Libraries
for
High-Performance Computing
and other purposes

Overview

❏ Why use libraries?

❏ Where to search?

❏ Commercial libraries

❏ Special purpose libraries

Why use libraries?

- ❏ Why should we invent the wheel again and again and again ...?
- ❏ Let us (re-)use what others have developed over many years ...
- ❏ ... with
  - ❏ reliable results
  - ❏ good performance
  - ❏ a lot of manpower

Where to search?

- ❏ Search engines like Google
  - ❏ need to know the name quite exactly
  - ❏ or a good description of what you want to achieve
  - ❏ a lot of irrelevant hits
- ❏ A better approach:
  - ❏ go to well known websites that have collected information over years
  - ❏ "Trust the old men!"

Places to start a search

❏ http://netlib.org

> ❏ Netlib is a collection of mathematical software, papers, and databases.

> ❏ Netlib is mainly dedicated to

>> ❏ Linear Algebra routines

>> ❏ the work by Jack Dongarra and friends

> ❏ up-to-date?

Places to start a search

Guide to Available Mathematical Software

❏ http://gams.nist.gov/

> ❏ extensive catalog of mathematical software

> ❏ nice division into classes and subclasses of problems

> ❏ other sites use the GAMS taxonomy as well, e.g. Netlib

Places to start a search

Collected Algorithms (CALGO)

❏ http://calgo.acm.org/

❏ Algorithms published in ACM journals:

  ❏ "This software is refereed for originality, accuracy, robustness, completeness, portability, and lasting value."

Places to start a search

Software/hardware vendors:

❏ Intel: http://software.intel.com/

  ❏ look for MKL (Math Kernel Library)

❏ AMD: http://developer.amd.com/

  ❏ look for ACML (Advanced Core Math Library)

Trust an "old" man

Nick Trefethen

- ❏ http://people.maths.ox.ac.uk/trefethen/
- ❏ Professor of Numerical Analysis at Oxford University Computing Laboratory
- ❏ Collection of links:
  - ❏ http://people.maths.ox.ac.uk/trefethen/tools.html

Commercial Libraries

- ❏ Numerical Algorithms Group (NAG): http://www.nag.co.uk/
  - ❏ well established general purpose library
- ❏ IMSL: http://www.roguewave.com/products-services/imsl-numerical-libraries
  - ❏ well established general purpose library
- ❏ Harwell Subroutine Library (HSL): http://www.hsl.rl.ac.uk/
  - ❏ free versions for academic research and teaching

A free library

GNU Scientific Library (GSL)

❏ http://www.gnu.org/software/gsl/

   ❏ *"A numerical library for C and C++ programmers. It is free software under the GNU General Public License."*

❏ has a lot of features, but not always optimized

❏ ships with many Linux distros

Special purpose libraries

Linear Algebra

❏ LAPACK & BLAS

   ❏ from Netlib.org or vendor

❏ ATLAS

   ❏ Automatically Tuned Linear Algebra Software

   ❏ http://math-atlas.sourceforge.net/

❏ GotoBLAS: fast implementation of BLAS

   ❏ by Kazushige Goto, TACC (now: Intel)

   ❏ now: OpenBLAS http://www.openblas.net/

Special purpose libraries

Linear Algebra

❏ ARPACK: library for large and sparse eigenvalue problems

  ❏ http://www.caam.rice.edu/software/ARPACK/

  ❏ ARPACK++: C++ interface to ARPACK

❏ MatrixMarket:

  ❏ http://math.nist.gov/MatrixMarket/

  ❏ collection of tools and data sets

Special purpose libraries

Fast Fourier Transforms

❏ FFTW: http://www.fftw.org/

  ❏ Fastest Fourier Transform in the West

  ❏ *"FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data."*

  ❏ state-of-the-art FFT library

  ❏ also in parallel (MPI and OpenMP)

Special purpose libraries

Parallel Solvers:

❏ PETSc: Portable, Extensible Toolkit for Scientific Computation

  ❏ http://www-unix.mcs.anl.gov/petsc/petsc-as/

❏ MUMPS: MUltifrontal Massively Parallel sparse direct Solver

  ❏ http://graal.ens-lyon.fr/MUMPS/

Good advice

If in doubt, don't hesitate to ask an expert, e.g. in your local Scientific Computing/Numerical Analysis group or some researchers working with similar problems