High-Performance Computing

Libraries
for
High-Performance Computing
and other purposes

Overview

❑ Why use libraries?

❑ Where to search?

❑ Commercial libraries

❑ Special purpose libraries

02614 – 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 people!"

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

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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 (emeritus) 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