# LAPACK Users' Guide

Second Edition

Many science and engineering applications require the solution of numerical linear algebra problems, for which well-developed and sophisticated algorithmic and software tools are now widely available. Most algorithms for solving such problems have been implemented in the Fortran language. Advantage was taken of the existing (public-domain) numerical linear algebra subroutine libraries: BLAS—Basic Linear Algebra Subprograms; LINPACK—for solving linear algebraic equations and least squares problems; and EISPACK—for solving algebraic eigenproblems. These collections have proven to perform efficient computations on conventional and vector computer architectures; but on modern high-performant computers often do they obtain only a small fraction of the peak performance.

The newly developed library LAPACK—Linear Algebra PACKage—(the first public release, version 1.0, February, 1992, and the second release, version 2.0, September, 1994), has been specially designed to supersede LINPACK and EISPACK, by achieving much greater efficiency on vector computers, high-performance "super-scalar" workstations and shared memory multiprocessors. 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. Versions for other modern computer architectures and programming languages (C and C++) are, or will soon be available.

LAPACK is more than a successor to LINPACK and EISPACK; it extends the functional capabilities of these packages by including equili-
bration, iterative refinement, error bounds, and driver routines for linear systems, routines for computing and re-ordering the Schur factorization, and condition estimation routines for eigenvalue problems. LAPACK also uses some improved or new algorithms; for instance, it includes highly accurate algorithms for finding singular values and eigenvalues of bidiagonal and tridiagonal matrices, respectively, that occur in singular value decomposition (SVD) and symmetric eigenvalue problems.

The LAPACK approach to combining efficiency with portability (on a wide range of machines) is to use the BLAS as a low-level interface to different computer architectures. The computation is performed as much as possible by calls to the BLAS. Beside the original *Level 1* BLAS, performing vector operations, *Level 2* BLAS—for matrix-vector operations, and *Level 3* BLAS—for matrix-matrix operations, are highly used. Level 2 BLAS, and especially Level 3 BLAS are in fact responsible for the efficient use of parallelism. Powerful machine-specific implementations of the BLAS are available for many modern high-performant computers.

The underlying philosophy of LAPACK as well as a detailed description of its usage are exposed in the *LAPACK Users' Guide*, published by the Society for Industrial and Applied Mathematics (SIAM). Specifically, this 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 driver and computational routines. The auxiliary routines are not covered, but detailed information about

their use is included in the comments on the corresponding codes.

The most important new routines and functions of Release 2.0 of LAPACK, documented in the reviewed book, are:

- the generalized nonsymmetric eigenproblem $Ax = \lambda Bx$;
- the generalized banded symmetric definite eigenproblem $Ax = \lambda Bx$;
- two generalized linear least squares problems (least squares with linear constraints, and the Gauss-Markov linear model problem);
- the generalized (quotient) singular value decomposition;
- faster routines for symmetric eigenproblems, based on divide-and-conquer techniques;
- a faster bidiagonal SVD (for singular values only);
- the reduction of a band matrix to bidiagonal form;
- improved linear system drivers, to better re-use existing factorizations, and return the reciprocal of the pivot growth factor;
- the least squares drivers return the residual root-sum-squares.

The second edition of the LAPACK Users' Guide reflects the above completions and improvements, by including a discussion of new or updated routines. Chapter 3 (Performance of LAPACK) has been updated with performance results for version 2.0, and extended to include an "LAPACK Benchmark" for selected driver routines. Chapter 4 (Accuracy and Stability) has been simplified and re-written. Of special interest there are the Fortran code segments illustrating the calculation of error bounds. Appendices A, B, and D have been expanded to cover the new routines. Appendix E lists over 40 added Working Notes, written during the LAPACK 2 and ScaLAPACK (or Scalable LAPACK) projects; these Notes are of special importance for those interested in various theoretical, algorithmic, and programming details related to these projects. Bibliography and Index have been placed to the end of the book. Over thirty new references have been included. The Index has been expanded to two indices: Index by Keyword and Index by Routine Name. The Index by Keywords has been extended as

to have two hierarchy levels. Occurrences of LAPACK, LINPACK, and EISPACK routine names have been cited in the Index by Routine Name.

The same as the first edition of the LAPACK Users' Guide, the second edition is remarkable in its material organization and support both expert and casual user. The LAPACK package itself has several levels of routines: driver routines, computational routines, and auxiliary routines. The Guide exposes the most general and frequently required information in the first sections of each chapter; more detailed and possibly seldom used information comes in the following sections. Many hints are provided to the reader for choosing the right routine for each particular problem and level of expertise. There are forty tables, presenting various routines or performance results for certain widely used computer platforms. Many included code segments extend the LAPACK functionality by some important calculations, as for instance evaluating approximate error bounds for the results computed by a specific solver. Topics of current research interest are mentioned whenever possible, and references to additional public-domain material are made.

Its unique features, partly mentioned above, make the second edition of *LAPACK Users' Guide* an extremely valuable reference book to anyone whose work involves numerical linear algebra. Excerpts from this Guide are available in Postscript or uncompressed Postscript form via SIAM's Gopher server by accessing `gopher.siam.org` or through the World Wide Web at `http://www.siam.org`.

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