

# 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 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



# 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