LAPACK ScaLAPACK

LAPACK is an open-source subroutine library for solving the most common problems in dense numerical linear algebra. It is designed to run efficiently on modern processors (including shared memory machines) by making extensive use of Level-3 BLAS. ScaLAPACK provides the same functionalities as LAPACK but for distributed memory parallel systems.

The goals of the **Sca/LAPACK** projects are to provide efficiency, portability, scalability, flexibility, reliability, ease of maintenance and ease of use software for computational science problems.

FUNCTIONALITIES

Sca/LAPACK provides routines for solving:

• Linear Equations (SV) for nonsymmetric, symmetric, symmetric positive definite matrices using respectively LU, LDL^T, Cholesky factorizations.

• Linear Least Squares (LLS)

• Generalized Linear Least Squares (LSE and GLM)

• Standard Eigenvalue and Singular Value Problems
  • Symmetric Eigenproblems (SEP)
  • Nonsymmetric Eigenproblems (NEP)
  • Singular Value Decomposition (SVD)

• Generalized Eigenvalue and Singular Value Problems
  • Generalized Symmetric Definite Eigenproblems (GSEP)
  • Generalized Nonsymmetric Eigenproblems (GNEP)
  • Generalized Singular Value Decomposition (GSVD)

Input matrix layout can be dense, banded, tridiagonal, bidiagonal or packed (for symmetric or triangular matrices).

For each driver, an expert version is provided, and subroutines are defined in four ways: real (s), complex (c), double precision (d), double complex (z).

DISTRIBUTION

The Sca/LAPACK source code are distributed through http://www.netlib.org/ and are publicly available. The libraries are regularly tested on numerous machines using multiple compilers.

The Sca/LAPACK APIs have been adopted by many vendors and the Sca/LAPACK public version provides a reference implementation of state of the art algorithms for a wide set of problems. LAPACK has been incorporated into the following commercial packages (often with some shared memory LAPACK implementations and the parallel distributed version of ScaLAPACK):AMD, Apple, Compaq, Cray, Fujitsu, Hewlett-Packard, Hitachi, IBM, Intel, MathWorks, NAG, NEC, PGI, SUN, Visual Numeric). It is also distributed in most Linux distributions (eg., Fedora, Debian,Cygwin, etc.).

ARCHITECTURE DESIGN

LAPACK makes extensive use of BLAS calls. This enables LAPACK to maintain its efficiency when ported from one platform to another.

ScaLAPACK software is multi-layered, enabling it to be portable and efficient. Matrices are in the 2D-block cyclic format, an important parameter for scalability and efficiency.
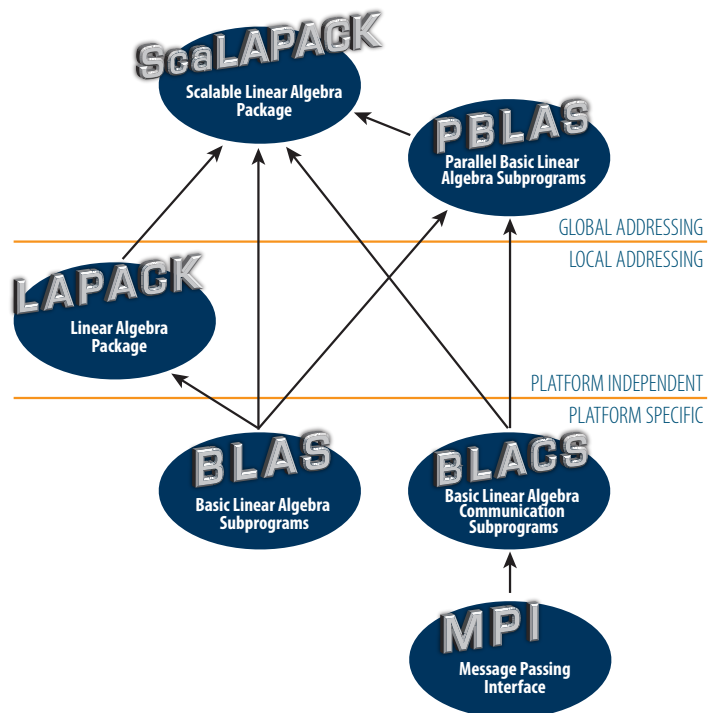

USERS

Sca/LAPACK is used on all DOE/DOD machines and by many others to provide efficient, easy to use and reliable numerical dense linear algebra methods. Many users do not even know that they are using Sca/LAPACK. For example, MUMPS, PETSc, MATLAB*P are using ScaLAPACK, while Matlab and Numeric Python are using LAPACK.

Sca/LAPACK is used for a number of applications of science and engineering in areas such as quantum chemistry and physics, electromechanics, geophysics and seismology, plasma physics, nonlinear mechanics, chemically reactive flows, helicopter flight control, atomic structure calculation, cardiomagnetism, radar cross-sections, and two-dimensional elastodynamics.

The package is used on matrices ranging from size 2 to 30,000 for LAPACK, and ScaLAPACK is now succesfully used on thousands of processors.

LAPACK   ScaLAPACK

One of the main strengths of Sca/LAPACK is the wide spread support and recognition from the international dense linear algebra community. Researchers, vendors, and individuals all over the world are regularly contributing to the Sca/LAPACK software library. The University of Tennessee (ICL) and the University of California Berkeley are responsible for the development, integration and verification of those contributions.

ON-GOING WORK

Current activity consists of including new algorithms and new functionalities in Sca/LAPACK while maintaining the library.

Below is a list of new algorithms that are being added in LAPACK:

Extended precision arithmetic (more accurate)

Recursive data structures (faster)

Ashcraft, Grimes and Lewis symmetric indefinite systems (more accurate)

Cholesky factorization with diagonal pivoting (more accurate)

Hessenberg QR-algorithm for the nonsymmetric GEEV (faster)

Multiple Relatively Robust Representations for SYEV (faster)

MRRR algorithm applied to the SVD (faster)

Reduction to bidiagonal form for the SVD using Level 2.5 BLAS (faster)

One-sided Jacobi algorithm for computing singular values with high relative accuracy (more accurate) (faster)

Successive Band Reduction (SBR) algorithm (faster)

High accuracy algorithms for the symmetric indefinite EVD (more accurate)

Updating matrix factorizations like Cholesky, LDL^T, LU, QR and SVD (new functionality)

Semi-separable matrices (new functionality)

Eigenvalue problems for matrix polynomials (new functionality)

Matrix functions (square root, exponential, sign function) (new functionality)

Eigenvalue and singular value decompositions of products and quotients of matrices (new functionality)

Out-of-core versions of matrix factorizations (new functionality)

DID YOU KNOW?

- LINPACK (ancestor of LAPACK) was one of the first libraries made publicly available.

- In 1979, the LINPACK benchmark was initially written for timing references. It has subsequently become the popular benchmark that is now used to rank the TOP500 computer list. A highly efficient implementation of the bench-mark is HPL from UTK, which is a tuned version of PDGESV from ScaALAPACK.

- Straightforward parallel progamming interfaces to ScaLAPACK are now available (eg., LFC from ICL at UTK). These enable scientists to easily use parallel distributed machines.

- LAPACK can solve the symmetric eigenvalue problem in five different ways. One can either use QR (STEQR), QR only eigenvalues (STERF), Bisection and Inverse Iteration (STEBZ+STEIN), Divide and Conquer (STEDC), or MRRR (STEGR). Each of these methods has its own importance and the LAPACK drivers are able to pick the appropriate one according to the user problem.

- LAPACK is written in F77 but a C version is also available: CLAPACK (via Netlib).

- LAPACK can run up to 100 times slower if it is not calling an optimized BLAS library.

- Matlab uses its own LAPACK library behind the scene. The performance of your Matlab is thus closely related to the performance of LAPACK

- The BLACS standard interface and the BLACS library were written before the MPI standard and before any MPI library ever existed.

- The BLAS/LAPACK/BLACS/ScaLAPACK test and timing suites provide a convenient and exhaustive way of testing and timing a third party library.

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