nag®

CSC / NAG Autumn School on

Core Algorithms in High-Performance Scientific Computing

Libraries IV

Ian Bush

Miscellaneous Libraries

Miscellaneous Libraries

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Other Libraries

- There are many libraries out there
  - Many free!
- We could not hope to cover them all
- In this talk I will give a few pointers as to what is out there
  - Google is your friend
- Not much technical detail in this talk
  - More pointers to (some of) what is out there
  - A lot of good stuff to deal with sparse systems

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Don't Reinvent The Wheel!

- If you have a problem to solve in all likelihood somebody else has had to solve it
  - They might have put up their solution somewhere
  - Don't reinvent the wheel!
- However be aware that not all software on the web is good software
  - In other news the Pope is a Catholic
  - Make sure you know how to test the software
    - Does it come with test cases ?
  - Make sure you know exactly how to use the software
    - How well is it documented ?
  - Many algorithms can be implemented in subtly different ways,
    - Normalization in FFTs
    - Direction in FFTs
    - Spherical harmonics

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So What Is Out There?

We've touched on quite a lot of important libraries already
- LAPACK, BLAS implementations, FFTW etc.

In the rest of this talk I shall simply mention a few of the more important libraries that are "out there"

- Not too much technical details
- More so you are aware of what they can do
- No nasty questions please, I haven't used all of these !

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MKL

- Intel Math Kernal Library
- "Intel® Math Kernel Library (Intel® MKL) is a library of highly optimized, extensively threaded math routines for science, engineering, and financial applications that require maximum performance"
- http://software.intel.com/en-us/intel-mkl/
- Version 10.2
- Commercial

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MKL - Features

- Functions include
  - BLAS
  - LAPACK
  - ScaLAPACK
  - Sparse Solvers
  - Fast Fourier Transforms
  - Vector Math
  - ...

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ACML

- AMD Core Math Library
- "ACML provides a free set of thoroughly optimized and threaded math routines for HPC, scientific, engineering and related compute-intensive applications. ACML is ideal for weather modeling, computational fluid dynamics, financial analysis, oil and gas applications and more."
- http://developer.amd.com/cpu/Libraries/acml/Pages/default.aspx
- Version 4.4.0
- Free!

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ACML Features

- ACML includes
  - 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.

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PLASMA

- Out of the University of Tennessee
  - Parallel Linear Algebra For Multicore Architectures
- "The Parallel Linear Algebra for Scalable Multi-core Architectures (PLASMA) project aims to address the critical and highly disruptive situation that is facing the Linear Algebra and High Performance Computing community due to the introduction of multi-core architectures.

  The development of programming models that enforce asynchronous, out of order scheduling of operations is the concept used as the basis for the definition of a scalable yet highly efficient software framework for Computational Linear Algebra applications."
- http://icl.cs.utk.edu/plasma/
- Version 2.1.0
- Free!

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PLASMA Features

- At present PLASMA implements a small subset of LAPACK and BLAS
  - Linear equation solves
  - LU, Cholesky, QR and LQ factorisations
- Main aim is efficiency on multicore architectures

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Blitz++

- "Blitz++ is a C++ class library for scientific computing which provides performance on par with Fortran 77/90. It uses template techniques to achieve high performance. The current versions provide dense arrays and vectors, random number generators, and small vectors and matrices"
- http://www.oonumerics.org/blitz/
- Version 0.9
- Free!

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HSL

- The Harwell Subroutine Library
- "HSL (formerly the Harwell Subroutine Library) is a collection of threadsafe ISO Fortran codes for large scale scientific computation."
- "**Among its best know codes are those for the solution of sparse linear systems of equations, optimization, and sparse eigenvalue problems.**"
- http://www.hsl.rl.ac.uk/
- Free to academics!

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Trilinos

- The Trilinos Project is a big effort coming out of Sandia National Lab
- "The Trilinos Project is an effort to develop algorithms and enabling technologies within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems. A unique design feature of Trilinos is its focus on packages."
- At release 10.4
- http://trilinos.sandia.gov/
- Free!

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Trilinos – Capability Areas

- Trilinos has defined 7 "Capability Areas"
  - See http://trilinos.sandia.gov/capability_areas.html
- They are:
  1. Framework & Tools
  2. Software Engineering Technologies and Integration
  3. Discretizations
  4. Meshes, Geometry, & Load Balancing
  5. Scalable Linear Algebra
  6. Linear & Eigen Solvers
  7. Embedded Nonlinear Analysis Tools

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Trilinos Package Summar

Objective	Package(s)
Distributed linear algebra objects	Epetra, Jpetra, Tpetra
Krylov solvers	AztecOO, Belos
ILU-type preconditioners	AztecOO, IFPACK
Multilevel preconditioners	ML, CLAPS
Eigenvalue problems	Anasazi
Block preconditioners	Meros
Direct sparse linear solvers	Amesos
Direct dense solvers	Epetra, Teuchos, Pliris
Abstract interfaces	Thyra
Nonlinear system solvers	NOX, LOCA
Complex linear systems	Komplex
C++ utilities, (some) I/O	Teuchos, EpetraExt, Kokkos, Galeri
Trilinos tutorial	Didasko
Python support	PyTrilinos
Time integrators/DAEs	Rythmos
Archetype package	NewPackage

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PETSc

- Comes out of Argonne National Lab
- "PETSc, **pronounced PET-see** (the S is silent), is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. It employs the MPI standard for parallelism."
- At release 3.1
- http://www.mcs.anl.gov/petsc/petsc-as/
- Free!

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PETSc – Features Include

- Parallel vectors
- Parallel matrices
  - several sparse storage formats
  - easy, efficient assembly.
- Scalable parallel preconditioners
- Krylov subspace methods
- Parallel Newton-based nonlinear solvers
- Parallel timestepping (ODE) solvers

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PETSc – Related Packages

- Related packages that use PETSc
  - TAO - Toolkit for Advanced Optimization.
  - SLEPc - Scalable Library for Eigenvalue Problems.
  - Prometheus - scalable unstructured finite element solver.
  - FreeCFD - general purpose CFD solver.
  - OpenFVM - finite volume based CFD solver.
  - OOFEM - object oriented finite element library.
  - LibMesh - adaptive finite element library.
  - DEAL.II - sophisticated C++ based finite element simulation package.
- Also Interoperability with Trilinos

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ARPACK and PARPACK

- From Rice University
- "ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems. The package is designed to compute a few eigenvalues and corresponding eigenvectors of a general n by n matrix A. It is most appropriate for large sparse or structured matrices A where structured means that a matrix-vector product w <- Av requires order n rather than the usual order n^2 floating point operations. This software is based upon an algorithmic variant of the Arnoldi process called the Implicitly Restarted Arnoldi Method (IRAM). When the matrix A is symmetric it reduces to a variant of the Lanczos process called the Implicitly Restarted Lanczos Method (IRLM)."
- http://www.caam.rice.edu/software/ARPACK/

Free!

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ARPACK - Features

- Important Features of ARPACK:
  - Reverse Communication Interface.
  - Single and Double Precision Real Arithmetic Versions for Symmetric, Non-symmetric,
  - Standard or Generalized Problems.
  - Single and Double Precision Complex Arithmetic Versions for Standard or Generalized Problems.
  - Routines for Banded Matrices - Standard or Generalized Problems.
  - Routines for The Singular Value Decomposition.
  - Example driver routines that may be used as templates to implement numerous Shift-Invert strategies for all problem types, data types and precision.

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Reverse Communication

- Reverse communication is an important tool for iterative methods
- The iterative method only knows that, say, a matrix vector product is needed. It doesn't know the exact data structure of your matrix
- Reverse communication isolates the product from the iterative method
  - Allows you, whose does know the structure, to write a really efficient matrix vector product
  - But you don't need to know the details of the iteration!

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Reverse Communication

```
Do
   call dsaupd ( ido, b, n, which, nev, tol, resid, ncv, &
                 v, ldv, iparam, ipntr, workd, workl,  lworkl, info )
   Select Case( ido )
   Case( -1 )
      ! w <- OP*v
   Case( 1 )
      ! w <- OP*B*v
   Case( 2 )
      ! w <- B*v
   Case Default
      Exit ! Converged
   End Select
End Do
```

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PARPACK

- PARPACK is the parallel version of ARPACK
- See
  - http://www.caam.rice.edu/software/ARPACK/denmark2.ps
  - http://www.caam.rice.edu/software/ARPACK/cm_writeup.ps
- Reverse communication is especially useful here!

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What ARPACK Is Being Used For

- Image Reconstruction Large Scale
- Molecular Dynamics Simulations
- Stability Analysis of Crystal Growth
- Reactive Scattering
- Iterative Determination of Vibrational Energy Levels
- Large-Scale Computation of Pseudospectra
- Large-Scale Electromagnetic Eigenvalue Problems
- etc.

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GSL - GNU Scientific Library

- "The GNU Scientific Library (GSL) is a numerical library for C and C++ programmers. It is free software under the GNU General Public License. The library provides a wide range of mathematical routines such as random number generators, special functions and least-squares fitting. There are over 1000 functions in total with an extensive test suite."
- At release 1.14
- http://www.gnu.org/software/gsl/
- Free!

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GSL

- Subjects include
  - Complex Numbers
  - Special Functions
  - Permutations
  - BLAS Support
  - Eigensystems
  - Quadrature
  - Quasi-Random Sequences
  - Statistics
  - N-Tuples
  - Simulated Annealing
  - Interpolation
  - Chebyshev Approximation
  - Discrete Hankel Transforms
  - Minimization
  - Physical Constants
  - Discrete Wavelet Transforms
  - Roots of Polynomials
  - Vectors and Matrices
  - Sorting
  - Linear Algebra
  - Fast Fourier Transforms
  - Random Numbers
  - Random Distributions
  - Histograms
  - Monte Carlo Integration
  - Differential Equations
  - Numerical Differentiation
  - Series Acceleration
  - Root-Finding
  - Least-Squares Fitting
  - IEEE Floating-Point
  - Basis splines

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IMSL

- Produced by Visual Numerics
- "The IMSL Numerical Libraries have been the cornerstone of high-performance and desktop computing as well as predictive analytics applications in science, technical and business environments for well over three decades."
- http://www.vni.com/products/imsl/
- Commercial

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IMSL Features

- These include:
  - Linear systems
  - Interpolation and approximation
  - Differential equations
  - Nonlinear equations
  - Matrix/vector operations
  - Utilities
  - Regression
  - Analysis of Variance
  - Nonparametric Statistics
  - Time Series and Forecasting
  - Survival Analysis
  - Random Number Generation
  - Eigensystem analysis
  - Integration and differentiation
  - Transforms
  - Optimization
  - Special Functions
  - Basic statistics
  - Correlation and Covariance
  - Categorical and Discrete Data Analysis
  - Goodness-of-Fit and Randomness
  - Multivariate analysis
  - Probability Distribution Functions and Inverses

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METIS and ParMETIS

- From the University of Minnesota
- "METIS is a family of programs for partitioning unstructured graphs and hypergraphs and computing fill-reducing orderings of sparse matrices. The underlying algorithms used by METIS are based on the state-of-the-art multilevel paradigm that has been shown to produce high quality results and scale to very large problems."
- http://glaros.dtc.umn.edu/gkhome/views/metis
- METIS 4.0.1, ParMETIS 3.1.1

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METIS and ParMETIS Functionality

- Functionality includes
  - Graph Partitioning
  - Mesh Partitioning
  - Graph Repartitioning
  - Matrix Reordering

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GPU accelerator libraries

- A number of libraries being developed to take advantage of GPUs as accelerators, by NAG and others (e.g. MAGMA)
- Don't really feel qualified to talk about this!
- But talk on it tomorrow

Summary

- There are many, many pieces of numerical software out there
  - Some good
  - Some not so
  - TEST!
- Don't reinvent the wheel!
- Google is your friend