# Parallel Libraries

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## Parallel Libraries

Public Domain

commercial

vendor specific

## Overview

- numerical libraries for linear systems
  - dense
  - sparse
- FFT
- support for parallelization



## netlib server

for all

public domain numerical programs and libraries

http://www.netlib.org

## LAPACK for linear systems

- for dense problems, fast
- Linear Equations, real and complex
  - Orthogonal Factorizations and Linear Least Squares Problems
  - Generalized Orthogonal Factorizations and Linear Least Squares Problems
- Eigenproblems
- Symmetric and nonsymmetric real eigenproblems
  - hermitian and nonhermitian complex
  - Generalized Symmetric Definite Eigenproblems
  - Generalized Nonsymmetric Eigenproblems
- Singular Value Decomposition
- Generalized (or Quotient) Singular Value Decomposition
- based on BLAS
- shared memory parallel versions



## Basic Linear Algebra Subroutines: BLAS

•BLAS-1

| | |
|---|---|
| vector x vector | saxpy |
| data transfer | 3*n |
| operations | 2*n-1 |
| FLOP/Word | 2/3 |

•BLAS-2

| | |
|---|---|
| matrix x vector | |
| data transfer | n*n+2*n |
| operations | n*(2*n-1) |
| FLOP/Word | 2 |

•BLAS-3

| | |
|---|---|
| matrix x matrix | |
| data transfer | 3*n*n |
| operations | n*n*(2*n-1) |
| FLOP/Word | 2/3*n |

## where to get BLAS

- as source code from netlib
- for PC/Windows  free Intel® Math Kernel Library
  http://developer.intel.com/software/products/mkl/index.htm
- vendor tuned versions on all platforms, also parallel



## ScaLAPACK

- Scalable Linear Algebra PACKage, or Scalable LAPACK
- handles dense and band matrices on distributed memory machines
- not general sparse matrices
- functionality is subset of LAPACK
- based on BLAS and BLACS
- http://www.netlib.org/scalapack/

## ScaLAPACK contents

- Linear Equations
  - Orthogonal Factorizations and Linear Least Squares Problems
    - **QR Factorization**
    - **LQ Factorization**
    - **QR Factorization with Column Pivoting**
    - **Complete Orthogonal Factorization**
    - **Other Factorizations**
  - Generalized Orthogonal Factorizations
    - **Generalized QR Factorization**
    - **Generalized RQ factorization**
- Symmetric and nonsymmetric Eigenproblems
  - Eigenvalues, Eigenvectors, and Schur Factorization
- Singular Value Decomposition
- Generalized Symmetric Definite Eigenproblems



## NAG Parallel Library, commercial

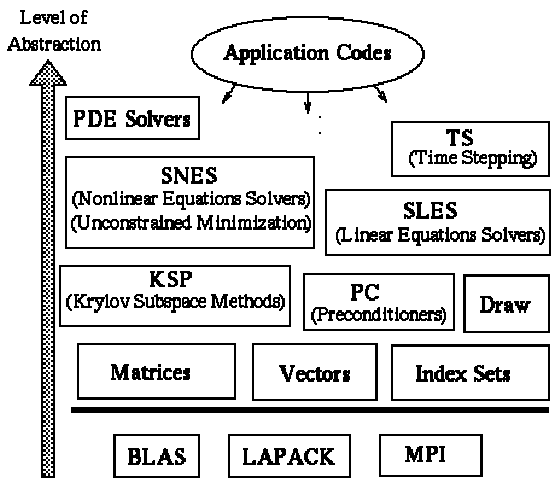
- distributed memory machine (MPI, PVM)
- http://www.nag.co.uk/numeric/fd/FDdescription.asp
- Dense linear algebra (including ScaLapack)
- Eigenvalue and singular value problems
- Input/Output, data distribution
- Optimisation
- Quadrature
- Random number generators
- Sparse linear algebra
- Sparse matrix solvers
- Support/utility routines
- contents in
  http://www.nag.co.uk/numeric/FD/manual/html/genint/FDlibconts.asp

## NAG SMP Library, commercial

- Zeros of Polynomials, Roots ofTranscendental Equations
- Quadrature, Numerical Differentiation, Interpolation, Approximation
- Ordinary Differential Equations,Partial Differential Equations
- Integral Equations
- Curve and Surface Fitting
- Minimizing or Maximizing a Function
- Matrix Factorizations
- Eigenvalues and Eigenvectors
- Orthogonalisation
- Linear Equations (LAPACK)
- Least-squares and Eigenvalue Problems (LAPACK)
- Sparse Linear Algebra
- Statistics
- Random Number Generators, sorting
- Time Series Analysis
- Operations Research



## PETSc Features (http://www-fp.mcs.anl.gov/petsc)



## PETSc components

- Vec vector operations, scatter, gather, ghostpoints for regular structures
- Mat data structures for parallel sparse matrices
- PC preconditioners (ILU(k), LU, block Jakobi, additive Schwarz)
- KSP Krylov subspace iterative methods (GMRES, CG, CGS, Bi-CG-Stab, TFQMR, CR, LSQR)
- SNES Newton-like methods for nonlinear systems
- TS (pseudo-) time evolution codes for solution of PDEs



## ParPre

- preconditioners for large sparse iterative solvers
- uses PETSc
- additive Schwarz
- multiplicative Schwarz
- block SSOR
- domain decomposition methods
- multilevel
- http://www.cs.utk.edu/~eijkhout/parpre.html

## PARPACK

- http://www.caam.rice.edu/software/ARPACK/
- http://www.caam.rice.edu/~kristyn/parpack_home.html
  Parallel version of ARPACK
- calculates a few eigenvalues of a large sparse matrix
- Implicitly Restarted Lanczos Method (IRLM)
- symmetric, nonsymmetric, and generalized eigenproblems
- Singular Value Decomposition.



## European Parasol project (Mumps)

- http://www.enseeiht.fr/lima/apo/mumps/European ESPRIT Activity MUMPS (MUltifrontal Massively Parallel sparse direct Solver )
- public domain
- symmetric positive definite matrices;
- general symmetric matrices;
- general unsymmetric matrices;
- Iterative refinement and backward error analysis;
- Input matrix in
  assembled format
  distributed assembled format
  elemental format

## Aztec

- iterative library for solution of large distributed sparse linear systems
- CG, GMRES, BiCGSTAB
- for systems arizing from discretization of partial differential equations
- Jakobi, polynomial, LU, ILU etc. preconditioning in processor domains
- distributed modified sparse row format (DMSR)
- distributed variable block row format (DVBR)
- matrix free interface, user defined preconditioning interface
- unknown numbering may be global
- free for research; license necessary
- http://www.cs.sandia.gov/CRF/aztec1.html



## MFACT

- multifrontal direct solver
- sparse symmetric positive definite linear systems
- Lapack style interface
- similar to CAPSS
- free
- http://www.cs.utk.edu/~padma/mfact.html

## SuperLU

- solves large sparse nonsymmetric systems
- direct solver
- SuperLU seriel
- SuperLU_MT shared memory parallel
- SuperLU_DIST distributed memory
- free
- http://www.nersc.gov/~xiaoye/SuperLU/



## FFTW

- Discrete Fourier Transform
- one and more dimension
- C, wrapper routines for Fortran
- free GPL
- http://www.fftw.org/

## ParMETIS

- graph partitioning
- mesh partitioning
- graph repartitioning
- graph partition refinement
- matrix reordering



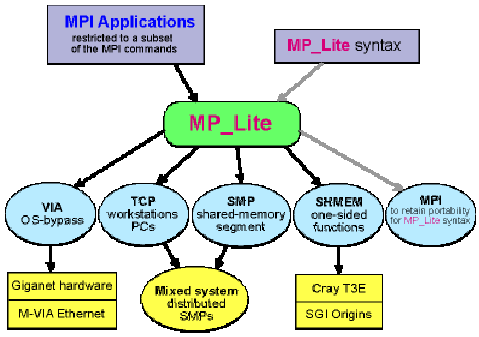
## global arrays

- shared memory programming interface for distributed memory machines
- asynchronously access of logical blocks of physically distributed dense multi-dimensional arrays
- cooperating with shared memory paradigm and MPI
- create a distributed array, controlling alignment and distribution; duplicate an array with properties of another existing array; destroy an array; synchronize.
- fetch, store and accumulate into a rectangular patch of global array; gather and scatter; atomic read and increment
  efficient access to local elements of global array (by a pointer).

- free
- http://www.emsl.pnl.gov:2080/docs/global/ga.html

## MP_Lite

- lightweight message-passing library
- http://www.scl.ameslab.gov/Projects/MP_Lite/



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