CS590C: Introduction to Computational Science

Lecture 8: Locating and Using Available CS&E Resources.

This lecture is intended to familiarize you with:

- ❑ Software repositories on the net.
- ❑ Tools for searching.
- ❑ Classification mechanisms and tools.

Netlib

The Netlib repository contains freely available software, documents, and databases of interest to the numerical, scientific computing, and other communities. The repository is maintained by AT&T Bell Laboratories, the University of Tennessee and Oak Ridge National Laboratory, and by colleagues world-wide. The collection is replicated at several sites around the world, automatically synchronized, to provide reliable and network efficient service to the global community.

World Wide Web (WWW): *http://www.netlib.org/*

email: *netlib@netlib.org*

ftp: *ftp.netlib.org*

gopher: *gopher.netlib.org*

Finding routines in Netlib

The most powerful search capabilities in Netlib are provided through the interface at

http://www.netlib.org/utk/misc/netlib_query.html

Software for solving specific problems

One way is to identify appropriate keywords and then use the Web search interface at

http://www.netlib.org/utk/misc/netlib_query.html

NHSE: National HPCC Software Exchange

The NHSE is a distributed collection of software, documents, data, and information of interest to the high performance and parallel computing community. The NHSE seeks to actively promote software sharing and reuse within and across HPCC agency programs on a sustainable basis. The NHSE facilitates the development of discipline-oriented software and document repositories, and promotes contributions and use via the World Wide Web.

URL: *http://nhse.cs.utk.edu/*

❏ Benchmark and Example Programs

❏ Data Analysis and Visualization

❏ Distributed Processing Tools

❏ Numerical Programs and Routines

❏ Parallel Processing Tools

❏ Scientific and Engineering Applications
(eg. 3D Acoustic Wave Propagation , 4D2, visualization tool for computational fluid dynamics data, Atmospheric Dynamics Benchmark Source Codes , CCP6 - Collaborative Computational Project in heavy particle dynamics, Computer Simulation of Nuclear Well Logging Tools, Cosmological Simulations Using Adaptive Particle-Mesh Methods)

Other Software Repositories:

- **Statlib:** http://lib.stat.cmu.edu: System for distributing statistical software, datasets, and information by electronic mail, FTP and WWW.

- **SymbolicNet:** http://symbolicnet.mcs.kent.edu: Distributing literature and software on Symbolic and Algebraic Computation (SAC), also known as Computer Algebra (CA).

- **NCSA SDG:** http://www.ncsa.uiuc.edu/SDG/SDGIntro.html: The Software Development Group (SDG) at the National Center for Supercomputing Applications develops computer programs to assist scientific discovery, including data analysis and visualization software (mostly visualization stuff).

- **ESS Software Exchange:** http://olympic.jpl.nasa.gov: Wide variety of numerical and scientific computing software.

- **Newsgroups and the such:** http://www.cis.ohio-state.edu/Services.html

- **More Info on software Repositories:** http://www.netlib.org/nhse/repositories.html

Searching for Information.

Web Search:

- AltaVista http://www.altavista.digital.com
- Lycos: http://lycos.cs.cmu.edu

Anon. FTP Search:

- Archie
- Veronica

Classification Mechanisms and Tools

Classification of Mathematical Software: GAMS (Guide to Available Mathematical Software) **http://gams.nist.gov/.** Search for software according to

- what problem it solves.
- package name.
- module name.
- text in module abstracts

Sample problem solving tree:

- Differential and integral equations
  - Ordinary differential equations (ODE's)
  - Partial differential equations
    - Initial boundary value problems
    - Elliptic boundary value problems
      - Linear
      - Nonlinear
      - Eigenvalue
      - Service routines
  - Integral equations

GAMS currently has about 10,000 problem solving modules in about 100 software packages.

The software is dynamically accessed from actual repositories.

Popular packages for numerical linear algebra.

Many problems in CS&E can be reduced to problems in linear algebra of the following forms:

- ❑ Solve a linear system of equations $Ax = b$
- ❑ Solve a least squares problem $\min \| Ax - b \|$
- ❑ Solve the eigenvalue problem $Ax = \lambda x$.

Solution techniques are influenced by

- ❑ Structure of matrix (sparse / dense / toeplitz)
- ❑ Qualitative structure of the matrix (reducing off-diagonal entries)
- ❑ Available computational resources (Direct solvers need more memory and computation)

Software for Dense Linear Algebra.

BLAS: Basic Linear Algebra Subroutines

Three levels of routines:

- ❏ BLAS1: Vector-vector operations
- ❏ BLAS2: Matrix-vector operations
- ❏ BLAS3: Matrix-Matrix Operations

EISPACK: Eigenvalues and Eigenvectors

LINPACK: collection of Fortran subroutines that analyze and solve linear equations and linear least-squares probles. The package solves linear systems whose matrices are general, banded, symmetric indefinite, symmetric positive definite, triangular, and tridiagonal square. In addition, the package computes the QR and singular value decompositions of rectangular matrices and applies them to least-squares problems.

LAPACK: above + more efficient operations on shared-memory parallel computers

ScaLAPACK: LAPACK on distributed memory parallel computers.