Appendix A

Some Software for Matrix Computations

In this appendix we list some most common mathematical software for matrix computations.

A.1 LAPACK

"LAPACK is a transportable library of Fortran 77 subroutines for solving the most common problems in numerical linear algebra: systems of linear equations, linear least squares problems, eigenvalue problems, and singular value problems. It has been designed to be efficient on a wide range of modern high-performance computers.

"LAPACK is designed to supersede LINPACK and EISPACK, principally by restructuring the software to achieve much greater efficiency on vector processors, high-performance 'superscalar' workstations, and shared memory multiprocessors. LAPACK also adds extra functionality, uses some new or improved algorithms, and integrates the two sets of algorithms into a unified package. The *LAPACK Users' Guide* gives an informal introduction to the design of the algorithms and software, summarizes the contents of the package, describes conventions used in the software and its documentation, and includes complete specifications for calling the routines." (Quoted from the cover page of *LAPACK Users' Guide*.)

A.1.1 LAPACK ++

This version of LAPACK is written in C++. It contains routines for solving systems of linear equations and eigenvalue problems on high-performance computer architectures. It does not, however, include all of the capabilities of original Fortran 77 LAPACK. "Emphasis is given to routines for solving linear systems consisting of non-symmetric matrices, symmetric positive definite systems, and solving linear systems." (Quoted from *http://math.nist.gov/lapack++/*.)

A.1.2 SCALAPACK

SCALAPACK (scalable LAPACK) includes a sublet of LAPACK routines redesigned for distributed memory MIMD parallel computers. "It implements block-oriented LAPACK linear algebra routines, adding a special set of communication routines to copy blocks of data between processors as required." (Quoted from *http://www.netlib.org/clapack/*.)

A.1.3 CLAPACK

"The CLAPACK library was built using a Fortran to C conversion utility called **fzc**. The entire Fortran 77 LAPACK library is run through **fzc** to obtain C code, and then modified to improve readability. CLAPACK's goal is to provide LAPACK for someone who does not have access to a Fortran compiler." (Quoted from *http://www.netlib.org/clapack/*.)

A.2 NAG

NAG stands for Numerical Algorithm Group. This group has developed a large software library (also called NAG) containing routines for most computational problems, including numerical linear algebra problems, numerical differential equations problems (both ordinary and partial), optimization problems, integral equations problems, statistical problems, etc.

A.3 IMSL

IMSL stands for International Mathematical and Statistical Libraries. As the title suggests, this library contains routines for almost all mathematical and statistical computations. The routines are written in C, C#, Java, and Fortran. It is now included as a part of Visual Numerics' Computational Technological Toolkit (CTT).

A.4 MATLAB

The name MATLAB stands for MATrix LABoratory. It is an interactive computing system designed for easy computations of various matrix-based scientific and engineering problems.

MATLAB can be used to solve a **linear system** and associated problems (such as inverting a matrix or computing the rank and determination of a matrix), to compute the **eigenvalues** and **eigenvectors** of a matrix, to find the **singular value decomposition** of a matrix, to compute the zeros of a polynomial, to compute generalized eigenvalues and eigenvectors, etc. MATLAB is an extremely useful and valuable package for testing algorithms for small problems and for use in the classroom. It has indeed become an indispensable tool for teaching applied and numerical linear algebra in the classroom. A remarkable feature of MATLAB is its graphic capabilities (see more about MATLAB in Appendix B).

Besides matrix computations, MATLAB can be used in a wide range of applications, including control design and analysis, signal processing, image processing, communications, financial modeling and analysis, and computational biology.

A.5 MATLAB Codes and MATLAB Toolboxes

MATLAB codes for selected algorithms described in this book are provided for beginning students in Appendix B.

Furthermore, there exists an interactive MATLAB Toolbox, called MATCOM, implementing all the major algorithms (to be taught in the first course) of this book, so that students can compare different algorithms for the same problem with respect to numerical efficiency, stability, accuracy, etc.

MATCOM is available from *http://www.siam.org/books/ot116*. Some major algorithms for linear systems and least-squares problems have also been implemented in the Matrix Computation Toolbox by N. Higham, which is available from *http://www.maths.manchester.ac.uk/∼higham/mctoolbox*.

A.6 The ACM Library

The ACM Library provided by the Association for Computing Machinery contains routines for basic matrix-vector operations, linear systems and associated problems, nonlinear systems, zeros of polynomials, etc. The journal *ACM Transactions on Mathematical Software* publishes these algorithms.

A.7 ITPACK (Iterative Software Package)

The package contains routines for solving iteratively mainly linear systems problems in large and sparse cases. The package was developed at the Center for Numerical Analysis of the University of Texas, Austin.

A.8 ARPACK

ARPACK stands for Arnoldi Package. It is a collection of Fortran routines for solving large-scale eigenvalue problems. There also exists a parallel version of ARPACK, called P_ARPACK, targeted for distributed memory architectures. Details can be found in *ARPACK Users' Guide* by Lehoucq, Sorensen, and Yang (1998).

A.9 SPARSKIT

This package is a general purpose Fortran library for sparse matrix computations, developed by Youcef Saad of the University of Minnesota. This is a basic toolkit for matrix computations. *http://www-users.cs.umn.edu/∼saad/software/SPARSKIT/sparskit.html.*

A.10 Sparse Software for Direct Methods

Although direct methods for sparse problems have not been discussed in this book, there exists a wide variety of software for direct sparse solvers; including HSL (formerly the Harwell Subroutine Library). A good source of finding a current list of the available sparse software for direct methods is the website of Prof. Timothy Davis of the University of Florida: *http://www.cise.ufl.edu/ davis*. Algorithms for direct sparse solvers are available from the book by Prof. Davis, *Direct Methods for Sparse Linear Systems* (Davis (2006)).

Then algorithms have been implemented in the package Csparse—a Concise Sparse Matrix Package. See Duff et al. (1989, 1992) for sparse matrix collections. For sparse matrices in MATLAB, see Gilbert et al. (1992).

A.11 NETLIB

NETLIB is a repository of mathematical software, papers, and databases.

In particular, all the software mentioned in this appendix, including LAPACK and the older packages LINPACK and EISPACK, are available from this site. *http://www.netlib.org*.

A.12 GAMS

GAMS stands for Guide to Available Mathematical Software: "A crop-index and virtual repository of mathematical and statistical software components of use in computational science and engineering." *http://gams.nist.gov*.

A.13 Users' Guides and Addresses

1. *LAPACK Users' Guide* (Third Edition) is available from
   SIAM (Society for Industrial and Applied Mathematics)
   3600 Market Street, 6th Floor
   Philadelphia, PA 19104-2688
   Tel: (215) 382-9800
   www.siam.org

2. The NAG Library and the associated users' manual can be obtained from
   The Numerical Algorithms Group, Ltd.
   Wilkinson House
   Jordan Hill Road
   Oxford, 0X28DR
   United Kingdom
   www.nag.co.uk

3. NAG North America Site
   The Numerical Algorithms Group, Inc.
   1431 Opus Place
   Suite 220
   Downers Grove, IL 60515-1362
   http://www.nag.com

4. IMSL: The IMSL software library and documentation are available from
   Visual Numerics Corporate Headquarters
   1300 W. Sam Houston
   Suite 150
   Houston, TX 77072
   info@houston.uni.com

5. MATLAB: The Corporate Headquarters for the Mathworks is
   The MathWorks, Inc.
   3 Apple Hill Drive
   Natick, MA 01760-2098
   Tel: (508) 647-7000; Fax: (508) 647-7001
   www.mathworks.com

MATLAB Simulink student version has just been released (Release 2007 a). It contains MATLAB, Simulink, Control Systems Toolbox, Signal Processing Toolbox, Statistical Toolbox, Optimization Toolbox, Symbolic Math Functions, and Signal Processing Blockset.

Several MATLAB guides are available. These include

- *MATLAB Guide* by Higham and Higham (2005),
- *MATLAB Premier* by Davis and Sigmon (2005),
- *Practical Introduction to MATLAB* by Mark S. Gockenbach, available from *http://www.math.mtu.edu/ ∼msgocken*,
- *MATLAB Manuals* from MathWorks,
- free online MATLAB tutorial available from *http://www.math.ufl.edu/help/matlab-tutorial*,

There also exists a MATLAB package, called FLAP, for Adjustable Precision Floating-Point Arithmetic by G.W. Stewart. The package can be obtained from an ftp site which has a link on Stewart's home page: *http://www.cs.umd.edu/∼stewart*.

6. MATCOM is available from *http://www.siam.org/books/ot116*.

A.14 Test Matrices

There are several collections of test matrices available which can be used to test algorithms for matrix computations. They include the following:

- Higham's Gallery, available from MATLAB.
- Matrix Market: *http://math.nist.gov/matrixmarket*
  (contains mostly large and sparse matrices arising in various applications).
- Harwell-Boeing package (see Duff et al. (1989) and (1992)).
- University of Florida Sparse Matrix Collection by T. Davis:
  http://www.cise. ufl.edu/research/sparse/matrices.