







# CSC / NAG Autumn School on Core Algorithms in High-Performance Scientific Computing

# Libraries IV

Ian Bush

Miscellaneous Libraries

### Miscellaneous Libraries

Numerical Algorithms Group Ltd, HECToR CSE





#### Other Libraries

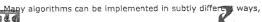
- ▶ There are many libraries out there
  - Many free!
- ▶ We could not hope to cover them all
- ▶ In this talk I will give a few pointers as to what is out there
  - Google is your friend
- ▶ Not much technical detail in this talk
  - More pointers to (some of) what is out there
  - A lot of good stuff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





#### 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 ?



- vormalization in FFTs Direction in FFTs
- · Spherical harmonics

#### 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 !





#### 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





RESEARCH COUNCILS UK

#### MKL - Features

- ▶ Functions include
  - · BLAS
  - LAPACK
  - ScalAPACK
  - · Sparse Solvers
  - · Fast Fourier Transforms Vector Math





#### ACML

- ► AMD Core Math Library
- ▶ "ACML provides a free set of thoroughly optimized and threaded math routines for HPC, scientific, engineering and related computeintensive 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





#### **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 doublecomplex data types.
- Fast scalar, vector, and array math transcendental brary routines optimized for high performance on MD Deteron processors Opteron processors.
  - Random Number Generators in both single- and thinks H

#### **PLASMA**

- ▶ Out of the University of Tennessee
  - Parallel Linear Aigebra 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/





#### 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





#### 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!





#### 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!





#### 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/





#### Trilinos - Capability Areas

- ▶ Trilinos has defined 7 "Capability Areas"
  - See <a href="http://trilinos.sandia.gov/capability">http://trilinos.sandia.gov/capability</a> 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





Objective	Package(s)	Trilinos
Distributed linear algebra objects	Epetra, Jpetra, Tpetra	Packag
Krylov solvers	AztecOO, Belos	Summa
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	
Triumas utorial	Didasko	7
Pylin Support	PyTrilinos	
THE chategrators/DAEs	Rythmos	RESEARCH
Archetype package	NewPackage	COUNCILS UK.

## 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!





#### 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





#### 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.
  - <u>DEAL.II</u> <u>sophisticated C++</u> based finite element <u>simulation package</u>.
- Also Interoperability with Trilinos



RESEARCH COUNCIES UK

#### ARPACK and PARPACK

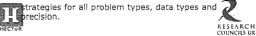
- From Rice University
- "ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems. The package is designed to compute a few eigenvalues and corresponding eigenvectors of a general n by n matrix A. It is most appropriate for large sparse or structured matrices A where structured means that a matrix-vector product w <- Av requires order n rather than the usual order n² 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)."</p>
- ▶ http://www.caam.rice.edu/software/ARPACK/





#### 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



#### 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!





#### 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





#### 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!





#### 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





#### 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!





#### GSL

#### ▶ Subjects include

- Complex Numbers
   Special Functions
- Permutations BLAS Support
- Eigensystems
- Ouadrature
- Quasi-Random Sequences
- Statistics
- Simulated Annealing
- •Interpolation •Chebyshev Approximation
- \*Discrete Hankel Transforms

mization. nis cui Constants

Wavelet Transforms Basis splines

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

#### **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





#### **IMSL** Features

#### ▶ These include:

- Linear systems
- 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

Interpolation and approximation 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

RESEARCH COUNCIES UK

#### 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/qkhome/views/metis
- ▶ METIS 4.0.1, ParMETIS 3.1.1





#### METIS and ParMETIS Functionality

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



### 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 goodSome not so
  - TEST!
- ▶ Don't reinvent the wheel!
- ▶ Google is your friend



