Libraries

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Libraries

- Why you should be interested
- What is available
- Issues
- Some results
- We have examples
Why?

- Many common problems have been solved
- Writing a good parallel routine is difficult
- “It’s not about the computer”
What?

- Intel-MKL

  - BLAS
  - BLACS
  - LAPACK
  - ScalAPACK
  - PBLAS
  - Sparse Solver
  - Vector Math Library (VML)
  - Vector Statistical Library (VSL)
  - Conventional DFTs and Cluster DFTs
  - Partial Differential Equations support
  - Optimization Solvers.

- Fourier Transforms

  - p3dfft
  - fftw

- NAG Library (Not installed)

  - Optimization, both Local and Global
  - Linear, quadratic, integer and nonlinear programming and least squares problems
  - Ordinary and partial differential equations, and mesh generation

- Solution of dense, banded and sparse linear equations and eigenvalue problems
- Solution of linear and nonlinear least squares problems
- Curve and surface fitting and interpolation
- Special functions
- Numerical integration and integral equations
- Roots of nonlinear equations (including polynomials)
- Option Pricing Formulae
- Wavelet Transforms
- Statistical facilities
- Random number generation
- Simple calculations on statistical data
- Correlation and regression analysis
- Multivariate methods
- Analysis of variance and contingency table analysis
- Time series analysis
- Nonparametric statistics

- PETSC

  - Solution of linear and non-linear partial differential equations
  - Focus on problems discretized using semi or fully implicit methods

- Cuda

  - CULA Linear Algebra Library from EMPhotonics
Issues

- Can be difficult to link
- Can be difficult to set up, especially parallel
- Portability
PETSc on RA

tar -xzf petsc-2.3.3-p13.tar.gz
cd petsc-2.3.3-p13
setenv PETSC_DIR $PWD
./config/configure.py
setenv PETSC_ARCH linux-gnu-c-debug
make all test

Builds fine. Test fails because it tries to run an MPI job on the front end
Sparse Linear Solve on RA

PETSc example /src/ksp/ksp/examples/tutorials/ex16.c on RA

M, where matrix size is (M x M)
Examples

- MKL LAPACK ScaLAPACK
- LAPACK & CUDA Cula
- I am starting from scratch...
  - http://geco.mines.edu/software/mkl/casestudy.html