Software Ecosystem for HPC

Murat Manguoğlu
Middle East Technical University
Computer Engineering

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Software Ecosystem

• Low level
  • BLAS
  • Lapack/Scalapack
  • Various Parallel Sparse Linear Solvers
  • PARPACK - eigensovlers
  • ....

• High level
  • General Purpose
    • PETSC
    • Trilinos
    • Julia
  • Domain specific
BLAS: Basic Linear Algebra Subroutines

• Basic dense matrix/vector operations
  • Vector-Vector (Level 1)
  • Matrix-Vector (Level 2)
  • Matrix-Matrix (Level 3)

• Usually optimized for a given platform usually multithreaded
  • Intel MKL BLAS
  • Atlas BLAS
  • Goto BLAS
  • cuBLAS
  • ....
LAPACK/ScaLAPACK: Scalable/ Linear Algebra Package

• Dense matrix operations that are higher level than the ones in BLAS, LAPACK/ScaLAPACK use BLAS
  • solving linear systems
  • solving least-square problems
  • solving eigenvalue problems
  • solving singular value problems

• Usually optimized for a given platform, LAPACK is sequential/multithreaded and ScaLAPACK is parallel using message passing
  • Intel MKL
  • MAGMA (~cuda LAPACK)
  • ...

...
Sparse Linear Solver Libraries

- SuperLU  http://crd-legacy.lbl.gov/~xiaoye/SuperLU/
- Pardiso  http://www.pardiso-project.org/
- MUMPS  http://mumps.enseeiht.fr/
Sparse Eigensolvers

- Parpack  http://www.caam.rice.edu/~kristyn/parpack_home.html
- Slepc  http://slepc.upv.es/
- FEAST  http://www.feast-solver.org/
- ...

PETSC: Portable, Extensible Toolkit for Scientific Computation

Structure of PETSc

https://www.mcs.anl.gov/petsc/
Trilinos: Algorithms and Enabling Technologies for Large-Scale Applications

Two-level design:
- Self-contained packages (50+)
- Leveraged common tools.
  - Version Control
  - Build System
  - Test Harness

http://trilinos.sandia.gov
Trilinos: A Layered Collection of C++ Libraries

- Standard C++, Not a language extension
  - *Not* a language extension: OpenMP, OpenACC, OpenCL, CUDA
  - In *spirit* of Intel’s TBB, NVIDIA’s Thrust & CUSP, MS C++AMP, ...
- Uses C++ template meta-programming
  - Previously relied upon C++1998 standard
  - Now require C++2011 for lambda functionality
    - Supported by Cuda 7.0; full functionality in Cuda 7.5
  - Participating in ISO/C++ standard committee for core capabilities

Application & Library Domain Layer(s)

- Trilinos Sparse Linear Algebra
- Kokkos Containers & Algorithms
- Kokkos Core

Back-ends: Cuda, OpenMP, pthreads, specialized libraries ...
**SU2: An open source CFD Code**

![SU2 diagram](http://su2.stanford.edu/)

**http://su2.stanford.edu/**
OpenFOAM: An open source CFD code

http://www.openfoam.com
LAMMPS: Molecular Dynamics Simulator

function mandel(z)
  c = z
  maxiter = 80
  for n = 1:maxiter
    if abs(z) > 2
      return n-1
    end
  end
  z = z^2 + c
end
return maxiter
end

function randmatstat(t)
  n = 5
  v = zeros(t)
  w = zeros(t)
  for i = 1:t
    a = randn(n,n)
    b = randn(n,n)
    c = randn(n,n)
    d = randn(n,n)
    P = [a b; c d]
    Q = [a b; c d]
    v[i] = trace((P.'*P)^4)
    w[i] = trace((Q.'*Q)^4)
  end
  std(v)/mean(v), std(w)/mean(w)
end
High Performance Fast Computing Challenge

• Do you want to help aerospace engineers solve problems faster? Does the phrase “nonlinear partial differential equations used for unsteady computations” excite you? Do you want to try yourself with the complex computational software that NASA scientists use? This might be the challenge for you.

• NASA’s Aeronautics Research Mission Directorate (ARMD) is responsible for developing technologies that will enable future aircraft to burn less fuel, generate fewer emissions and make less noise. Every U.S. aircraft and U.S. air traffic control tower has NASA-developed technology on board. It's why we like to say, NASA is with you when you fly!

• We need to increase the speed of computations on the Pleiades supercomputer, specifically for computational fluid dynamics, by orders of magnitude, and could use your help!

• This isn’t a quest for the faint of heart. As a participant, you’ll need to gain access to FUN3D software through an application process with the US Government. Although this software usually runs on the Pleiades supercomputer, you can download and run it locally after applying HERE.

• TOTAL PRIZE AMOUNT $55,000  

https://herox.com/HPFCC