Numerisk programvara

Olika typer av programvara:

- Paket som Matlab, Maple, Mathematica.

- Generella rutinbibliotek, NAG, IMSL. Får tillhandahålla huvudprogram etc. och länka till en biblioteksfil.

- Bibliotek för speciella problemområden.
  Lapack (RISC-optimerat) rutiner för $Ax = b$,
  $\min_x \; ||Ax - b||_2$ och $Ax = \lambda x$.
  (Linpack äldre bibliotek för CISC.)

  BLAS, t.ex. $\sigma = x^T y$, $y = Ax$ och $C = AB$.
  Finns i NAG, IMSL men även i:

- Datorspecifika bibliotek, t.ex.

  - AMD: ACML (AMD Core Math Library)
  - Intel: MKL (Intel Math Kernel library).
  - Sun: Sunperf (Sun Performance Library).
  - SGI: complib.sgimath
    (Scientific and Mathematical Library).
  - IBM: ESSL
    (Engineering and Scientific Subroutine Library).

- Rutiner för speciella tillämpningar. Finns samlingar på www. Netlib (där man även finner Lapack),

Rutinerna är normalt skrivna i Fortran (finns Fortran66, 77, 90, 95). En mindre del i C/C++. Än mindre andel i Java etc.

Enkelt att blanda Fortran med C/C++ (om enkel lagring).

För anrop av Fortran, C/C++ från Java, se:
Java Native Interface,
`java.sun.com/docs/books/tutorial/native1.1/index.html`

NAG - The Numerical Algorithms Group Ltd

`http://www.nag.com/`

NAG offers libraries in Fortran 77, Fortran 90, C, as well as an SMP Library and a Parallel Library for shared memory and distributed memory parallel computing respectively. We have most recently added Data Mining Components to our product range.

Innehåller så där 1100 rutiner.

List of Contents, Release 4

Chapter 1: Utilities
Chapter 3: Special Functions
Chapter 4: Matrix and Vector Operations

Chapter 5: Linear Equations

Module 5.1: Solves a general real or complex system of linear equations with one or many right-hand sides

Module 5.2: Solves a real or complex, symmetric or Hermitian system of linear equations with one or many right-hand sides

Module 5.3: Solves a real or complex triangular system of linear equations

Module 5.4: Solves a general real or complex banded system of linear equations, with one or many right-hand sides

Module 5.5: Solves a real symmetric or complex Hermitian positive definite banded system of linear equations, with one or many right-hand sides

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Module 5.6: Sparse matrix preconditioner Set-up and Solve

Module 5.7: Iterative Solvers
General sparse linear system solver

Chapter 6: Eigenvalue and Least-squares Problems
Chapter 7: Transforms
Chapter 8: Curve and Surface Fitting
Chapter 9: Optimization
Chapter 10: Nonlinear Equations
Chapter 11: Quadrature
Chapter 12: Ordinary Differential Equations (ODE's)
Chapter 13: Partial Differential Equations (PDE's)
Chapter 19: Operations Research
Chapter 20: Statistical Distribution Functions
Chapter 21: Random Number Generation
Chapter 22: Basic Descriptive Statistics
Chapter 25: Correlation and Regression Analysis
Chapter 28: Multivariate Analysis

Ett annat kommersiellt paket är IMSL (The International Mathematical and Statistical Library),
`http://www.vni.com/products/imsl/index.html` .

Finns i Fortran, C men även i Java:
`http://www.vni.com/products/imsl/jmsl.html` .

Netlib

`http://www.netlib.org`

Main Index of Software Libraries
Netlib Libraries:

a	fishpack	matlab	research
access	fitpack	mds	scalapack
aicm	floppy	microscope	sched
alliant	fmm	minpack	scilib
amos	fn	misc	seispack
ampl	fortran	mpfun	sequent
anl-reports	fortran-m	mpi	sfmm
apollo	fp	na-digest-html	shpcc94
benchmark	gcv	napack	slap
bib	gmat	netsolve	slatec
bibnet	gnu	news	sminpack
bihar	go	numeralgo	sodepack
blacs	graphics	ode	sparse
blas	harwell	odepack	sparse-blas
blast	hence	odrpack	sparspak
bmp	hompack	opt	specfun
c	hpf	p4	spin
c++	hypercube	paragraph	srwn
cephes	ieeecss	paranoia	stoeplitz
chammp	ijsa	parkbench	stringsearch
cheney-kincaid	image	parmacs	svdpack
clapack	intercom	pascal	templates
commercial	itpack	pbwg	tennessee
confdb	jakef	pdes	textbook
conformal	kincaid-cheney	performance	toeplitz
contin	la-net	photo	toms
control	lanczos	picl	tomspdf
crc	lanz	pltmg	transform
cumulvs	lapack	poly2	typesetting
ddsv	lapack90	polyhedra	uncon
dierckx	laso	popi	vanhuffel
diffpack	lawson-hanson	port	vfftpack
domino	linalg	posix	vfnlib
eispack	linpack	pppack	voronoi
elefunt	list	presto	xmagic
env	lp	problem-set	xnetlib
f2c	machines	pvm3	y12m
fdlibm	magic	quadpack	
fftpack	maspar	random	

ode innehåller 51 paket (jag har inte listat alla). Jag har också
avlägsnat en del rader i de paket jag tagit med.

```
file      daspk.tgz
for       differential-algebraic system solver
by        Brown, Hindmarsh, Petzold
prec      double and single
alg       BDF methods with direct and preconditioned
          Krylov linear solvers
ref       SIAM J. Sci. Comp.: 15, 6, 1467 (1994) and 19, 5,

lib       rksuite
alg       Runge-Kutta
for       initial value problem for first order ordinary
          differential equations. A suite of codes for
          solving IVPs in ODEs. A choice of RK methods
          is available. Includes an error assessment
          facility and a sophisticated stiffness checker.
          Template programs and example results provided.
by        R.W. Brankin (NAG), I. Gladwell and L.F. Shampine
lang      Fortran
prec      double

file      colnew.f
by        Ascher and Bader
for       ordinary differential equation boundary-value
          problem solver
alg       truncated powers collocation

file      ddverk.f
by        Enright and Hayashi <hiroshi@cs.toronto.edu>
for       delay differential equations
```

```
file      parsodes.tar.gz
by        Claus.Bendtsen@uni-c.dk
for       large systems of stiff ordinary differential
          equations
alg       multiimplicit Runge-Kutta with "across the
          method" parallelization
lang      Fortran90, MPI

file      odeToJava.tgz
for       initial-value problems for stiff and non-stiff
          ordinary differential equations
alg       explicit Runge-Kutta, linearly implicit
          implicit-explicit (IMEX)
by        Murray Patterson and Raymond J. Spiteri <spiteri(
lang      Java
```

odepack

ODEPACK is a collection of Fortran solvers for the initial va-
lue problem for ordinary differential equation systems. It con-
sists of nine solvers, namely a basic solver called LSODE and
eight variants of it – LSODES, LSODA, LSODAR, LSODPK,
LSODKR, LSODI, LSOIBT, and LSODIS. The collection is su-
itable for both stiff and nonstiff systems. It includes solvers for
systems given in explicit form, $dy/dt = f(t,y)$, and also solvers
for systems given in linearly implicit form, $A(t,y) \, dy/dt = g(t,y)$.
Two of the solvers use general sparse matrix solvers for the li-
near systems that arise. Two others use iterative (preconditio-
ned Krylov) methods instead of direct methods for these linear
systems. The most recent addition is LSODIS, which solves im-
plicit problems with general sparse treatment of all matrices
involved.

1. LSODE (Livermore Solver for Ordinary Differential Equa-
tions) is the basic solver of the collection. It solves stiff and
nonstiff systems of the form $dy/dt = f$. In the stiff case, it tre-
ats the Jacobian matrix df/dy as either a dense (full) or a ban-
ded matrix, and as either user-supplied or internally approxima-
ted by difference quotients. It uses Adams methods (predictor-
corrector) in the nonstiff case, and Backward Differentiation For-
mula (BDF) methods in the stiff case. The linear systems that
arise are solved by direct methods (LU factor/solve).

2. LSODES, written jointly with A. H. Sherman, solves systems
$dy/dt = f$ and in the stiff case treats the Jacobian matrix in
general sparse form. It determines the sparsity structure on its
own, or optionally accepts this information from the user. It then
uses parts of the Yale Sparse Matrix Package (YSMP) to solve
the linear systems that arise, by a sparse (direct) LU factoriza-
tion/backsolve method.

3. LSODA, written jointly with L. R. Petzold, solves systems
$dy/dt = f$ with a dense or banded Jacobian when the problem is
stiff, but it automatically selects between nonstiff (Adams) and
stiff (BDF) methods. It uses the nonstiff method initially, and
dynamically monitors data in order to decide which method to
use.

4. LSODAR, also written jointly with L. R. Petzold, is a variant
of LSODA with a rootfinding capability added. Thus it solves
problems $dy/dt = f$ with dense or banded Jacobian and automa-
tic method selection, and at the same time, it finds the roots of
any of a set of given functions of the form $g(t,y)$. This is often
useful for finding stop conditions, or for finding points at which
a switch is to be made in the function f.

5. LSODPK, written jointly with Peter N. Brown, is a variant of
LSODE in which the direct solvers for the linear systems have
been replaced by a selection of four preconditioned Krylov (ite-
rative) solvers. The user must supply a pair of routine to evalu-
ate, preprocess, and solve the (left and/or right) preconditioner
matrices. LSODPK also includes an option for a user-supplied
linear system solver to be used without Krylov iteration.

6. LSODKR is a variant of LSODPK with the addition of the
same rootfinding capability as in LSODAR, and also of auto-
matic switching between functional and Newton iteration. The
nonlinear iteration method-switching differs from the method-
switching in LSODA and LSODAR, but provides similar sa-
vings by using the cheaper method in the non-stiff regions of
the problem. LSODKR also improves on the Krylov methods in
LSODPK by offering the option to save and reuse the approxi-
mate Jacobian data underlying the preconditioner.

BLAS - Basic Linear Algebra Subprograms

- Blas 1: vektor-vektor-rutiner.

  $y := y + a\ x$ **daxpy**.

  Innerprodukt, skalning.

- Blas 2: matris-vektor-rutiner.

  $y := \alpha A x + \beta y$ eller $y := \alpha A^T x + \beta y$ **dgemv**

  (eller $y := \alpha A^H x + \beta y$ om komplext. $A^H = \bar{A}^T$).

- Blas 3: matris-matris-rutiner.

  $C := \alpha\ op(A)\ op(B) + \beta C$ **dgemm**, där

  $op(M) = M$, $op(M) = M^T$ eller $op(M) = M^H$.

Fyra datatyper, **namn = gemm** t.ex.:

- **snamn** enkel precision
- **dnamn** dubbel precision
- **cnamn** enkel precision komplex
- **znamn** dubbel precision komplex

De datorspecifika biblioteken innehåller optimerade BLAS-rutiner. BLAS från Netlib är inte optimerat.

LAPACK - Linear Algebra PACKage

Ickeglesa problem, men finns stöd för bandmatriser.

- $Ax = b$
- $\min_x\ ||Ax - b||_2$
- $Ax = \lambda x$.

(plus en del närliggande problem vi ej har pratat om).

Två slag av rutiner:

- "driver routines", <u>ett</u> anrop för att lösa ett fullständigt problem. Det finns "simple drivers" med standardvärden på vissa parametrar respektive "expert drivers" med fler inställningsmöjligheter. Kan få tillbaks en uppskattning av konditionstalet till exempel.
- "computational routines", som utför delsteg i en beräkning, t.ex. LU-faktorisering eller lösning givet LU-faktoriseringen.
- "auxiliary routines", diverse hjälprutiner på låg nivå

Drivers för $Ax = b$:

- general
- general band
- general tridiagonal
- symmetric/Hermitian positive definite
- symmetric/Hermitian positive definite (packed storage)
- symmetric/Hermitian positive definite band
- symmetric/Hermitian positive definite tridiagonal
- symmetric/Hermitian indefinite
- complex symmetric
- symmetric/Hermitian indefinite (packed storage)
- complex symmetric (packed storage)

Här är en lista över "computational routines" för "symmetric/Hermitian positive definite":

- factorize, **POTRF**
- solve using factorization, **POTRS**
- estimate condition number, **POCON**
- error bounds for solution, **PORFS**
- invert using factorization, **POTRI**
- equilibrate, **POEQU**

Samma namngivningskonvention som för BLAS.

AMD Core Math Library (ACML)

Från hemsidan: **http://developer.amd.com/acml.jsp**

- A full implementation of Level 1, 2 and 3 Basic Linear Algebra Subroutines (BLAS), with key routines optimized for high performance on AMD Opteron processors.
- A full suite of Linear Algebra (LAPACK) routines. As well as taking advantage of the highly-tuned BLAS kernels, a key set of LAPACK routines has been further optimized to achieve considerably higher performance than standard LAPACK implementations.
- A comprehensive suite of Fast Fourier Transforms (FFTs) in both single-, double-, single-complex and double-complex data types.
- Fast scalar, vector, and array math transcendental library routines optimized for high performance on AMD Opteron processors.
- Random Number Generators in both single- and double-precision.

Tillgängligt för flera system och kompilatorer:
Linux & Windows: gnu, Intel, PGI.
Linux: gfortran, NAG, PathScale
Sun: Solaris

Intel Math Kernel Library (Intel MKL), Linux & Windows

Från:
`http://www.intel.com/cd/software/products/asmo-na`
`/eng/307757.htm`

Optimerat för Intels processorer.
Känner av vilken CPU som används.
Trådat och färdigt för CPUer med flera kärnor.
Fortran- och C-interface.

Innehåller (bland annat):

- BLAS and LAPACK. Optimerade för Intels CPUer.

- ScaLAPACK, parallell Lapack. Available in the Cluster Edition only.

- Sparse solvers. Solve large, sparse, symmetric, and asymmetric linear systems of equations on shared-memory multiprocessors with the PARDISO Direct Sparse Solver...
  Intel MKL also includes a Conjugate Gradient iterative solver...

- Fast Fourier Transforms (FFT).

- Vector Math Library. Increase application speeds with vectorized implementations of computationally intensive core mathematical functions (power, trigonometric, exponential, hyperbolic, logarithmic, and so on).

- Vector Random Number Generators.