The Future of LAPACK and ScaLAPACK

Jason Riedy, Yozo Hida, James Demmel

EECS Department
University of California, Berkeley

November 18, 2005
Outline

Survey responses: What users want

Improving LAPACK and ScaLAPACK
  Improved Numerics
  Improved Performance
  Improved Functionality
  Improved Engineering and Community

Two Example Improvements
  Numerics: Iterative Refinement for $Ax = b$
  Performance: The MRRR Algorithm for $Ax = \lambda x$
Survey: What users want

- Survey available from
  http://www.netlib.org/lapack-dev/.
- 212 responses, over 100 different, non-anonymous groups
- Problem sizes:
  100  1K  10K  100K  1M  (other)
  8%  26%  24%  12%  6%  (24%)
- >80% interested in small-medium SMPs
- >40% interested in large distributed-memory systems
- Vendor libs seen as faster, buggier
- over 20% want > double precision, 70% out-of-core
- Requests: High-level interfaces, low-level interfaces, parallel redistribution* and tuning
Participants

- UC Berkeley
  - Jim Demmel, Ming Gu, W. Kahan, Beresford Parlett, Xiaoye Li, Osni Marques, Christof Vömel, David Bindel, Yozo Hida, Jason Riedy, Jianlin Xia, Jiang Zhu, undergrads, ...
- U Tennessee, Knoxville
  - Jack Dongarra, Julien Langou, Julie Langou, Piotr Luszczek, Stan Tomov, ...
- Other Academic Institutions
  - UT Austin, UC Davis, U Kansas, U Maryland, North Carolina SU, San Jose SU, UC Santa Barbara, TU Berlin, FU Hagen, U Madrid, U Manchester, U Umeå, U Wuppertal, U Zagreb
- Research Institutions
  - CERFACS, LBL, UEC (Japan)
- Industrial Partners
  - Cray, HP, Intel, MathWorks, NAG, SGI

You?
Improved Numerics

Improved accuracy with standard asymptotic speed: Some are faster!

▶ Iterative refinement for linear systems, least squares
  Demmel / Hida / Kahan / Li / Mukherjee / Riedy / Sarkisyan
▶ Pivoting and scaling for symmetric systems
  ▶ Definite and indefinite
▶ Jacobi SVD (and faster) — Drmač / Veselić
▶ Condition numbers and estimators
  Higham / Cheng / Tisseur
▶ Useful approximate error estimates
Improved Performance

Improved performance with at least standard accuracy

- MRRR algorithm for eigenvalues, SVD
  Parlett / Dhillon / Vömel / Marques / Willems / Katagiri
- Fast Hessenberg QR & QZ
  Byers / Mathias / Braman, Kågström / Kressner
- Fast reductions and BLAS2.5
  van de Geijn, Bischof / Lang, Howell / Fulton
- Recursive data layouts
  Gustavson / Kågström / Elmroth / Jonsson
- generalized SVD — Bai, Wang
- Polynomial roots from semi-separable form
  Gu / Chandrasekaran / Zhu / Xia / Bindel / Garmire / Demmel
- Automated tuning, optimizations in ScaLAPACK, . . .
Improved Functionality

Algorithms

- Updating / downdating factorizations — Stewart, Langou
- More generalized SVDs: products, CSD — Bai, Wang
- More generalized Sylvester, Lyupanov solvers
  Kågström, Jonsson, Granat
- Quadratic eigenproblems — Mehrmann
- Matrix functions — Higham

Implementations

- Add “missing” features to ScaLAPACK
- Generate LAPACK, ScaLAPACK for higher precisions
Improved Engineering and Community

Use new features without a rewrite

- Use modern Fortran 95, maybe 2003
  - DO ... END DO, recursion, allocation (in wrappers)
- Provide higher-level wrappers for common languages
  - F95, C, C++
- Automatic generation of precisions, bindings
  - Full automation (FLAME, etc.) not quite ready for all functions
- Tests for algorithms, implementations, installations

Open development

Need a community for long-term evolution.
http://www.netlib.org/lapack-dev/
Lots of work to do, research and development.
Two Example Improvements

Recent, locally developed improvements

Improved Numerics
Iterative refinement for linear systems $Ax = b$:

- Extra precision $\Rightarrow$ small error, dependable estimate
- Both normwise and componentwise
- (See LAWN 165 for full details.)

Improved Performance
MRRR algorithm for eigenvalue, SVD problems

- Optimal complexity: $O(n)$ per value/vector
- (See LAWNs 162, 163, 166, 167... for more details.)
**Numerics: Iterative Refinement**

Improve solution to \( Ax = b \)

Repeat: \( r = b - Ax, \ dx = A^{-1}r, \ x = x + dx \)

Until: good enough

Not-too-ill-conditioned \( \Rightarrow \) error \( O(\sqrt{n} \varepsilon) \)
Numerics: Iterative Refinement

Improve solution to $A x = b$

Repeat: $r = b - A x$, $d x = A^{-1} r$, $x = x + d x$

Until: good enough

Dependable normwise relative error estimate
Numerics: Iterative Refinement

Improve solution to $Ax = b$

Repeat: $r = b - Ax$, $dx = A^{-1}r$, $x = x + dx$

Until: good enough

Also small componentwise errors and dependable estimates
Relying on Condition Numbers

Need condition numbers for dependable estimates.
Picking the right condition number and estimating it well.
Performance: The MRRR Algorithm

Multiple Relatively Robust Representations

- 1999 Householder Award honorable mention for Dhillon
- Optimal complexity with small error!
  - $O(nk)$ flops for $k$ eigenvalues/vectors of $n \times n$ tridiagonal matrix
  - Small residuals: $\|Tx_i - \lambda_i x_i\| = O(n\varepsilon)$
  - Orthogonal eigenvectors: $\|x_i^T x_j\| = O(n\varepsilon)$
- Similar algorithm for SVD.
- Eigenvectors computed independently $\Rightarrow$ naturally parallelizable
- (LAPACK r3 had bugs, missing cases)
Performance: The MRRR Algorithm

"fast DC": Wilkinson, deflate like crazy
Summary

- LAPACK and ScaLAPACK are open for improvement!
- Planned improvements in
  - numerics,
  - performance,
  - functionality, and
  - engineering.
- Forming a community for long-term development.