Online Appendix C

Guide to Literature

C.1 Introduction

For many readers numerical analysis is studied as an important applied subject. Therefore, we shall give here a more complete overview of the literature than is usually given in textbooks. We restrict ourselves to books written in English. Further, only a restricted guide to literature on numerical linear algebra and differential equations is given here. These topics will be covered elsewhere.

The bibliography which we give is by necessity a subjective selection and by no means complete. We hope, however, that it can serve as a good guide for a reader who out of interest (or necessity!) wishes to deepen his or her knowledge.

Besides the reference periodicals such as *Mathematical Reviews*, *SIAM Review* and *Mathematics of Computation* publish extensive reviews of most books of interest. The weekly electronic newsletter *NA Digest* is a valuable source of information about current topics. To subscribe and for archives visit `www.netlib.org/na-net`.

MathSciNet (`http://www.ams.org/mathscinet`), an electronic index, is the basic source for mathematics published in the United States, with coverage on an international scope beginning in 1940. *Web of Science* (`http://scientific.thomsom.com/products/wos`) is an electronic multidisciplinary index in which mathematical journals are indexed. Coverage starts with 1945.

C.2 Textbooks in Numerical Analysis

We restrict ourselves to books published after 1965. A valuable source book to the literature before 1956 is Parke [25]. An interesting account of the history of numerical analysis from the sixteenth through the nineteenth centuries can be found in Goldstine [13].

Many outstanding textbooks in numerical analysis were originally published in the 1960s and 70s. The classical text by Hildebrand [18] can still be used as an introduction. Isaacson and Keller [19] give a rigorous mathematical treatment of classical topics, including differential equations and orthogonal polynomials. The authors' previous textbook [6] was used at many universities in the USA and is still available.

Hamming [16] is a more applied text and aims at combining mathematical theory, heuristic analysis, and computing methods. It emphasizes the message that *the purpose of computing is insight, not numbers*. An in-depth treatment of several areas such as numerical quadrature and approximation is found in the comprehensive book by Ralston and Rabinowitz [29]. This book also contains a great number of interesting and fairly advanced problems.

A popular introductory textbook is Fröberg [11], a revised and updated version of an earlier Swedish textbook. The book by Forsythe, Malcolm, and Moler [10] is notable in that it includes a set of Fortran subroutines of unusually high quality. It is not surprising to note that Cleve Moler, the creator of MATLAB, is one of the coauthors. Conte and de Boor [5] is a well-written introductory text, with a particularly good treatment of polynomial approximation.

Kahaner, Moler, and Nash [20] comes with a disk containing software. A good introduction to scientific computing is given by Golub and Ortega [14]. A matrix-vector approach is used in the MATLAB-oriented text of Van Loan [35]. Analysis is complemented with computational experiments using a package of more than 200 m-files. Another good introductory text using MATLAB is Eldén, Wittmeyer-Koch, and Nielson [9]. Cheney and Kincaid [4] is an undergraduate text with many examples and exercises. Kincaid and Cheney [21] is a related textbook but more mathematically oriented.

Heath [17] is a popular, more advanced, comprehensive text. Gautschi [12] is an elegant introductory text containing a wealth of computer exercises. Much valuable and hard-to-find information is included in notes after each chapter. The bestseller by Press et al. [27] gives a good survey of contemporary numerical methods for the applied scientist, but is weak on analysis.

Several good textbooks have been translated from German, notably the excellent book by Stoer and Bulirsch [32]. This is particularly suitable for a reader with a good mathematical background. Deuflhard and Hohmann [8] is less comprehensive but with a modern and careful treatment. Schwarz [31] is a mathematically oriented text which also covers ordinary and partial differential equations. Rutishauser [30] is an annotated translation of a highly original textbook by one of the pioneers of numerical analysis. Although brief, the book by Tyrtychnikov [33] is original and thorough. It also contains references to Russian literature unavailable in English.

Ueberhuber [34] is a two-volume introduction to numerical computation, which also emphasizes software aspects. It is notable for its thorough coverage of numerical integration. A modern textbook which covers iterative methods for linear systems as well as ordinary and partial differential equations is Quarteroni, Sacco, and Saleri [28].

The problem of adapting algorithms to run efficiently on modern parallel computer architecture is an important and nontrivial part of scientific computing. The textbook by Petersen and Arbenz [26] gives a good introduction to this topic.

We finally mention two standard references. For topics on linear spaces and approximation theory the comprehensive monograph by Davis [7] is invaluable. For a background in modern analysis including analytic functions, the classical textbook by Apostol [2] is recommended.

[1] F. S. Acton. *Numerical Methods That (Usually) Work*, Harper and Row, New York, 1970, 541 pages. Reprinted by the Mathematical Association of America, Washington, DC, 1990.

[2] Tom M. Apostol. *Mathematical Analysis*. Addison Wesley, Reading, MA, second edition, 1974. ISBN-13 0201002881. (Cited on p. C-2.)

[3] Kendall E. Atkinson. *An Introduction to Numerical Analysis*. John Wiley, New York, second edition, 1989, 712 pages. ISBN 0-471-62489-6

[4] Ward Cheney and David Kincaid. *Numerical Mathematics and Computing*. Brooks/Cole, Pacific Grove, CA, fourth edition, 1999. 562 pages. ISBN 0-534-04356-9 (Cited on p. C-2.)

[5] Samuel D. Conte and Carl de Boor. *Elementary Numerical Analysis. An Algorithmic Approach*. McGraw-Hill, New York, third edition, 1980, 432 pages. ISBN 0-07-012447-7 (Cited on p. C-2.)

[6] Germund Dahlquist and Åke Björck. *Numerical Methods*. Prentice-Hall, Englewood Cliffs, NJ., 1974, 573 pages. Republished by Dover, Mineola, NY, 2003. ISBN 0-486-42807-9 (Cited on p. C-1.)

[7] Philip J. Davis. *Interpolation and Approximation*. Blaisdell, New York, 1963. (Cited on p. C-2.)

[8] Peter Deuflhard and Andreas Hohmann. *Numerical Analysis in Modern Scientific Computing*. Springer, Berlin, second edition, 2003, 337 pages. ISBN 0-387-95410-4 (Cited on p. C-2.)

[9] Lars Eldén, Linde Wittmeyer-Koch, and Hans Bruun Nielsen. *Introduction to Numerical Computation*. Studentlitteratur, Lund, Sweden, 2004, 375 pages. ISBN 91-44-03727-9 (Cited on p. C-2.)

[10] George E. Forsythe, Michael A. Malcolm, and Cleve B. Moler. *Computer Methods for Mathematical Computations*. Prentice-Hall, Englewood Cliffs, NJ, 1977, 259 pages. ISBN 0-13-165332-6 (Cited on p. C-2.)

[11] Carl-Erik Fröberg. *Numerical Mathematics. Theory and Computer Applications*. Benjamin/Cummings, Menlo Park, CA, 1985, 436 pages. ISBN 0-8053-2530-1 (Cited on p. C-2.)

[12] Walter Gautschi. *Numerical Analysis. An Introduction*. Birkhäuser, Boston, MA, 1997, 506 pages. ISBN 0-8176-3895-4 (Cited on p. C-2.)

[13] Herman H. Goldstine. *A History of Numerical Analysis from the 16th through the 19th Century*. Stud. Hist. Math. Phys. Sci., Vol. 2. Springer-Verlag, New York, 1977, 348 pages. ISBN 0-387-90237-5. (Cited on p. C-1.)

[14] Gene H. Golub and James M. Ortega. *Scientific Computing and Differential Equations. An Introduction to Numerical Methods*. Academic Press, San Diego, CA, 1992, 337 pages. ISBN 0-12-289253-4 (Cited on p. C-2.)

[15] Gene H. Golub and James M. Ortega. *Scientific Computing. An Introduction with Parallel Computing*. Academic Press, San Diego, CA, 1993, 442 pages. ISBN 0-12-289255-0

[16] Richard W. Hamming. *Numerical Methods for Scientists and Engineers*. McGraw-Hill, New York, second edition, 1974, 721 pages. Republished by Dover, Mineola, NY, 1986. ISBN 0-486-65241-6 (Cited on p. C-2.)

[17] Michael T. Heath. *Scientific Computing. An Introductory Survey*. McGraw-Hill, Boston, MA, second edition, 2002, 563 pages. ISBN 0-07-239910-4 (Cited on p. C-2.)

[18] F. B. Hildebrand. *Introduction to Numerical Analysis*. McGraw-Hill, New York, second edition, 1974, 669 pages. Republished by Dover, Mineola, NY, 1987. ISBN 0-486-65363-3 (Cited on p. C-1.)

[19] Eugene Isaacson and Herbert B. Keller. *Analysis of Numerical Methods*. John Wiley, New York, 1966, 541 pages. Republished by Dover, Mineola, NY, 1994. ISBN 0-486-63029-0 (Cited on p. C-1.)

[20] David Kahaner, Cleve B. Moler, and Stephen G. Nash. *Numerical Methods and Software*. Prentice-Hall, Englewood Cliffs, NJ, 1989, 495 pages + disk. (Cited on p. C-2.)

[21] David Kincaid and Ward Cheney. *Numerical Analysis*. Brooks/Cole, Pacific Grove, CA, third edition, 2002, 804 pages. ISBN 0-534-38905-8. (Cited on p. C-2.)

[22] Cornelius Lanczos. *Applied Analysis*. Prentice-Hall, Englewood Cliffs, NJ, 1956, 559 pages. Republished by Dover, Mineola, NY, 1988. ISBN 0-486-65656-0

[23] G. I. Marchuk. *Methods in Numerical Mathematics*. Springer-Verlag, Berlin, second edition, 1982, 510 pages. ISBN 0-387-90614-2

[24] James Ortega. *Numerical Analysis: A Second Course*. Academic Press, New York, 1972. Republished by SIAM, Philadelphia, PA, 1990. ISBN 0-89871-5.

[25] N. G. Parke. *Guide to the Literature of Mathematics and Physics*. Dover, Mineola, NY, second edition, 1958. (Cited on p. C-1.)

[26] W. P. Petersen and P. Arbenz. *Introduction to Parallel Computing. A Practical Guide with Examples in C*. Oxford Texts in Applied and Engineering Mathematics. Oxford University Press, Oxford, UK, 2004. ISBN 0 19 851577 4. (Cited on p. C-2.)

[27] William H. Press, Brian P. Flannery, Saul A. Teukolsky, and William T. Vetterling. *Numerical Recipes in Fortran* 77: *The Art of Scientific Computing*. Cambridge University Press, Cambridge, UK, second edition, 1992. (Cited on p. C-2.)

[28] Alfio Quarteroni, Riccardo Sacco, and Fausto Saleri. *Numerical Mathematics*. Springer-Verlag, New York, 2000, 654 pages. ISBN 0-387-98959-5 (Cited on p. C-2.)

[29] Anthony Ralston and Philip Rabinowitz. *A First Course in Numerical Analysis*. McGraw-Hill, New York, second edition, 1978. Republished by Dover, Mineola, NY, 2001. ISBN 0-486-41454-0 (Cited on p. C-2.)

[30] Heinz Rutishauser. *Lectures on Numerical Mathematics* Band 1 & 2. Birkhäuser, Boston, MA, 1990, 164 + 228 pages. (Cited on p. C-2.)

[31] H.-R. Schwarz. *Numerical Analysis: A Comprehensive Introduction*. John Wiley, New York, 1989, 517 pages. ISBN 0-471-92064-9 (Cited on p. C-2.)

[32] Joseph Stoer and Roland Bulirsch. *Introduction to Numerical Analysis*. Springer-Verlag, New York, third edition, 2002, 744 pages. (Cited on p. C-2.)

[33] E. Tyrtychnikov, *A Brief Introduction to Numerical Analysis*. Birkhäuser, Boston, 1997. ISBN: 0-8176-3916-0 6501 (Cited on p. C-2.)

[34] Christoph W. Ueberhuber. *Numerical Computation: Methods, Software, and Analysis. Volumes* 1 & 2. Springer-Verlag, Berlin, 1997, 474 + 495 pages. ISBN 3-540-62058-3, 3-540-62057-5 (Cited on p. C-2.)

[35] Charles F. Van Loan. *Introduction to Scientific Computing*. Prentice-Hall, Upper Saddle River, NJ, second edition, 2000 367 pages. ISBN 0-13-125444-8 (Cited on p. C-2.)

C.3 Handbooks and Collections

A series of conferences on the State of the Art in Numerical Analysis were organized by the Institute of Mathematics and Its Applications with the aim of accounting for recent developments in the field. Proceedings from the last two held in 1986 (Iserles and Powell [5]) and 1996 (Duff and Watson [3]) contain excellent surveys of many topics.

Another source of survey articles on topics of current interest can be found in *Acta Numerica*, a Cambridge University Press Annual started in 1992. The journal *SIAM Review* also publishes high-quality review papers.

The *Journal of Computational and Applied Mathematics* published in Volumes 121–128 (2000–2001) a series of papers on "Numerical Analysis of the 20th Century," with the aim of presenting the historical development of numerical analysis and reviewing current research. The papers were arranged in seven-volume book set:

Vol. I: Approximation Theory.

Vol. II: Interpolation and Extrapolation.

Vol. III: Linear Algebra.

Vol. IV: Nonlinear Equations and Optimisation.

Vol. V: Quadrature and Orthogonal Polynomials.

Vol. VI: Ordinary Differential Equations and Integral Equations.

Vol. VII: Partial Differential Equations.

A collection of outstanding survey papers on special topics are being published in a multivolume sequence in the *Handbook of Numerical Analysis* [2], edited by Philippe G. Ciarlet and Jacques-Louis Lions. It offers comprehensive coverage in all areas of numerical analysis as well as many actual problems of contemporary interest. Each volume concentrates on one to three particular subjects under the following headings:

- Solution of Equations in R^n.
- Finite Difference Methods.
- Finite Element Methods.
- Techniques of Scientific Computing.
- Optimization Theory and Systems Science.
- Numerical Methods for Fluids.
- Numerical Methods for Solids.

Other topics covered include meteorology, seismology, petroleum mechanics and celestial mechanics. By 2005, 13 volumes had appeared.

We also mention here some additional useful references which do not fit into any of the above categories. Knuth [6] is the ultimate reference on number systems and arithmetic. The book by Gander and Hřebiček [4] contains a collection of well-chosen problems in scientific computing and their solutions via modern software tools like MATLAB and Maple. Another collection of solved problems which is entertaining and highly instructive is contained in *The SIAM* 100-*Digit Challenge* [1]. Strang [7] gives an excellent modern introduction to applied mathematics.

[1] Folkmar Bornemann, Dirk Laurie, Stan Wagon, and Jörg Waldvogel. *The SIAM* 100-*Digit Challenge. A Study in High-Accuracy Numerical Computing*. SIAM, Philadelphia, PA, 2004. (Cited on p. C-6.)

[2] Philippe G. Ciarlet and Jacques Louis Lions. *Handbook of Numerical Analysis*, volume I–XIII. North-Holland, Amsterdam, 1990–2005. (Cited on p. C-5.)

[3] Iain S. Duff and G. Alistair Watson, editors. *The State of the Art in Numerical Analysis*. Clarendon Press, Oxford, 1997. (Cited on p. C-5.)

[4] W. Gander and J. Hřebiček. *Solving Problems in Scientific Computing using Maple and Matlab*. Springer-Verlag, Berlin, fourth edition, 2004. (Cited on p. C-6.)

[5] Arieh Iserles and M. J. D. Powell, editors. *The State of the Art in Numerical Analysis*. Clarendon Press, Oxford, 1987. (Cited on p. C-5.)

[6] Donald E. Knuth. *The Art of Computer Programming, Volume* 2: *Seminumerical Algorithms*. Addison-Wesley, Reading, MA, third edition, 1998. (Cited on p. C-6.)

[7] Gilbert Strang. *Introduction to Applied Mathematics*. Wellesley-Cambridge Press, Wellesley, MA, 1986. (Cited on p. C-6.)

C.4 Encyclopedias, Tables, and Formulas

Although mathematical tables no longer play the same role in computing as they used to, occasionally they can be an aid in checking or planning calculations on a computer. Fletcher, Miller, and Rosenhead [3] list nearly every table of mathematical functions published up to approximately 1959. Many excellent tables were produced in Russia; see Lebedev and Federova [7].

Advice about the use and choice of tables is given in Todd [13, pp. 93–106]. He distinguishes between tables that should be on one's desk and those which should be available in a library. Among tables in the first category is Comrie [2]. Comrie's book also contains a handy collection of useful formulas for trigonometric and hyperbolic functions. The tables of higher functions by Jahnke, Emde, and Lösch [5] were first published in 1909. This collection is now dated, but contains some amazing hand calculated two- and three-dimensional graphs showing the behavior of different functions in the complex plane. A modern version is the *Atlas of Functions* [12], which contains computer-generated color graphs of families of functions. It comes with a CD containing software that can provide values of functions in the *Atlas*.

The most comprehensive source of information on useful mathematical functions and formulas is the *Handbook of Mathematical Functions, with Formulas, Graphs, and Mathe-*

matical Tables, edited by Milton Abramowitz and Irene Stegun [1]. This was first published in 1964 by the National Bureau of Standards (renamed National Institute of Standards and Technology (NIST) in 1988), and more than 150,000 copies have been sold. Although still available and among one of the most cited references, it is becoming increasingly out of date. A replacement more suited to today's needs is being developed at NIST. This is planned to be made available soon both in print and as a free electronic publication on the World Wide Web; see the mockup version at `http://dlmf.nist.gov`.

An outline of the features of new NIST Digital Library of Mathematical functions is given by D. W. Lozier [9]. The internet version will come with hyperlinks, interactive graphics, and tools for downloading and searching. The part of the old *Handbook* devoted to massive tables of values will be superseded. To summarize, data-intensive and operation-preserving methods are replaced by data-conserving and operation-intensive techniques. A good overview of software for mathematical special functions is given by Lozier and Olver [8].

The *James & James Mathematics Dictionary* [6] is a high-quality general mathematics dictionary that covers arithmetic to calculus and includes a multi-lingual index. *CRC Concise Encyclopedia of Mathematics* [14] by Eric Weisstein is a comprehensive compendium of mathematical definitions, formulas, and references. A free Web encyclopedia containing surveys and references is Eric Weisstein's World of Mathematics at `mathworld.wolfram.com`.

[1] Milton Abramowitz and Irene A. Stegun (eds.). *Handbook of Mathematical Functions*. Dover, New York, NY, 1965. (Cited on p. C-7.)

[2] L. J. Comrie. *Chamber's Shorter Six-Figure Mathematical Tables*. W. & R. Chambers, Edinburgh, 1968. (Cited on p. C-6.)

[3] A. Fletcher, J. C. P. Miller, and L. Rosenhead. *Index of Mathematical Tables. Two volumes*. Blackwell's, Oxford, UK, second edition, 1962. (Cited on p. C-6.)

[4] I. S. Gradshteyn and I. M. Ryzhik. *Table of Integrals, Series and Products*. Academic Press, London, UK, fifth edition, 1993.

[5] Eugene Jahnke, Fritz Emde, and Friedrich Lösch. *Tables of Higher Functions*. McGraw-Hill, New York, sixth edition, 1960. (Cited on p. C-6.)

[6] Glenn James and Robert C. James, editors. *James & James Mathematics Dictionary*. Van Nostrand, Princeton, NJ, fifth edition, 1992. (Cited on p. C-7.)

[7] A. V. Lebedev and R. M. Federova. *A Guide to Mathematical Tables*. Van Nostrand, New York, 1960. (Cited on p. C-6.)

[8] D. W. Lozier and F. W. J. Olver. Numerical evaluation of special functions. In W. Gautschi, editor, *Mathematics of Computation* 1943–1993: *A Half-Century of Computational Mathematics*, volume 48 of *Proc. Symposium Appl. Math.*, pages 79–125, Amer. Math. Soc., Providence, RI, 1994. (Cited on p. C-7.)

[9] Daniel W. Lozier NIST digital library of mathematical functions. *Annals of Mathematics and Artificial Intelligence*, 38:105–119, 2003. (Cited on p. C-7.)

[10] A. P. Prudnikov, Y. A. Brychkov, and O. I. Marichev. *Integrals and Series. Volume* 1: *Elementary Functions*. Gordon and Breach, New York, 1986.

[11] A. P. Prudnikov, Yu. A. Brychkov, and O. I. Marichev. *Integrals and Series. Volume 2: Special Functions*. Gordon and Breach, New York, 1986.

[12] Jerome Spanier, Keith B. Oldham, and Jan Myland. *An Atlas of Functions*. Springer-Verlag, Berlin, second edition, 2008. (Cited on p. C-6.)

[13] John Todd, editor. *Survey of Numerical Analysis*, McGraw-Hill, New York, 1962. (Cited on p. C-6.)

[14] Eric W. Weisstein, editor. *CRC Concise Encyclopedia of Mathematics*. CRC Press, Boca Raton, FL, 1999. (Cited on p. C-7.)

C.5 Selected Journals

We list here a selection of journals covering the areas of numerical analysis and mathematical software. Most journals are now available in electronic form. There are several journal platforms: *Science Direct* for Elsevier's journals; *Springer Link* for Springer's journals, including *Lecture Notes in Mathematics*; and *Wiley Interscience* for Wiley's electronic journal platform. The SIAM journals are published by the Society for Industrial and Applied Mathematics and are available electronically at `epubs.siam.org`. JSTOR at `www.jstor.org` contains back issues of several numerical journals, e.g., *Mathematics of Computation*, and some SIAM journals.

The early issues of *The Computer Journal* contain many classical papers, but lately few papers are relevant to numerical methods.

ACM Transactions on Mathematical Software (1975–), Association for Computing Machinery.

Acta Numerica (1992–), Cambridge University Press.

Applied Numerical Mathematics (1985–), Elsevier.

BIT Numerical Mathematics (1961–), Springer.

Calcolo (1964–), Springer Milan.

Chinese Journal of Numerical Mathematics and Applications (1979–), Allerton Press.

Computing (1966–), Springer Wien.

IMA Journal on Numerical Analysis (1981–), Oxford University Press.

Journal of Computational and Applied Mathematics (1975–), North–Holland.

Linear Algebra and Its Applications (1968–), Elsevier.

Mathematics of Computation (1960–), American Mathematical Society; previously called *Mathematical Tables and Other Aids to Computing* (1943–1959).

Numerical Algorithms (1991–), Springer.

Numerical Linear Algebra with Applications (1994–), Wiley Interscience.

Numerische Mathematik (1959–), Springer.

SIAM Journal on Matrix Analysis and Applications (1988–), SIAM.

SIAM Journal on Numerical Analysis (1996–), SIAM.

SIAM Journal on Scientific Computing (1994–), SIAM; previously called *SIAM Journal on Scientific & Statistical Computing* (1980–1993).

SIAM Review (1959–), SIAM.

The Computer Journal (1959–), The British Computer Society.

Several journals only available in electronic form are also of interest. *Electronic Transactions on Numerical Analysis* (ETNA) is available at `etna.math.kent.edu` and at several mirror sites. *Electronic Journal of Linear Algebra* is available at `www.math.technion.ac.il/iic/ela/` and at several mirror sites.

C.6 Algorithms and Software

Some principal questions concerning the production of software for mathematical computation are discussed by Rice [3, 4].

Starting in the 1960s much general purpose software, often collected in large libraries or packages, has been developed. There are two large suppliers of commercial scientific subroutine libraries. Numerical Algorithms Group (NAG), based in England, started in 1970 as an interuniversity collaboration; see `www.nag.co.uk`. IMSL, now part of Visual Numerics (`www.vni.com`) was founded about the same time in the USA. Both companies offer a wide range of software in Fortran and C.

MATLAB, developed by The Mathworks (`www.mathworks.com`), is a widespread interactive system for matrix computations. It offers many "toolboxes" for specific application areas, e.g., control problems. Maple, developed by Maplesoft (`www.maplesoft.com`), offers symbolic computation. It is available as a MATLAB toolbox, which makes it possible to combine numerical and symbolic computations.

Mathematica, developed by Wolfram Research (`www.wolfram.com`), also integrates numerical and symbolical computing. It can handle symbolical calculations that involve hundreds of thousands of terms. Wolfram Research also sponsors the free resource MathWorld (`www.mathworld.com`), an encyclopedia of mathematics on the Web. COMSOL (`www.comsol.com`), started by students of the first author, has developed a unique modular software package for multiphysics simulation.

The book *Numerical Recipes in Fortran* 77, by Press et al. (see Sec. C.2) exists in several other versions with programs in Fortran 90, Pascal, C++, and C. The programs printed in the book are, however, for reading purposes only, and the copyrighted software is sold separately and can be downloaded from an online store. The book [2] is a complement to the original *Fortran* 77 book. It contains reworked versions of all the original codes adapted to the parallel computing facilities in Fortran 90.

Many programs and packages are available in the public domain and can be downloaded for free. A prime example is LAPACK, which superseded LINPACK and EISPACK in the mid-1990s, and contains programs for solving linear systems and eigenvalue problems. Other packages, such as DASSL, are available for solving ordinary systems of differential equations.

The National Institute of Standards and Technology (NIST) Guide to Available Mathematical Software (GAMS) is available at `gams.nist.gov`. GAMS is an online cross-index of mathematical and statistical software providing abstracts, documentation, and source codes of software modules, and it provides access to multiple repositories operated by others. Currently four repositories are indexed, three within NIST and one on Netlib. Both public domain and proprietary software are indexed although source codes of proprietary software are not redistributed by GAMS.

Netlib is a repository of public domain mathematical software, data, address lists, and other useful items for the scientific computing community. Access Netlib is via `www.netlib.org`. Background about Netlib is given in [1].

A top-level index which describes the chapters of Netlib, each of which has an individual index, file is available. Note that many of these codes are designed for use by professional numerical analysts who are capable of checking for themselves whether an algorithm is suitable for their needs. One routine can be superb and the next awful. So be careful!

[1] Jack. J. Dongarra and Eric Grosse. Distribution of mathematical software via electronic mail. *Comm. ACM*, 30:403–407, 1987. (Cited on p. C-10.)

[2] William H. Press, Brian P. Flannery, Saul A. Teukolsky, and William T. Vetterling. *Numerical Recipes in Fortran* 90: *The Art of Parallel Scientific Computing*. Cambridge University Press, Cambridge, UK, 1996. (Cited on p. C-9.)

[3] John R. Rice, editor. *Mathematical Software*. Academic Press, New York, 1971. (Cited on p. C-9.)

[4] John R. Rice. *Numerical Methods, Software, and Analysis*. Academic Press, Boston-New York, second edition, 1993. (Cited on p. C-9.)

C.7 Public Domain Software

Below is a selective list indicating the scope of software available from Netlib. The first few libraries here are widely regarded as being of high quality. The likelihood of your encountering a bug is relatively small; if you do, report it by email to `ehg@research.att.com`

Algorithms published in *ACM Transactions on Mathematical Software* can also be downloaded from `www.acm.org/pubs/calgo`. As of October 2007, 866 algorithms were available.

BLAS: Basic Linear Algebra Subprograms levels 1, 2, and 3, and machine constants.

FFTPACK: A package of Fortran programs for the fast Fourier transform of periodic and other symmetric sequences. This package consists of programs which perform fast Fourier transforms for both complex and real periodic sequences and certain other symmetric sequences. Developed by Paul Swarztrauber, NCAR.

VFFTPK: A vectorized version of FFTPACK for multiple sequences. Developed by Sweet, Lindgren, and Boisvert.

FISHPACK: A package of Fortran subprograms providing finite difference approximations for elliptic boundary value problems. Developed by Paul Swarztrauber and Roland Sweet.

FN: Wayne Fullerton's special function library (single and double).

GO: Golden Oldies: Routines that have been widely used but aren't available through the standard libraries.

HARWELL: Sparse matrix routine MA28 from the Harwell library made available by Iain Duff.

LAPACK: For the most common problems in numerical linear algebra such as linear equations, linear least squares problems, eigenvalue problems, and singular value problems. Designed to be efficient on a wide range of modern high-performance computers. Developed by Ed Anderson, Z. Bai, Chris Bischof, Jim Demmel, Jack Dongarra, Jeremy Du Croz, Anne Greenbaum, Sven Hammarling, Alan McKenney, Susan Ostrouchov, and Danny Sorensen.

PPPACK: Subroutines from the book *A Practical Guide to Splines*, by Carl de Boor. Some calling sequences differ slightly from those in the book.

TOMS: Collected algorithms of the ACM. When requesting a specific item, please refer to the algorithm number.

In contrast to the above libraries, the following are collections of codes from a variety of sources. Most are excellent, but you should exercise caution. We include research codes that we haven't tested and codes that may not be state of the art but are useful for comparisons. The following list is alphabetical, not by merit:

AMOS: Bessel and Airy functions of complex arguments and nonnegative order.

BIHAR: Biharmonic solver in rectangular geometry and polar coordinates. Made available by Petter Bjørstad, University of Bergen.

BMP: Multiple precision package. By Richard P. Brent.

C++: Miscellaneous codes written in C++. Eric Grosse, editor, Bell Laboratories.

C: Miscellaneous codes written in C. Not all C software is in this miscellaneous library. If it clearly fits into a domain-specific library, it is assigned there. Eric Grosse, editor.

CONFORMAL: Routines to solve the "parameter problem" associated with conformal mapping. Includes SCPACK (polygons with straight sides) from Nick Trefethen; CAP (circular arc polygons) from Petter Bjorstad and Eric Grosse; gear-like domains by Kent Pearce, and CONFPACK (Symm's integral equation) by Hough and Gutknecht.

CONTIN: Methods for continuation and limit points, notably PITCON, by Werner Rheinboldt and John Burkardt, University of Pittsburgh.

DDSV: Programs from *Linear Algebra Computations on Vector and Parallel Computers*, by Jack Dongarra, Iain Duff, Danny Sorensen, and Henk Van der Vorst.

DIERCKX: Spline fitting routines for various kinds of data and geometries. Paul Dierckx, Leuven.

ELEFUNT: Transportable Fortran programs for testing the elementary function programs provided with Fortran compilers. Reference: *Software Manual for the Elementary Functions* by W. J. Cody and W. Waite, Prentice–Hall, 1980.

FITPACK: Splines under tension (an early version). Developed by Alan K. Cline.

FMM: Routines from the book *Computer Methods for Mathematical Computations*, by George Forsythe, Mike Malcolm, and Cleve Moler.

GCV: Generalized cross validation spline smoothing and ridge regression. Developed by Grace Wahba.

HOMPACK: Fortran 77 subroutines for solving nonlinear systems of equations by homotopy methods. There are subroutines for fixed point, zero finding, and general homotopy curve tracking problems, utilizing both dense and sparse Jacobian matrices. Three different algorithms are implemented: ODE-based, normal flow, and augmented Jacobian. Layne T. Watson, Blacksburg, VA.

ITPACK: Iterative linear system solver based on a number of methods: Jacobi method, SOR, and SSOR with conjugate gradient or Chebyshev (semi-iteration) acceleration. David Young, David Kincaid, and the group at the University of Texas, Austin.

JAKEF: A precompiler that analyzes a given Fortran 77 source code for the evaluation of a scalar or vector function and then generates an expanded Fortran subroutine that simultaneously evaluates the gradient or Jacobian, respectively. For scalar functions the ratio between the run time of the resulting gradient routine and that of the original evaluation routine is never greater than a fixed bound of about five. The storage requirement may be considerable, as it is also proportional to the run time of the original routine. Since no differencing is done, the partial derivative values obtained are exact up to roundoff errors. By Andreas Griewank.

LANZ: Large Sparse Symmetric Generalized Eigenproblem. Mark T. Jones, Argonne National Laboratory and Merrell L. Patrick, Duke University.

LANCZOS: For computing a few eigenvalues/eigenvectors of large (sparse) real symmetric and Hermitian matrices, and singular values and vectors of rectangular matrices. By Jane Cullum and Ralph Willoughby.

LAWSON–HANSON: Least squares codes from the book *Solving Least Squares Problems*, by C. L. Lawson and R. J. Hanson, SIAM, 1995.

LP: A set of test problems for linear programming in MPS format. David Gay, Bell Laboratories.

MINPACK: Solution of systems of nonlinear equations and nonlinear least squares problems. Consists of five algorithmic paths, each including a core subroutine and an easy-to-use driver. The algorithms proceed either from an analytic specification of the Jacobian matrix or directly from the problem functions. The paths include facilities for systems of equations with a banded Jacobian matrix, for least squares problems with a large amount of data, and for checking the consistency of the Jacobian matrix with the functions. Developed by Jorge Moré, Burt Garbow, and Ken Hillstrom, Argonne National Laboratory.

MISC: Contains various pieces of software collected over time. Jack Dongarra.

MPFUN: Multiple precision arithmetic. David Bailey.

NAPACK: Solving linear systems; estimating the condition number or the norm of a matrix; computing determinants, matrix inverse, least squares problems. Also for performing unconstrained minimization, compute eigenvalues, eigenvectors, the singular value decomposition, or the QR decomposition. The package has special routines for general, band, symmetric, indefinite, tridiagonal, upper Hessenberg, and circulant matrices. By Bill Hager, University of Florida, Gainesville. Related book: *Applied Numerical Linear Algebra*, Prentice–Hall, 1988.

NUMERALGO: Algorithms from the journal *Numerical Algorithms*.

ODE: Various initial and boundary value ordinary differential equation solvers: colsys, dverk, rksuite, ode. Erik Grosse.

ODEPACK: The ODE package from Hindmarch and others. Alan Hindmarch, Lawrence Livermore National Laboratory.

ODRPACK: Orthogonal Distance Regression. A portable collection of Fortran subprograms for fitting a model to data. It is designed primarily for instances when the independent as well as the dependent variables have significant errors, implementing a highly efficient algorithm for solving the weighted orthogonal distance regression problem, i.e., for minimizing the sum of the squares of the weighted orthogonal distances between each data point and the curve described by the model equation. By Boggs, Byrd, Rogers, and Schnabel.

PARANOIA: A program to explore the floating-point system on your computer. Devised by W. Kahan, University of California, Berkeley.

PDES: A compact package for solving systems of linear equations using multigrid or aggregation–disaggregation methods. Imbedded in the algorithms are implementations for sparse Gaussian elimination and symmetric Gauss–Seidel (unaccelerated or accelerated by conjugate gradients or Orthomin(1)). This package is particularly useful for solving problems which arise from discretizing partial differential equations, regardless of whether finite differences, finite elements, or finite volumes are used. Craig Douglas.

PLTMG: Elliptic partial differential equations in general regions of the plane. It features adaptive local mesh refinement, multigrid iteration, and a pseudoarclength continuation option for parameter dependencies. The package includes an initial mesh generator and several graphics packages. By Randy Bank. Reference: *PLTMG*: *A Software Package for Solving Elliptic Partial Differential Equations*: *Users' Guide* 8.0, SIAM, 1998.

POLYHEDRA: A database of angles, vertex locations, and so on for over 100 hundred geometric solids. Compiled by Andrew Hume.

PORT: Public subset of the PORT library, which includes the latest version of David Gay's NL2SOL nonlinear least squares. The rest of the PORT3 library is available by license from Lucent Technologies.

RANDOM: Random number generators. Eric Grosse, editor.

QUADPACK: Univariate quadrature. By Robert Piessens (Leuven), Elise de Donker (Leuven), and David Kahaner (National Bureau of Standards).

SLAP: Sparse linear algebra package for iterative symmetric and nonsymmetric linear system solutions. Included are core routines to do iterative refinement, preconditioned conjugate gradient, preconditioned conjugate gradient on the normal equations, preconditioned biconjugate gradient, preconditioned biconjugate gradient squared, orthomin, and generalized minimum residual. Mark K. Seager and Anne Greenbaum.

SLATEC: Comprehensive software library containing over 1400 general purpose mathematical and statistical routines written in Fortran 77.

SPARSPAK: Subroutines from the book *Computer Solution of Large Sparse Positive Definite Systems* by Alan George and Joseph Liu, Prentice–Hall, 1981.

SPARSE: Subroutines written in C that solve large sparse systems of linear equations using LU factorization. The package is able to handle arbitrary real and complex square matrix equations. Besides being able to solve linear systems, it solves transposed systems, finds determinants, multiplies a vector by a matrix, and estimates errors due to ill-conditioning in the system of equations and instability in the computations. SPARSE does not require or assume symmetry and is able to perform numerical pivoting (either diagonal or complete) to avoid unnecessary error in the solution. SPARSE also has an optional interface that allow it to be called from FORTRAN programs. Ken Kundert, Alberto Sangiovanni-Vincentelli, Berkeley.

SPARSE-BLAS: An extension to the set of Basic Linear Algebra Subprograms (BLAS). The extension is targeted at sparse vector operations, with the goal of providing efficient, but portable, implementations of algorithms for high-performance computers. By Dave Dodson.

SPECFUN: Fortran programs for special functions, and accompanying test programs similar in concept to those in ELEFUNT. W. J. Cody, Argonne National Laboratory.

SVDPACK: Singular values and singular vectors of large sparse matrices. By Mike Berry.

TEXTBOOK: Codes associated with numerical analysis textbooks. Erik Grosse, editor.

TOEPLITZ: Solution of Toeplitz or circulant systems of linear equations and for orthogonal factorization of column-circulant matrices. A Soviet–American collaborative effort. Burt Garbow, Argonne National Laboratory,

TRANSFORM: Fast Fourier Transform (FFT) and other digital processing tools. Erik Grosse, editor.

UNCON: Unconstrained optimization. Problems from Moré, Garbow, and others.

VANHUFFEL: Total least squares (TLS) problem by using a partial singular value decomposition (PSVD). By Sabine Van Huffel.