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

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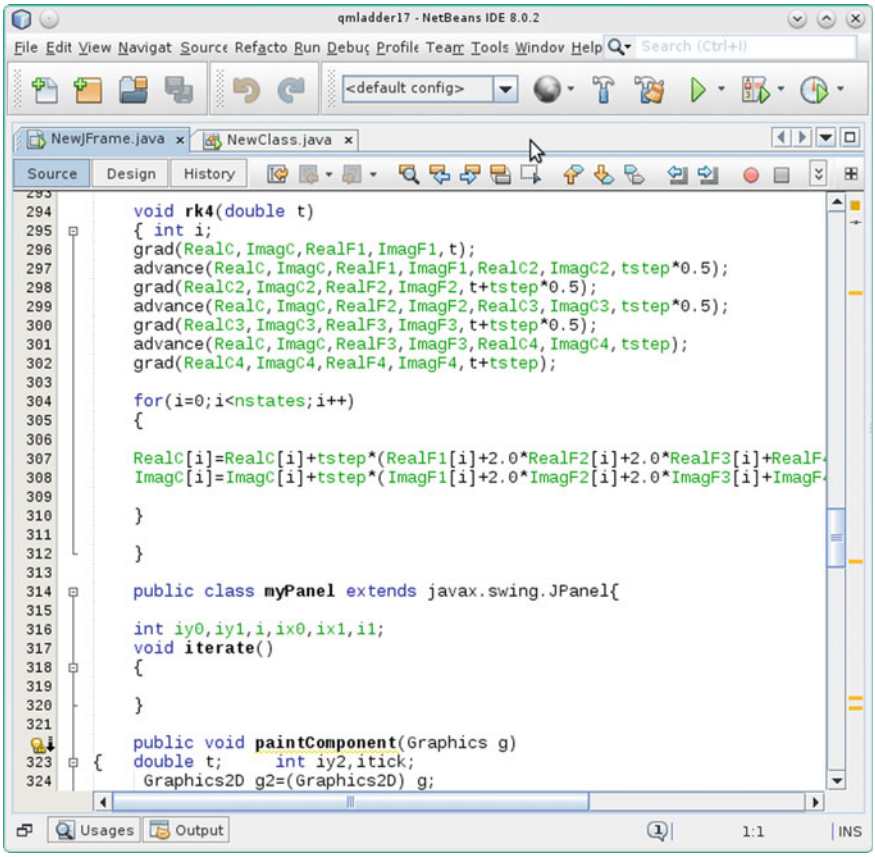

Fig. A.1 Screenshot of the source code

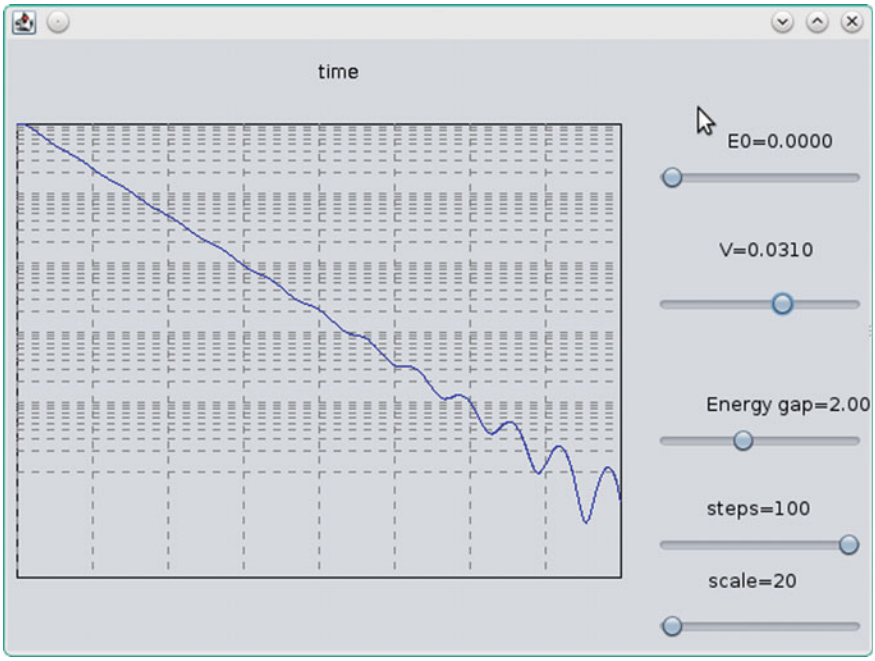

Fig. A.2 Screenshot of computer experiment 23.4

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

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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	98
	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 Lax-Wendroff	highly accurate for advection	449
	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

References

1. IEEE 754-2008: Standard for Floating-Point Arithmetic, IEEE Standards Association (2008)
2. J. Stoer, R. Bulirsch, *in Introduction to Numerical Analysis*, 3rd edn. (Springer, New York, 2010). ISBN 978-1441930064
3. H. Jeffreys, B.S. Jeffreys, in *Lagrange's Interpolation Formula. §9.011 in: Methods of Mathematical Physics*, 3rd ed. (Cambridge University Press, Cambridge, 1988), p. 260
4. J.-P. Berrut, L.N. Trefethen, Barycentric Lagrange interpolation. SIAM Rev. **46**(3), 501–517 (2004)
5. H. Jeffreys, B.S. Jeffreys, in *Divided Differences §9.012 in: Methods of Mathematical Physics*, 3rd edn. (Cambridge University Press, Cambridge, 1988), pp. 260–264
6. W. Werner, Math. Comput. **43**, 205 (1984)
7. E.H. Neville, Indian Math. Soc. **20**, 87 (1933)
8. C.T.H. Baker, Numer. Math. **15**, 315 (1970)
9. I.J. Schoenberg, Q. Appl, Math. **4**(45–99), 112–141 (1946)
10. G. Nürnberger, *in Approximation by Spline Functions* (Springer, Berlin, 1989). ISBN 3-540-51618-2
11. M.S. Floater, K. Hormann, Numer. Math. **107**, 315 (2007)
12. J.P. Berrut, R. Baltensperger, H.D. Mittelmann, Int. Ser. Numer. Math. **151**, 27 (2005)
13. C. Schneider, W. Werner, Math. Comput. **47**, 285 (1986)
14. G.A. Baker Jr., P. Graves-Morris, *in Padé Approximants* (Cambridge University Press, New York, 1996)
15. J.P. Berrut, Comput. Math. Appl. **14**, 1 (1988)
16. L.F. Richardson, Philos. Trans. R. Soc. Lond. Ser. A **210**, 307–357 (1911)
17. L.N. Trefethen, SIAM Rev. **50**, 67–87 (2008)
18. M. Novelinkova, in *WDS'11 Proceedings of Contributed Papers, Part I* (2011), p. 67. ISBN 978-80-7378-184-2
19. C.W. Clenshaw, A.R. Curtis, Numer. Math. **2**, 197 (1960)
20. J. Waldvogel, B.I.T. Numer, Math. **46**, 195 (2006)
21. A. Sommariva, *submitted to Comput* (Math, Appl, 2012)
22. G.H. Golub, J.H. Welsch, Math. Comput. **23**, 221 (1969)
23. R.Z. Iqbal, Master Thesis, School of Mathematics (University of Birmingham, 2008)
24. H. Wilf, *in Mathematics for the Physical Sciences* (Wiley, New York, 1962)
25. M.R. Hestenes, E. Stiefel, J. Res. Natl. Bur. Stand. **49**, 435 (1952)
26. Y. Saad, M. Schultz, SIAM, J. Sci. Stat. Comput. **7**, 856–869 (1986)
27. R. Fletcher, Conjugate gradient methods for indefinite systems, in *Numerical Analysis, vol. 506*, Lecture Notes in Mathematics, ed. by G.A. Watson (Springer, Berlin, 1976), pp. 73–89

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28. H.A. Van der Vorst, SIAM, J. Sci. Stat. Comput. **13**(2), 631–644 (1992)
29. Y. Saad, *in Iterative Methods for Sparse Linear Systems*, 2nd edn. (SIAM, Philadelphia, 2003), p. 194
30. C. Paige, S.I.A.M.J. Saunders, Numer. Anal. **12**, 617–629 (1975)
31. R. Freund, N. Nachtigal, Numer. Math. **60**, 315–339 (1991)
32. C. Paige, B. Parlett, H. van der Vorst, Numer. Linear Algebra Appl. **29**, 115–134 (1995)
33. C. Brezinski, H. Sadok, Appl. Numer. Math. **11**, 443–473 (1993)
34. M.H. Gutknecht, Acta Numer. **6**, 271–397 (1997)
35. S.-L. Zhang, SIAM, J. Sci. Stat. Comput. **18**, 537–551 (1997)
36. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *LU decomposition and its applications, in Numerical Recipes, the Art of Scientific Computing*, 3rd edn. (Cambridge University Press, Cambridge, 2007), pp. 48–55
37. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *Cholesky decomposition, in Numerical Recipes, the Art of Scientific Computing*, 3rd edn. (Cambridge University Press, Cambridge, 2007), pp. 100–101
38. L.N. Trefethen, D. Bau III, *in Numerical Linear Algebra (Society for Industrial and Applied Mathematics* (SIAM, Philadelphia, 1997)
39. G.H. Golub, C.F. Van Loan, *in Matrix Computations*, 3rd edn. (Johns Hopkins, Baltimore, 1976). ISBN 978-0-8018-5414-9
40. J.W. Daniel, W.B. Gragg, L. Kaufmann, G.W. Stewart, Math. Comput. **30**, 772 (1976)
41. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *Cyclic tridiagonal systems, in Numerical Recipes, the Art of Scientific Computing*, 3rd edn. (Cambridge University Press, Cambridge, 2007), p. 79
42. J. Sherman, W.J. Morrison, Ann. Math. Stat. **20**, 621 (1949)
43. I.N. Bronshtein, K.A. Semendyayev, *in Handbook of Mathematics*, 3rd edn. (Springer, New York, 1997), p. 892
44. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *Relaxation methods for boundary value problems, in Numerical Recipes, the Art of Scientific Computing*, 3rd edn. (Cambridge University Press, Cambridge, 2007), pp. 1059–1065
45. H. Jeffreys, B.S. Jeffreys, *in Methods of Mathematical Physics*, 3rd edn. (Cambridge University Press, Cambridge, 1988), pp. 305–306
46. J.H. Wilkinson, J. ACM **8**, 281 (1961)
47. D. Hilbert, L. Nordheim, J. von Neumann, John. Math. Ann. **98**, 1 (1927)
48. A. Bermann, S. Gueron, Math. Gaz. **86**, 274 (2002)
49. B. Beckermann, Numer. Math. **85**, 553 (2000)
50. I.R. Savage, E. Lukacs, in *Contributions to the Solution of Systems of Linear Equations and the Determination of Eigenvalues.* National Bureau of Standards, Applied Mathematics Series, vol. 39, ed. by O. Taussky (1954)
51. R.L. Burden, J.D. Faires, *in Numerical Analysis* (Brooks Cole Publishing Company, Boston, 2010)
52. J.A. Ford, Improved Algorithms of Illinois-type for the Numerical Solution of Nonlinear Equations. Technical Report CSM-257. University of Essex Press (1995)
53. J.Y. Tjalling, Historical development of the Newton-Raphson method. SIAM Rev. **37**, 531 (1995)
54. J.M. Papakonstantinou, A historical development of the (n+1)-point secant method, M.A. thesis, Rice University Electronic Theses and Dissertations, 2007
55. D.E. Muller, Math. Tables Aids Comput. **10**, 208 (1956)
56. R.P. Brent, Comput. J. **14**, 422 (1971)
57. T.R. Chandrupatla, Adv. Eng. Softw. **28**, 145 (1997)
58. T.J. Dekker, Finding a zero by means of successive linear interpolation, in *Constructive Aspects of the Fundamental Theorem of Algebra*, ed. by B. Dejon, P. Henrici (Wiley-Interscience, London, 1969)
59. J.C.P. Bus, T.J. Dekker, A.C.M. Trans, Math. Softw. **1**, 330 (1975)

60. R.P. Brent, *Algorithms for Minimization without Derivatives* (Prentice-Hall, Englewood Cliffs, 1973)
61. A. Quarteroni, R. Sacco, F. Saleri, *Numerical Mathematics*, 2nd edn. (Springer, Berlin, 2007)
62. C.G. Broyden, Math. Comput. **19**, 577 (1965)
63. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Section 10.2. golden section search in one dimension, in *Numerical Recipes: The Art of Scientific Computing*, 3rd edn. (Cambridge University Press, New York, 2007). ISBN 978-0-521-88068-8
64. J. Kiefer, Proc. Am. Math. Soc. **4**, 502–506 (1953)
65. R. Fletcher, C. Reeves, Comput. J. **7**, 149 (1964)
66. C.G. Broyden, J. Inst. Math. Appl. **6**, 76 (1970)
67. R. Fletcher, Comput. J. **13**, 317 (1970)
68. D. Goldfarb, Math. Comput. **24**, 23 (1970)
69. D.F. Shanno, Math. Comput. **24**, 647 (1970)
70. Z. Wang, B.R. Hunt, Appl. Math. Comput. **16**, 19 (1985)
71. N. Ahmed, T. Natarajan, K.R. Rao, IEEE Trans. Comput. **C-23**, 90 (1974)
72. K.R. Rao, P. Yip, *Discrete Cosine Transform: Algorithms, Advantages, Applications* (Academic Press, Boston, 1990)
73. F.j. Harris, Proc. IEEE **66**, 51 (1978)
74. G. Goertzel, Am. Math. Mon. **65**, 34 (1958)
75. E.I. Jury, *in Theory and Application of the Z-Transform Method* (Krieger Publishing Company, New York, 1973). ISBN 0-88275-122-0
76. P. Duhamel, M. Vetterli, Signal Process. **19**, 259 (1990)
77. H.J. Nussbaumer, *in Fast Fourier Transform and Convolution Algorithms* (Springer, Berlin, 1990)
78. J.W. Cooley, J.W. Tukey, Math. Comput. **19**, 297 (1965)
79. D. Gabor, J. Inst. Electr. Eng. **93**, 429 (1946)
80. M.J. Bastiaans, Appl. Opt. **33**, 5241 (1994)
81. M.J. Bastiaans, Proc. IEEE **68**, 538 (1980)
82. R.S. Orr, I.E.E.E. Trans, Sign. Proc. **41**, 122 (1993)
83. S. Qian, I.E.E.E. Trans, Signal Proc. **41**, 2429 (1993)
84. J. Ashmead, Quanta **1**, 58 (2012)
85. A. Grossmann, J. Morlet, SIAM. J. Math. Anal. **15**, 723 (1984)
86. S.G. Mallat, Trans. Am. Math. Soc. **315**, 69 (1989)
87. S.G. Mallat, I.E.E.E. Trans, Pattern Anal. Mach. Intell. **11**, 674 (1989)
88. A. Haar, Math. Ann. **69**, 331 (1910)
89. I. Daubechies, A. Grossmann, Y. Meyer, J. Math. Phys. **27**, 1271 (1986)
90. Y. Meyer, *in Wavelets and Operators*, vol. I (Cambridge University Press, Cambridge, 1995)
91. V. Vermehren Valenzuela, H.M. de Oliveira, OALib J. (2015), arXiv.org/abs/1502.00161v1
92. D. Esteban, C. Galand, in *Proceedings of the IEEE International Conference on Acoustics, Speech, and Signal Processing* (1977)
93. I. Daubechies, Commun. Pure Appl. Math. **16**, 909 (1988)
94. N. Metropolis, S. Ulam, J. Am. Stat. Assoc. **44**, 335 (1949)
95. G.S. Fishman, in *Monte Carlo: Concepts, Algorithms, and Applications* (Springer, New York, 1995, 1996). ISBN 038794527X
96. C.P. Robert, G.C. Casella, *in Monte Carlo Statistical Methods*, 2nd edn. (Springer, New York, 2004). ISBN 0387212396
97. R.E. Caflisch, in *Monte Carlo and Quasi-Monte Carlo Methods*. Acta Numerica, vol. 7 (Cambridge University Press, Cambridge, 1998), pp. 1–49
98. R.D. Richtmyer, *in Principles of Modern Mathematical Physics*, vol. I (Springer, New York, 1978)
99. H. Pollard, Q. J. Pure Appl. Math. **49**, 1 (1920)
100. J. Rice, *in Mathematical Statistics and Data Analysis*, 2nd edn. (Duxbury Press, Belmont, 1995). ISBN 0-534-20934-3
101. True random number service at RANDOM.ORG

102. J. Kelsey, B. Schneier, N. Ferguson, *Yarrow-160 notes on the design and analysis of the yarrow cryptographic pseudorandom number generator, in Sixth Annual Workshop on Selected Areas in Cryptography* (Springer, Berlin, 1999)
103. N. Ferguson, B. Schneier, *in Practical Cryptography* (Wiley, New York, 2003)
104. The Marsaglia Random Number CDROM including the Diehard Battery of Tests of Randomness, http://stat.fsu.edu/pub/diehard/
105. G. Marsaglia, J. Mod. Appl. Stat. Methods **1**, 2 (2003)
106. The TestU01 website, http://simul.iro.umontreal.ca/testu01/tu01.html
107. P. L'Ecuyer, R. Simard, A.C.M. Trans, Math. Softw. **33**, 22 (2007)
108. M. Matsumoto, T. Nishimura, A.C.M. Trans, Modeling Comput. Simul. **8**, 3 (1998)
109. K. Entacher, A.C.M. Trans, Modeling Comput. Simul. **8**, 61 (1998)
110. G.E.P. Box, M.E. Muller, Ann. Math. Stat. **29**, 610 (1958)
111. N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, E. Teller, J. Chem. Phys. **21**, 1087 (1953)
112. E. Bonomi, J.-L. Lutton, SIAM Rev. **26**, 551 (1984)
113. B.N. Parlett, *in The Symmetric Eigenvalue Problem* (Society for Industrial and Applied Mathematics, Philadelphia, 1998)
114. H.W. Chang, S.E. Liu, R. Burridge, Linear Algebra Appl. **430**, 999 (2009)
115. S. Kouachi, Electron. J. linear Algebra **15**, 115 (2006)
116. W.C. Yueh, Appl. Math. E-Notes **5**, 66 (2005)
117. J.G.F. Francis, Comput. J. **4**, 265 (1961); **4**, 332 (1962)
118. C. Lanczos, J. Res. Natl Bur. Stand. **45**, 255 (1950)
119. H.D. Simon, Linear Algebra Appl. **61**, 101 (1984)
120. B.N. Parlett, D.S. Scott, Math. Comput. **33**, 217 (1979)
121. D. Calvetti, L. Reichel, D.C. Sorensen, Electron. Trans. Numer. Anal. **2**, 1 (1994)
122. D.C. Sorenson, NASA contractor report 198342 (1996)
123. J. Wolberg, *in Data Analysis Using the Method of Least Squares: Extracting the Most Information from Experiments* (Springer, Berlin, 2005)
124. J.A. Richards, *in Remote Sensing Digital Image Analysis* (Springer, Berlin, 1993)
125. A.E. Garcia, Phys. Rev. Lett. **86**, 2696 (1992)
126. T.D. Romo et al., Proteins **22**, 311 (1995)
127. D.P. Derrarr et al., *in A Practical Approach to Microarray Data Analysis* (Kluwer, Norwell, 2003)
128. DGESVD routine from the freely available software package LAPACK, http://www.netlib.org/lapack
129. G. Golub, W. Kahan, J.S.I.A.M. Numer, Anal. B **2**, 205 (1965)
130. G.W. Stewart, SIAM Rev. **35**, 551 (1993)
131. J. Mandel, Am. Stat. **36**, 15 (1982)
132. A. Ben-Israel, T.N.E. Greville, *in Generalized Inverses* (Springer, Berlin, 2003). ISBN 0-387-00293-6
133. J. Peiro, S. Sherwin, in *Handbook of Materials Modeling*, vol. 1, ed. by S. Yip (Springer, Berlin, 2005), pp. 1–32
134. H.P. Langtangen, *in Computational Partial Differential Equations: Numerical Methods and Diffpack Programming* (Springer, Berlin, 2003)
135. W. Ames, *in Numerical Methods for Partial Differential Equations* (Academic Press Inc., New York, 1992)
136. F. John, Duke Math. J. **4**, 300 (1938)
137. D.J. Acheson, *in Elementary Fluid Dynamics* (Oxford University Press, Oxford, 1990)
138. B.G. Galerkin, On electrical circuits for the approximate solution of the Laplace equation. Vestn. Inzh. **19**, 897–908 (1915)
139. R. Eymard, T. Galloue, R. Herbin, in *Finite Volume Methods. Handbook of Numerical Analysis*, ed. by P.G. Ciarlet, J.L. Lions (Elsevier, Amsterdam, 2000), pp. 713–1020
140. E.L. Ortiz, SIAM. J. Numer. Anal. **6**, 480 (1969)
141. B.-N. Jiang, *in The Least-Squares Finite Element Method* (Springer, Berlin, 1998)

142. P. Bochev, M. Gunzburger, *in Least Squares Finite Element Methods* (Springer, Berlin, 2009)
143. C.A.J. Fletcher, *in Computational Galerkin Methods* (Springer, Berlin, 1984)
144. J.P. Boyd, *in Chebyshev and Fourier Spectral Methods* (Dover Publications, New York, 2001)
145. J. Fish, T. Belytschko, *in A First Course in Finite Elements* (Wiley, New York, 2007)
146. S.S. Rao, *in The Finite Element Method in Engineering* (Elsevier, Amsterdam, 2011)
147. C.A.J. Fletcher, in *Computational Techniques for Fluid Dynamics*, vol. I, 2nd edn. (Springer, Berlin, 1991)
148. G. Beer, I. Smith, C. Duenser, *in The Boundary Element Method with Programming: For Engineers and Scientists* (Springer, Berlin, 2008)
149. L.C. Wrobel, M.H. Aliabadi, *in The Boundary Element Method* (Wiley, New Jersey, 2002)
150. G. Wunsch, *in Feldtheorie* (VEB Technik, Berlin, 1973)
151. A. Nordsieck, Math. Comput. **16**, 22 (1962)
152. C.W. Gear, *in Numerical Initial Value Problems in Ordinary Differential Equations* (Prentice-Hall, Englewood Cliffs, 1971)
153. G.J. Martyna, M.E. Tuckerman, J. Chem. Phys. **102**, 8071 (1995)
154. J.C. Butcher, *in The Numerical Analysis of Ordinary Differential Equations: Runge-Kutta and General Linear Methods* (Wiley, New York, 1987)
155. W.B. Gragg, SIAM. J. Numer. Anal. **2**, 384 (1965)
156. L.F. Shampine, IMA. J. Numer. Anal. **3**, 383 (1983)
157. L.F. Shampine, L.S. Baca, Numer. Math. **41**, 165 (1983)
158. C.W. Gear, I.E.E.E. Trans, Circuit Theory **18**, 89–95 (1971)
159. C.W. Gear, Math. Comput. **21**, 146 (1967)
160. I.P. Omelyan, I.M. Mryglod, R. Folk, Comput. Phys. Commun. **151**, 272 (2003)
161. S.-H. Tsai et al., Braz. J. Phys. **34**, 384 (2004)
162. M. Tuckerman, B.J. Berne, J. Chem. Phys. **97**, 1990 (1992)
163. M.P. Allen, D.J. Tildesley, *in Computer Simulation of Liquids* (Oxford University Press, Oxford, 1989). ISBN 0-19-855645-4
164. L. Verlet, Phys. Rev. **159**, 98 (1967)
165. E. Hairer, C. Lubich, G. Wanner, Acta Numer. **12**, 399 (2003)
166. W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, in Section 17.4. second-order conservative equations, in *Numerical Recipes: The Art of Scientific Computing*, 3rd edn. (Cambridge University Press, Cambridge, 2007)
167. P. Schofield, Comput. Phys. Commun. **5**, 17 (1973)
168. D. Beeman, J. Comput. Phys. **20**, 130 (1976)
169. R. Sonnenschein, A. Laaksonen, E. Clementi, J. Comput. Chem. **7**, 645 (1986)
170. B.K.P. Horn, H.M. Hilden, S. Negahdaripour, J. Opt. Soc. Am. A **5**, 1127 (1988)
171. I.P. Omelyan, Phys. Rev. **58**, 1169 (1998)
172. I.P. Omelyan, Comput. Phys. Commun. **109**, 171 (1998)
173. H. Goldstein, *inKlassische Mechanik* (Akademische Verlagsgesellschaft, Frankfurt/Main, 1974)
174. I.P. Omelyan, Comput. Phys. **12**, 97 (1998)
175. D.C. Rapaport, *in The Art of Molecular Dynamics Simulation* (Cambridge University Press, Cambridge, 2004). ISBN 0-521-44561-2
176. D. Frenkel, B. Smit, *in Berend: Understanding Molecular Simulation: From Algorithms to Applications* (Academic Press, San Diego, 2002)
177. J.M. Haile, *in Molecular Dynamics Simulation: Elementary Methods* (Wiley, New York, 2001). ISBN 0-471-18439-X
178. A. Leach, *in Molecular Modelling: Principles and Applications*, 2nd edn. (Prentice Hall, Publisher, Harlow, 2001). ISBN 978-0582382107
179. T. Schlick, *in Molecular Modeling and Simulation* (Springer, Berlin, 2002). ISBN 0-387-95404-X
180. R. Car, M. Parrinello, Phys. Rev. Lett. **55**, 2471 (1985)
181. T. Kühne, M. Krack, F. Matthias, M.P. Mohamed, Phys. Rev. Lett. **98**, 066401 (2007)

182. W.D. Cornell, P. Cieplak, C.I. Bayly, I.R. Gould, K.M. Merz Jr., D.M. Ferguson, D.C. Spellmeyer, T. Fox, J.W. Caldwell, P.A. Kollman, J. Am. Chem. Soc. **117**, 5179 (1995)
183. A.D. MacKerell Jr., B. Brooks, C.L. Brooks III, L. Nilsson, B. Roux, Y. Won, M. Karplus, CHARMM: the energy function and its parameterization with an overview of the program, in *The Encyclopedia of Computational Chemistry*, vol. 1, ed. by P.v.R. Schleyer, et al. (Wiley, Chichester, 1998), pp. 271–277
184. W.F. van Gunsteren, S.R. Billeter, A.A. Eising, P.H. Hünenberger, P. Krüger, A.E. Mark, W.R.P. Scott, I.G. Tironi, *Biomolecular Simulation: The GROMOS96 Manual and User Guide*. vdf Hochschulverlag AG an der ETH Zürich and BIOMOS b.v.: Zürich, Groningen, 1996
185. M. Christen, P.H. Hünenberger, D. Bakowies, R. Baron, R. Bürgi, D.P. Geerke, T.N. Heinz, M.A. Kastenholz, V. Kräutler, C. Oostenbrink, C. Peter, D. Trzesniak, W.F. van Gunsteren, J. Comput. Chem. **26**, 1719 (2005)
186. IUPAC-IUB Commission on Biochemical Nomenclature, Biochemsistry **9**, 3471 (1970)
187. B.R. Brooks, C.L. Brooks III, A.D. Mackerell Jr., L. Nilsson, R.J. Petrella, B. Roux, Y. Won, G. Archontis, C. Bartels, S. Boresch, A. Caflisch, L. Caves, Q. Cui, A.R. Dinner, M. Feig, S. Fischer, J. Gao, M. Hodoscek, W. Im, K. Kuzcera, T. Lazaridis, J. Ma, V. Ovchinnikov, E. Paci, R.W. Pastor, C.B. Post, J.Z. Pu, M. Schaefer, B. Tidor, R.M. Venable, H.L. Woodcock, X. Wu, W. Yang, D.M. York, M. Karplus, J. Comput. Chem. **30**, 1545 (2009)
188. B.R. Brooks, R.E. Bruccoleri, B.D. Olafson, D.J. States, S. Swaminathan, M. Karplus, J. Comput. Chem. **4**, 187 (1983)
189. K.J. Bowers, E. Chow, H. Xu, R.U. Dror, M.P. Eastwood, B.A. Gregersen, J.L. Klepeis, I. Kolossvary, M.A. Moraes, F.D. Sacerdoti, J.K. Salmon, Y. Shan, D.E. Shaw, Scalable algorithms for molecular dynamics simulations on commodity clusters, in SC. Conference. Proceedings of the ACM/IEEE **2006**, 43 (2006)
190. A.K. Rappe, C.J. Casewit, K.S. Colwell, W.A. Goddar, W.M. Skiff, J. Am. Chem. Soc. **115**, 10024 (1992)
191. E.J. Bautista, J.M. Seminario, Int. J. Quantum Chem. **108**, 180 (2008)
192. R.E. Tuzun, D.W. Noid, B.G. Sumpter, Macromol. Theory Simul. **5**, 771 (1996)
193. R.E. Tuzun, D.W. Noid, B.G. Sumpter, J. Comput. Chem. **18**, 1804 (1997)
194. C. Lavor, Phys. D **227**, 135 (2007)
195. V.S. Allured, C.M. Kelly, C.R. Landis, J. Am. Chem. Soc. **113**, 1 (1991)
196. T. Schlick, J. Comput. Chem. **10**, 951 (1989)
197. S. Chynoweth, U.C. Klomp, L.E. Scales, Comput. Phys. Commun. **62**, 297 (1991)
198. H. Bekker, H.J.C. Berendsen, W.F. van Gunsteren, J. Comput. Chem. **16**, 527 (1995)
199. J.P. Hansen, L. Verlet, Phys. Rev. **184**, 151 (1969)
200. J.J. Nicolas, K.E. Gubbins, W.B. Streett, D.J. Tildesley, Mol. Phys. **37**, 1429 (1979)
201. J.K. Johnson, J.A. Zollweg, K.E. Gubbins, Mol. Phys. **78**, 591 (1993)
202. H. Watanabe, N. Ito, C.K. Hu, J. Chem. Phys. **136**, 204102 (2012)
203. C. Muguruma, Y. Okamoto, M. Mikami, Croat. Chemica Acta **80**, 203 (2007)
204. S.A. Khrapak, M. Chaudhuri, G.E. Morfill, Phys. Rev. B **82**, 052101 (2010)
205. B. Smit, J. Chem. Phys. **96**, 8639 (1992)
206. H.J.C. Berendsen, J.P.M. Postma, W.F. van Gunsteren, A. DiNola, J.R. Haak, J. Chem. Phys. **81**, 3684 (1984)
207. P.H. Huenenberger, Adv. Polym. Sci. **173**, 105 (2005)
208. F. Schwabl, *in Statistical Mechanics* (Springer, Berlin, 2003)
209. J.R. Errington, P.G. Debenedetti, S. Torquato, J. Chem. Phys. **118**, 2256 (2003)
210. H. Risken, *in The Fokker-Planck Equation* (Springer, Berlin, 1989)
211. D. Levesque, L. Verlet, Phys. Rev. A **2**, 2514 (1970)
212. T. Tsang, H. Tang, Phys. Rev. A **15**, 1696 (1977)
213. E. Ising, Beitrag zur Theorie des Ferromagnetismus. Z. Phys. **31**, 253–258 (1925). doi:10.1007/BF02980577
214. K. Binder, in *"Ising Model" Encyclopedia of Mathematics* (Suppl.), vol. 2, ed. by R. Hoksbergen (Kluwer Academic Publishers, Dordrecht, 2000), pp. 279–281
215. L. Onsager, Phys. Rev. **65**, 117 (1944)

216. B.M. McCoy, T.T. Wu, *in The Two-Dimensional Ising Model* (Harvard University Press, Cambridge, 1973). ISBN 0674914406
217. K. Pearson, The problem of the Random Walk. Nature **72**, 294 (1905)
218. A.A. Markov, Theory of Algorithms. [Translated by Jacques J. Schorr-Kon and PST staff] Imprint Moscow, Academy of Sciences of the USSR, 1954 [Jerusalem, Israel Program for Scientific Translations, 1961; available from Office of Technical Services, United States Department of Commerce] Added t.p. in Russian Translation of Works of the Mathematical Institute, Academy of Sciences of the USSR, v. 42. Original title: Teoriya algorifmov. [QA248.M2943 Dartmouth College library. U.S. Dept. of Commerce, Office of Technical Services, number OTS 60-51085.] (1954)
219. A.A. Markov, Extension of the limit theorems of probability theory to a sum of variables connected in a chain reprinted in Appendix B of: R. Howard, in *Dynamic Probabilistic Systems, volume 1: Markov Chains* (Wiley, New York, 1971)
220. G. Schaftenaar, J.H. Noordik, J. Comput.-Aided Mol. Design **14**, 123 (2000)
221. W.L. Mattice, U.W. Suter, *in Conformational Theory of Large Molecules* (Wiley Interscience, New York, 1994). ISBN 0-471-84338-5
222. R. Brown, Philos. Mag. **4**, 161 (1828)
223. A. Einstein, Annalen der Physik **17**, 549 (1905)
224. A. Einstein, *in Investigations on the Theory of Brownian Movement* (Dover, New York, 1956)
225. S. Yang, M.K. Gobbert, Appl. Math. Lett. **22**, 325 (2009)
226. Y. Zhu, A.C. Cangellaris, in *Multigrid Finite Element Methods for Electromagnetic Field Modeling* (Wiley, New York, 2006), p. 132 ff. ISBN 0471741108
227. M.T. Heath, in *§11.5.7 Multigrid Methods. Scientific Computing: An Introductory Survey* (McGraw-Hill Higher Education, New York, 2002), p. 478 ff. ISBN 007112229X
228. G. Skollermo, Math. Comput. **29**, 697 (1975)
229. P.N. Swarztrauber, R.A. Sweet, in *Handbook of Fluid Dynamics and Fluid Machinery*, ed. by J.A. Schetz, A.E. Fuhs (Wiley, New York, 1996)
230. M. Oevermann, R. Klein, J. Comput. Phys. **219**, 749 (2006)
231. M. Oevermann, C. Scharfenberg, R. Klein, submitted to J. Comput. Phys
232. R.E. Bruccoleri, J. Novotny, M.E. Davis, K.A. Sharp, J. Comput. Chem. **18**, 268 (1997)
233. P. Debye, E. Hueckel, Phys. Z. **24**, 185 (1923)
234. G.L. Gouy, J. Phys. **9**, 457 (1910)
235. D.L. Chapman, Philos. Mag. **25**, 475 (1913)
236. F. Fogolari, A. Brigo, H. Molinari, J. Mol. Recognit. **15**, 377 (2002)
237. A. Nicholls, B. Honig, J. Comput. Chem. **12**, 435 (1990)
238. A.H. Boschitsch, M.O. Fenley, H.X. Zhou, J. Phys. Chem. B **106**, 2741 (2002)
239. A.H. Juffer et al., J. Phys. Chem. B **101**, 7664 (1997)
240. J.S. Bader et al., J. Chem. Phys. **106**, 2372 (1997)
241. T. Simonson, Rep. Prog. Phys. **66**, 737 (2003)
242. J.G. Kirkwood, J. Chem. Phys. **2**, 351 (1934)
243. R. Courant, K. Friedrichs, H. Lewy, Math. Ann. **100**, 32 (1928)
244. Y. Li, C. Trenchea, J. Comput. Phys. **259**, 23 (2014)
245. P.D. Williams, Mon. Weather Rev. **139**, 1996 (2011)
246. R.J. LeVeque, *in Finite-Volume Methods for Hyperbolic Problems* (Cambridge University Press, Cambridge, 2004)
247. S.K. Godunov, Math. Sbornik **47**, 271 (1959) (translated US Joint Publ. Res. Service, JPRS 7225 Nov. 29, 1960)
248. E.F. Toro, *in Riemann Solvers and Numerical Methods for Fluid Dynamics* (Springer, Berlin, 1999)
249. J. Donea, Int. J. Numer. Meth. Eng. **20**, 101 (1984)
250. J. Donea, L. Quartapelle, V. Selmin, J. Comput. Phys. **70**, 463 (1987)
251. B. Roig, J. Comput. Appl. Math. **204**, 95 (2007)
252. E.F. Toro, S.J. Billet, College of Aeronautics Report 9312 (1993). ISBN 1-871564-65-4

253. H. Ibach, H. Lüth, *in Solid-State Physics: An Introduction to Principles of Materials Science (Advanced Texts in Physics)* (Springer, Berlin, 2003)
254. L. Lynch, in *Numerical Integration of Linear and Nonlinear Wave Equations*. Bachelor Thesis, Florida Atlantic University (Digital Commons@University of Nebraska-Lincoln, 2004)
255. S.A. Teukolsky, Phys. Rev. D **61**, 067503 (2000)
256. Y.A. Cengel, in *Heat Transfer-A Practical Approach*, 2nd edn. (McGraw Hill Professional, New York, 2003), p. 26. ISBN 0072458933, 9780072458930
257. J. Fourier, in *The Analytical Theory of Heat* (Cambridge University Press, Cambridge University Press, 1878) (Cambridge University Press, Cambridge, 2009; ISBN 978-1-108-00178-6)
258. A. Fick, Philos. Mag. **10**, 30 (1855)
259. J. Crank, P. Nicolson, Proc. Camb. Philos. Soc. **43**, 50 (1947)
260. J.W. Thomas, *in Numerical Partial Differential Equations: Finite Difference Methods, Texts in Applied Mathematics*, vol. 22 (Springer, New York, 1995)
261. D. Hinrichsen, A.J. Pritchard, *in Mathematical Systems Theory I - Modelling, State Space Analysis, Stability and Robustness* (Springer, Berlin, 2005). ISBN 0-978-3-540-441250
262. H.K. Khalil, *in Nonlinear Systems* (Prentice Hall, Englewood Cliffs, 2001). ISBN 0-13-067389-7
263. I. Vasile, *in Istratescu in Fixed Point Theory, An Introduction* (D. Reidel Publishing Company's, London, 1981)
264. S.H. Strogatz, in *Nonlinear dynamics and Chaos: Applications to Physics, Biology, Chemistry, and Engineering* (Perseus, 2001). ISBN 0-7382-0453-6
265. J.D. Murray, in *Mathematical Biology: I. An Introduction*, 3rd edn., vol. 2 (Springer, Berlin, 2002). ISBN 0-387-95223-3
266. E. Renshaw, in *Modelling Biological Populations in Space and Time* (C.U.P., 1991). ISBN 0-521-44855-7
267. P. Grindrod, *in Patterns and Waves: The Theory and Applications of Reaction-Diffusion Equations* (Clarendon Press, Oxford, 1991)
268. P.C. Fife, *in Mathematical Aspects of Reacting and Diffusing Systems* (Springer, Berlin, 1979)
269. A.M. Lyapunov, *in Stability of Motion* (Academic Press, New York, 1966)
270. P.F. Verhulst, Mémoires de l'Académie Royale des Sciences et Belles Lettres de Bruxelles. 18, Bruxelles (1845), pp. 1–42
271. A.J. Lotka, *in Elements of Physical Biology* (Williams and Wilkins, Baltimore, 1925)
272. V. Volterra, Mem. R. Accad. Naz. dei Lincei **2**, 31 (1926)
273. C.S. Holling, Can. Entomol. **91**, 293 (1959)
274. C.S. Holling, Can. Entomol. **91**, 385 (1959)
275. J.T. Tanner, Ecology **56**, 855 (1975)
276. A.M. Turing, Philos. Trans. R. Soc. B **237**, 37 (1952)
277. F. Schwabl, *in Quantum Mechanics*, 4th edn. (Springer, Berlin, 2007)
278. E. Schrödinger, Phys. Rev. **28**, 1049 (1926)
279. X. Antoine, A. Arnold, C. Besse, M. Erhardt, A. Schädle, Commun. Comput. Phys. **4**, 729 (2008)
280. C. Leforestier, R.H. Bisseling, C. Cerjan, M.D. Feit, R. Friesner, A. Guldberg, A. Hammerich, G. Jolicard, W. Karrlein, H.-D. Meyer, N. Lipkin, O. Roncero, R. Kosloff, J. Comput. Phys. **94**, 59 (1991)
281. B. Fornberg, Geophysics **52**, 4 (1987)
282. B. Fornberg, Math. Comput. **51**, 699 (1988)
283. R. Guantes, S.C. Farantos, J. Chem. Phys. **111**, 10827 (1999)
284. R. Guantes, A. Nezis, S.C. Farantos, J. Chem. Phys. **111**, 10836 (1999)
285. A. Castro, M.A.L. Marques, A. Rubio, J. Chem. Phys. **121**, 3425 (2004)
286. Z.A. Anastassi, T.E. Simos, Phys. Rep. **482–483**, 1 (2009)
287. K. Yabana, G.F. Bertsch, Phys. Rev. B **54**, 4484 (1996)
288. A. Goldberg, H.M. Schey, J.L. Schwartz, Am. J. Phys. **35**, 177 (1967)
289. E.A. McCullough Jr., R.E. Wyatt, J. Chem. Phys. **51**, 1253 (1969)
290. E.A. McCullough Jr., R.E. Wyatt, J. Chem. Phys. **54**, 3592 (1971)

291. T. Iitaka, Phys. Rev. E **49**, 4684 (1994)
292. T. Iitaka, N. Carjan, T. Strottman, Comput. Phys. Commun. **90**, 251 (1995)
293. A. Askar, A.S. Cakmak, J. Chem. Phys. **68**, 2794 (1978)
294. H. De Raedt, Comput. Phys. Rep. **7**, 1 (1987)
295. H. De Raedt, B. De Raedt, Phys. Rev. A **28**, 3575 (1983)
296. A.D. Bandrauk, H. Shen, Chem. Phys. Lett. **176**, 428 (1991)
297. L.A. Collins, J.D. Kress, R.B. Walker, Comput. Phys. Commun. **114**, 15 (1998)
298. C. Cerjan, K.C. Kulander, Comput. Phys. Commun. **63**, 529 (1991)
299. H. TalEzer, R. Kosloff, J. Chem. Phys. **81**, 3967 (1984)
300. R. Chen, H. Guo, J. Chem. Phys. **111**, 9944 (1999)
301. T.J. Park, J.C. Light, J. Chem. Phys. **85**, 5870 (1986)
302. B.I. Schneider, J.A. Collins, J. Non-Cryst, Solids **351**, 1551 (2005)
303. I. Allonso-Mallo, N. Reguera, J. Comput. Phys. **220**, 409 (2006)
304. S.E. Koonin, C.M. Dawn, *in Computational Physics* (Perseus Books, New York, 1990). ISBN 978-0201127799
305. W. van Dijk, F.M. Toyama, Phys. Rev. E **75**, 036707 (2007)
306. D. Kosloff, R. Kosloff, J. Comput. Phys. **52**, 35 (1983)
307. W. Magnus, Commun. Appl. Math. **7**, 649 (1954)
308. M. Suzuki, Commun. Math. Phys. **51**, 183 (1976)
309. M.D. Feit, J.A. Fleck Jr., A. Steiger, J. Comput. Phys. **47**, 412 (1982)
310. P.W. Anderson, Phys. Rev. **79**, 350 (1950)
311. J. Halpern, L.E. Orgel, Discuss. Faraday Soc. **29**, 32 (1960)
312. P. Bocchieri, A. Loinger, Phys. Rev. **107**, 337 (1957)
313. M. Bixon, J. Jortner, J. Chem. Phys. **48**, 715 (1986)
314. B.I. Stepanov, V.P. Grobkovskii, *in Theory of Luminescence* (Butterworth Publications, London, 1986)
315. L. Landau, Phys. Soviet Union **2**, 46–51 (1932)
316. C. Zener, Proc. R. Soc. Lond. A **137**(6), 696–702 (1932)
317. A. Yariv, *in Quantum Electronics* (Wiley, New York, 1975)
318. L.M.K. Vandersypen, I.L. Chuang, Rev. Mod. Phys. **76**, 1037 (2004)
319. M. Nielsen, I. Chuang, *in Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000)
320. L. Diosi, *in A Short Course in Quantum Information Theory* (Springer, Berlin, 2007)
321. R.P. Feynman, F.L. Vernon, R.W. Hellwarth, J. Appl. Phys. **28**, 49 (1957)
322. S.E. Economou, T.L. Reinecke, in *Optical Generation and Control of Quantum Coherence in Semiconductor Nanostructures*, ed. by G. Slavcheva, P. Roussignol (Springer, Berlin, 2010), p. 62
323. F. Bloch, Nucl. Induction Phys. Rev. **70**, 460 (1946)
324. D. Pines, C.P. Slichter, Phys. Rev. **100**, 1014 (1955)
325. R.K. Wangsness, F. Bloch, Phys. Rev. **89**, 728 (1953)
326. S.J. Nettel, A. Kempicki, Am. J. Phys. **47**, 987 (1979)
327. I. Zutic, J. Fabian, S. Das, Sarma. Rev. Mod. Phys. **76**, 323 (2004)
328. G. Burkard, R.H. Koch, D.P. DiVincenzo, Phys. Rev. B **69**, 64503 (2004)
329. M. Fox, *in Quantum Optics, An Introduction* (Oxford University Press, Oxford, 2006)
330. F.-Y. Hong, S.-J. Xiong, Chin. J. Phys. **46**, 379 (2008)
331. C.P. Williams, *in Explorations in Quantum Computing* (Springer, Berlin, 2011)
332. C.J. Umrigar, K.G. Wilson, W. Wilkins, Phys. Rev. Lett. **60**, 1719 (1988)
333. P.J. Reynolds, D.M. Ceperley, B.J. Alder, J. Chem. Phys. **77**, 5593 (1982)
334. R. Jastrow, Phys. Rev. **98**, 1479 (1955)
335. T. Kato, Commun. Pure Appl. Math. **10**, 151 (1957)
336. N.D. Drummond, M.D. Towler, R.J. Needs, Phys. Rev. B **70**, 235119 (2004)
337. H.J. Flad, A. Savin, J. Chem. Phys. **103**, 691 (1995)
338. T. Kobayashi, *in J-Aggregates* (World Scientific, Singapore, 1996)
339. R.J. Cogdell, A. Gall, J. Köhler, Q. Rev, Biophysics **39**, 227 (2006)

340. P.O.J. Scherer, E.W. Knapp, S.F. Fischer, Chem. Phys. Lett. **106**, 101 (1984)
341. R.E. Merrifield, J. Chem. Phys. **40**, 445 (1964)
342. P.O.J. Scherer, S.F. Fischer, Chem. Phys. **86**, 269 (1984)
343. R. Kunz, K. Timpmann, J. Southall, R.J. Cogdell, A. Freiberg, J. Köhler, J. Phys. Chem. B **116**, 11017 (2012)
344. A.S. Davydov, Physica **3D**, 1 (1981)
345. G. Venzl, S.F. Fischer, Phys. Rev. B **32**, 6437 (1985)

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