Numerical Libraries

Uwe Küster
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Numerical Libraries

Public Domain

commercial

vendor specific

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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

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

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)

Commercial Libraries

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

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

end

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