国际著名数学图书——影印版

LAPACK95 Users' Guide

LAPACK95用户指南

V. A. Barker, L. S. Blackford
J. Dongarra, J. Du Croz
S. Hammarling, M. Marinova
J. Waśniewski, and P. Yalamov
著

TSINGHUA UNIVERSITY PRESS
siam

LAPACK95 Users' Guide

LAPACK95用户指南

V. A. Barker, L. S. Blackford
J. Dongarra, J. Du Croz
S. Hammarling, M. Marinova
J. Waśniewski, and P. Yalamov

TSINGHUA UNIVERSITY PRESS
北京
siam

V. A. Barker, L. S. Blackford, J. Dongarra, J. Du Croz, S. Hammarling, M. Marinova, J. Waśniewski, and P. Yalamov
LAPACK95 Users' Guide
ISBN: 0-89871-504-0

图书在版编目(CIP)数据

LAPACK95用户指南 = LAPACK95 Users' Guide：英文/(美)巴克(Barker, V.A.)等著.-- 影印本. -- 北京：清华大学出版社，2011.2
(国际著名数学图书)
ISBN 978-7-302-24503-2

Ⅰ.①L…　Ⅱ.①巴…　Ⅲ.①线性代数-计算机辅助计算-应用软件-英文　Ⅳ.①O151.2-39

中国版本图书馆CIP数据核字(2011)第006645号

责任编辑：陈朝晖
责任印制：王秀菊
出版发行：清华大学出版社　　**地　址**：北京清华大学学研大厦A座
http://www.tup.com.cn　　**邮　编**：100084
社 总 机：010-62770175　　**邮　购**：010-62786544
投稿与读者服务：010-62776969,c-service@tup.tsinghua.edu.cn
质 量 反 馈：010-62772015,zhiliang@tup.tsinghua.edu.cn
印 装 者：北京鑫海金澳胶印有限公司
经　销：全国新华书店
开　本：175×245　**印　张**：17.5
版　次：2011年2月第1版　　**印　次**：2011年2月第1次印刷
印　数：1～3000
定　价：38.00元

产品编号：027802-01

Preface

Fortran has always been a principal language in the fields of scientific, numerical, and engineering computing. A series of revisions to the standard defining successive versions of the language has progressively enhanced its power and kept it competitive with several generations of rivals. The present Fortran standard is Fortran 95. The new features contained in Fortran 95 ensure that the Fortran language will continue to be used successfully for a long time to come. The fact that it contains the whole of Fortran 77 as a subset means that conversion to Fortran 95 is as simple as conversion to another Fortran 77 compiler. For more information on Fortran 95, see [31].

The development of LAPACK was a natural step after specifications of the Level 2 and 3 BLAS were drawn up in 1984–86 and 1987–88. Research on block algorithms had been ongoing for several years, but agreement on the BLAS made it possible to construct a new software package, to take the place of LINPACK and EISPACK, which would achieve much greater efficiency on modern high-performance computers. The new package, LAPACK, written in Fortran 77, also contained a number of algorithmic advances that had been made since LINPACK and EISPACK were written in the 1970's. The proposal for LAPACK was submitted while the Level 3 BLAS were still being developed, and funding was obtained from the National Science Foundation (NSF) beginning in 1987. Since its completion, four follow-up projects, LAPACK 2, ScaLAPACK, ScaLAPACK 2 and LAPACK 3 have been funded in the U.S. by the NSF and ARPA in 1990–1994, 1991–1995, 1995–1998, and 1998–2001, respectively.

This book describes LAPACK95 [12, 6, 14], yet another step in the development of LAPACK. LAPACK95 is a Fortran 95 interface to the Fortran 77 LAPACK library. It is relevant for anyone who writes in the Fortran 95 language and needs reliable software for basic numerical linear algebra. It may be regarded as a sequel to [1], the official reference for LAPACK, and as such, it assumes a basic knowledge of LAPACK and frequently refers to the LAPACK Users' Guide [1] for specific details. This book is divided into three parts. *Part I: GENERAL INFORMATION* contains chapters providing a thorough explanation of the design and functionality of the LAPACK95 library. *Part II: DRIVER ROUTINES* contains detailed specifications of the driver routines, including numerical examples. *Part III: COMPUTATIONAL ROUTINES* contains brief specifications of the computational routines. A *Bibliography* is also provided, as well as two indexes– *Index by Keyword* and *Index by Routine Name.*

A number of technical reports were written during the development of LAPACK95 and published as technical reports at UNI•C, Denmark, and as LAPACK Working Notes by the University of Tennessee. These reports are available in postscript and pdf format.

`http://www.netlib.org/lapack/lawns/`

The performance results presented in this book were obtained using computer resources at the Danish Computing Center for Research and Education, UNI•C.

This work was supported by the Danish Natural Science Research Council through a grant for the EPOS project (Efficient Parallel Algorithms for Optimization and Simulation) and by the Oak Ridge National Laboratory, managed by UT/Battelle, LLC for the U.S. Department of Energy, under contract number DE-AC05-96OR22464.

The cover was designed by David Rogers at the Innovative Computing Laboratory, Department of Computer Science, University of Tennessee.

Finally, we would like to thank all those who have contributed code, criticism, ideas and encouragement. We wish especially to express our gratitude to the LAPACK authors, Bjarne Stig Andersen, Zohair Maany, Antoine Petitet, John Reid, Clint Whaley, and Adam Zemła. The base-files for the LAPACK95 library are kept in the *extract* system developed by Clint Whaley.

The royalties from the sales of this book are being placed in a fund to help students attend SIAM meetings and other SIAM related activities. This fund is administered by SIAM and qualified individuals are encouraged to write directly to SIAM for guidelines.

Contents

List of Tables

List of Figures

Part I

GENERAL INFORMATION

Chapter 1

Essentials

1.1 LAPACK95

LAPACK95 [6, 14] is a Fortran 95 [31] interface to the Fortran 77 LAPACK library [1]. It improves upon the original user-interface to the LAPACK package, taking advantage of the considerable simplifications which Fortran 95 allows. The design of LAPACK95 exploits assumed-shape arrays, optional arguments, and generic interfaces. The Fortran 95 interface has been implemented by writing Fortran 95 "wrappers" to call existing routines from the LAPACK package. This interface can persist unchanged even if the underlying Fortran 77 LAPACK code is rewritten to take advantage of the new features of Fortran 95.

The LAPACK95 home page, which is maintained at *netlib* [18], is

```
http://www.netlib.org/lapack95/
```

A list of LAPACK95 Frequently Asked Questions (FAQ) can be found at

```
http://www.netlib.org/lapack95/faq.html
```

1.2 Problems that LAPACK95 can Solve

LAPACK95 provides interfaces to all LAPACK driver and computational routines. Driver routines are for the major tasks of solving systems of linear equations, linear least squares problems, eigenvalue problems and singular value problems. For details see Chapter 2 and Part II. Computational routines are for smaller computational tasks; each driver typically calls a sequence of computational routines. The computational routines are documented briefly in Part III.

As with LAPACK, dense and band matrices are provided for but not general sparse matrices. In all areas, similar functionality is provided for real and complex matrices and single and double precision.

1.3 Computers for which LAPACK95 is Suitable

Since LAPACK95 is an interface to LAPACK, its efficiency is closely related to that of LAPACK. LAPACK is designed to give high efficiency on vector processors, high-performance "super-scalar" workstations, and shared memory multiprocessors. It can also be used satisfactorily on all types of scalar machines (PC's, workstations, mainframes). Section 4.1.2 gives some examples of the performance achieved by LAPACK with the LAPACK95 interface routines.

1.4 LAPACK and the BLAS

LAPACK routines are written so that as much as possible of the computation is performed by calls to the Basic Linear Algebra Subprograms (BLAS) [30, 16, 15] . Highly efficient machine-specific implementations of the BLAS are available for many modern high-performance computers. Alternatively, machine-specific implementations can be generated using the ATLAS system mentioned in Section 1.5.3 below. The BLAS enable LAPACK routines to achieve high performance with portable code. The methodology for constructing LAPACK routines in terms of calls to the BLAS is described in Chapter 3 of the LAPACK Users' Guide [1].

1.5 Availability and Installation of Software

1.5.1 LAPACK95

The LAPACK95 software can be downloaded from the LAPACK95 home page

```
http://www.netlib.org/lapack95/lapack95.tgz
```

and is also available via ftp as follows:

```
anon ftp to www.netlib.org
cd lapack95
binary
get lapack95.tgz
```

This distribution tar file does *NOT* contain an LAPACK library or a BLAS library. *Note that LAPACK, version 3.0 or later, is required for the installation of LAPACK95.* LAPACK95 assumes that an LAPACK library and a BLAS library are installed on the machine to which the user is installing LAPACK95. If either of these libraries is not already installed, refer to the downloading and installation instructions in sections 1.5.2 and 1.5.3, respectively.

After downloading the software, the user enters the following command to extract the files:

```
gunzip -c lapack95.tgz | tar xvf -
```