, no extra storage	74
	Chessboard (black-red)	two independent subgrids, especially for Poisson equation	307
	Damping and Successive over-relaxation	speeds up convergence for proper relaxation parameter	75
	Multigrid	fast convergence but more complicated	307
	Conjugate gradients	for symmetric positive definite matrices, preconditioning often necessary	76
	Special LU decomposition	Tridiagonal linear equations	69
	Sherman-Morrison formula	Cyclic tridiagonal systems	71
Root finding	Bisection	reliable but slow continuous functions	84
	Regula falsi (false position)	speed and robustness between bisection and interpolation	85
	Newton-Raphson	continuous derivative necessary, converges fast if starting point is close to a root	85
	Interpolation (secant)	no derivative necessary, but slower than Newton	87
	Inverse interpolation	mainly used by combined methods	88
	Dekker's combined method	Combination of bisection and secant method	91
	Brent's combined method	Combination of bisection, secant, and quadratic inverse interpolation methods, very popular	92
	Chandrupatla's combined method	Uses quadratic interpolation whenever possible, faster than Brent's method, especially for higher order roots	95

Purpose	Method	Comments	Pages
Multidimensional root finding	Newton-Raphson	Needs full Hessian	97
	Quasi-Newton (Broyden)	Hessian not needed, no matrix inversion	98
Function minimization	Ternary search	no gradient needed, very simple, for unimodal functions	99
	Golden section search (Brent)	faster than ternary search but more complicated	101
Multidimensional minimization	Steepest descent	simple but slow	106
	Conjugate gradients	faster than steepest descent	107
	Newton-Raphson	fast, if starting point close to minimum, needs full Hessian	107
	Quasi-Newton (BFGS,DFP)	Hessian not needed, very popular	108
Fourier transformation	Görtzel's algorithm	efficient if only some Fourier components are needed	120
	Fast Fourier transform	much faster than direct discrete Fourier transform	121
Random numbers	Linear congruent mapping	simple pseudo-random number generator	135
	Marsaglia-Zamann	higher quality random numbers but more complicated	135
	RN with given distribution	inverse of cumulative distribution function needed	136
	Random points on unit sphere	random directions	137
	Gaussian RN (Box-Muller)	Gaussian random numbers	138
Thermodynamic average	Simple sampling	inefficient	141
	Importance sampling	samples preferentially important configurations	142
	Metropolis algorithm	generates configurations according to a canonical distribution	142
Eigenvalue problems	Direct solution	only for very small dimension	148
	Tridiagonal matrices	explicit solutions for some special tridiagonal matrices	150
	Jacobi	simple but not very efficient	148
	QL	efficient method for not too large matrices, especially in combination with tridiagonalization by Householder transformations	156
	Lanczos	iterative method for very large matrices or if only a few eigenvalues are needed	159
	Singular value decomposition (SVD)	Generalization for arbitrary matrices	167

Purpose	Method	Comments	Pages
Data fitting	Least square fit	fit a model function to a set of data	162
	Linear least square fit with normal equations	simple but less accurate	163
	Linear fit with orthogonalization	better numerical stability	165
	Linear fit with SVD	expensive but more reliable, also for rank deficient matrices	172
	Low rank matrix approximation	data compression, total linear least squares	170
Discretization	Method of lines	continuous time, discretized space	183
	Eigenvector expansion		
	Finite differences	simplest discretization, uniform grids	180
	Finite volumes	partial differential equations with a divergence term (conservation laws), flux conservative, allows unstructured meshes and discontinuous material parameters	185
	Finite elements	very flexible and general discretization method but also more complicated	196
	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	193
	Dual grid	for finite volumes	185, 314
	Weighted residuals	general method to determine the expansion coefficients	190
	Point collocation	simplest criterion, often used for nonlinear problems and spectral methods	191
	Sub-domains	more general than finite volumes	191
	Least square	popular for computational fluid dynamics and electrodynamics	192
	Galerkin	most widely used criterion, leads often to symmetric matrices	192
	Fourier pseudo-spectral method	very useful whenever a Laplacian is involved, reduces dispersion	193
	Boundary elements	if the Green's function is available	204
Time evolution	Explicit forward Euler	low error order and unstable, mainly used as predictor step	210
	Implicit backward Euler	low error order but stable, used for stiff problems and as corrector step	212
	Improved Euler (Heun, predictor-corrector)	higher error order	213
	Nordsieck predictor-corrector	implicit method, has been used for molecular dynamics	215
	Gear predictor-corrector	optimized for molecular dynamics	217
	Explicit Runge Kutta (2nd, 3rd, 4th)	general and robust methods, easy step size and quality control	217

Purpose	Method	Comments	Pages
	Extrapolation (Gragg-Bulirsch-Stör)	very accurate and very slow	221
	Explicit Adams-Bashforth	high error order but not self-starting, for smooth functions, can be used as predictor	222
	Implicit Adams-Moulton	better stability than explicit method, can be used as corrector	223
	Backward differentiation (Gear)	implicit, especially for stiff problems	223
	Linear multistep predictor-corrector	General class, includes Adams-Bashforth-Moulton and Gear methods	224
	Verlet integration	symplectic, time reversible, for molecular dynamics	225
	Position Verlet	less popular	227
	Velocity Verlet	often used	227
	Störmer-Verlet	if velocities are not needed	228
	Beeman's method	velocities more accurate than for Störmer-Verlet	230
	Leapfrog	simple but two different grids	231, 231, 343
	Crank-Nicolson	implicit, stable, diffusion and Schrödinger equation	357, 347
	Lax-Wendroff	hyperbolic differential equations	345
	Two-step	differential equation with second order time derivative	338
	Reduction to a first order equation	Derivatives treated as additional variables	340
	Two-variable	transforms wave equation into a system of two first order equations	343
	Split operator	approximates an operator by a product	360, 226, 399
Unitary time evolution	Rational approximation	implicit,unitary	392
	Second order differencing	explicit, not exactly unitary	396
	Split operator Fourier	low dispersion, needs fast Fourier transformation	399
	Real space product formula	fast but less accurate, useful for wavepackets in coupled states	399
Rotation	Reorthogonalization	restore orthogonality of rotation matrix	250
	Quaternions	optimum parametrization of the rotation matrix	256
	Euler angles	numerical singularities	255
	Explicit method	low accuracy, reorthogonalization needed	250
	Implicit method	higher accuracy, orthogonal transformation	251
Molecular dynamics	Force field gradients	needed for molecular dynamics	270
	Normal mode analysis	small amplitude motion around an equilibrium	274
	Behrendsen thermostat	simple method to control temperature	281
	Langevin dynamics	Brownian motion	301

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