Numerical and Parallel Libraries

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Numerical Libraries

Public Domain

commercial

vendor specific

Overview

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

Public Domain

Lapack-3	linear equations, eigenproblems
BLAS	fast linear kernels
Linpack	linear equations
Eispack	eigenproblems
Slatec	old library, large functionality
Quadpack	numerical quadrature
Itpack	sparse problems
pim	linear systems
PETSc	linear systems
Netlib Server	best server

http://www.netlib.org/utk/papers/iterative-survey/packages.html

netlib server

for all

public domain numerical programs and libraries

http://www.netlib.org

Contents of netlib

access aicm alliant amos ampl anl-reports apollo atlas
benchmark bib bibnet bihar blacs blas blast bmp
c c++ cephes chammp cheney-kincaid clapack commercial confdb
conformal contin control crc cumulvs ddsv dierckx diffpack
domino eispack elefunt env f2c fdlibm fftpack fishpack
fitpack floppy fmm fn fortran fortran-m fp gcv
gmat gnu go graphics harwell hence hompack hpf
hypercube ieeecss ijsa image intercom itpack jakef java
kincaid-cheney la-net lanczos lanz lapack lapack++ lapack90 laso
lawson-hanson linalg linpack list lp machines magic maspar
mds microscope minpack misc mpfun mpi mpicl na-digest-html
napack netsolve news numeralgo ode odepack odrpack opt
p4 paragraph paranoia parkbench parmacs pascal pdes performance
photo picl pltmg poly2 polyhedra popi port posix
pppack presto problem-set pvm3 quadpack random research scalapack
sched scilib seispack sequent sfmm slap slatec sminpack
sodepack sparse sparse-blas sparspak specfun spin srwn stoeplitz
stringsearch svdpack templates tennessee textbook toeplitz toms tomspdf
transform typesetting uncon vanhuffel vfftpack vfnlib voronoi xmagic
xnetlib y12m

VSIPL

Vector/Signal/Image Processing Library

http://www.vsipl.org/
C,C++
FFT, histogram, density, median,convolution,
gradient edge detection,morphological operators,
expand, shrink, padding
matrix product, -transpose, -LU, -Cholesky, QR,
toeplitz solver, least squares,
vector operations

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

tuned versions on all platforms

getting BLAS by ATLAS:

generates tuned versions of e.g. BLAS code

Automated Emprical Optimization of Software (AEOS)

http://www.netlib.org/atlas/

available for LAPACK Fortran and C: (◊: S,D,C,Z)

- ◊GESV (lin. equ.)
- ◊GETRF (lin. equ. LU)
- ◊GETRS (lin. equ. solve)
- ◊POSV (sym. pos. lin. equ.)
- ◊POTRF (sym. pos. lin. equ. LU)
- ◊POTRS (sym. pos. lin. equ. solve)

ScaLAPACK http://www.netlib.org/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

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 Eigenproblems
Nonsymmetric Eigenproblems
- Eigenvalues, Eigenvectors, and Schur Factorization

Singular Value Decomposition
Generalized Symmetric Definite Eigenproblems

Commercial Libraries

- IMSL
  - Fortran 77 Library
- NAG
  - Fortran 77 Library
  - F90 Library
  - Parallel Library
  - SMP Library

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

Vendor specific Libraries

CRAY SciLib

IBM ESSL

Hitachi MSL

NEC ASL

NEC MPACK

NEC Mathkeisan

NEC MathKeisan (ASL) contents 1

- linear equations, eigenvalues and eigenvectors

  direct, iterative, parallel

  sparse, banded and dense

  multiple right hand sides

  real and complex

  (non)symmetric, (non)hermitian

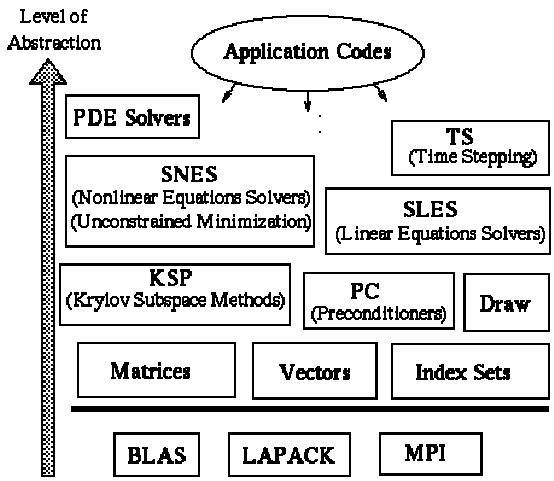
NEC MathKeisan (ASL) contents 2

Fast Fourier Transform
Wavelet Transform
Interpolation, Approximation
Integration
Roots of equations
Ordinary Differential equations
Random numbers, Sorting
Special functions
Statistics

NEC MathKeisan (MPACK) contents

BLAS	Basic Linear Algebra Subprograms
LAPACK	Linear algebra for high performance computers
ScaLAPACK	Scalable Linear Algebra package (contains PBLAS)
BLACS	Basic Linear Algebra Communication Subprograms
PARBLAS	Shared memory Parallel BLAS
ARPACK	Solution of large scale eigenvalue problems
FFT	HP's VECLIB and SGI/CRAY LIBSCI 3.1 interface
SOLVER	Direct solver for sparse SPD systems
METIS	Matrix/Graph ordering and partitioning library
ParMETIS	Parallel Matrix/Graph ordering and partition library

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

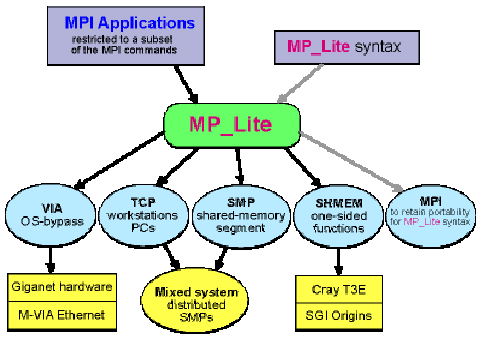
global arrays

- 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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