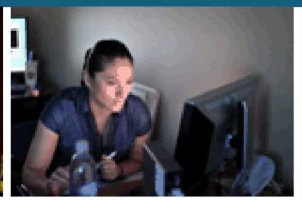
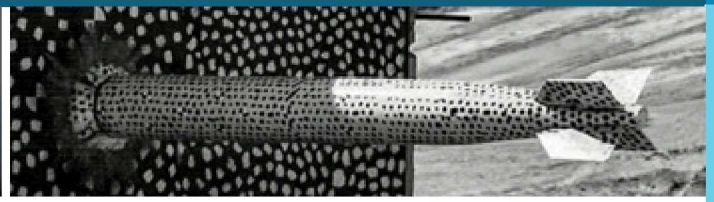
SAND2019-8034PE

SNL+DOE need/ask for NVIDIA Math Libraries





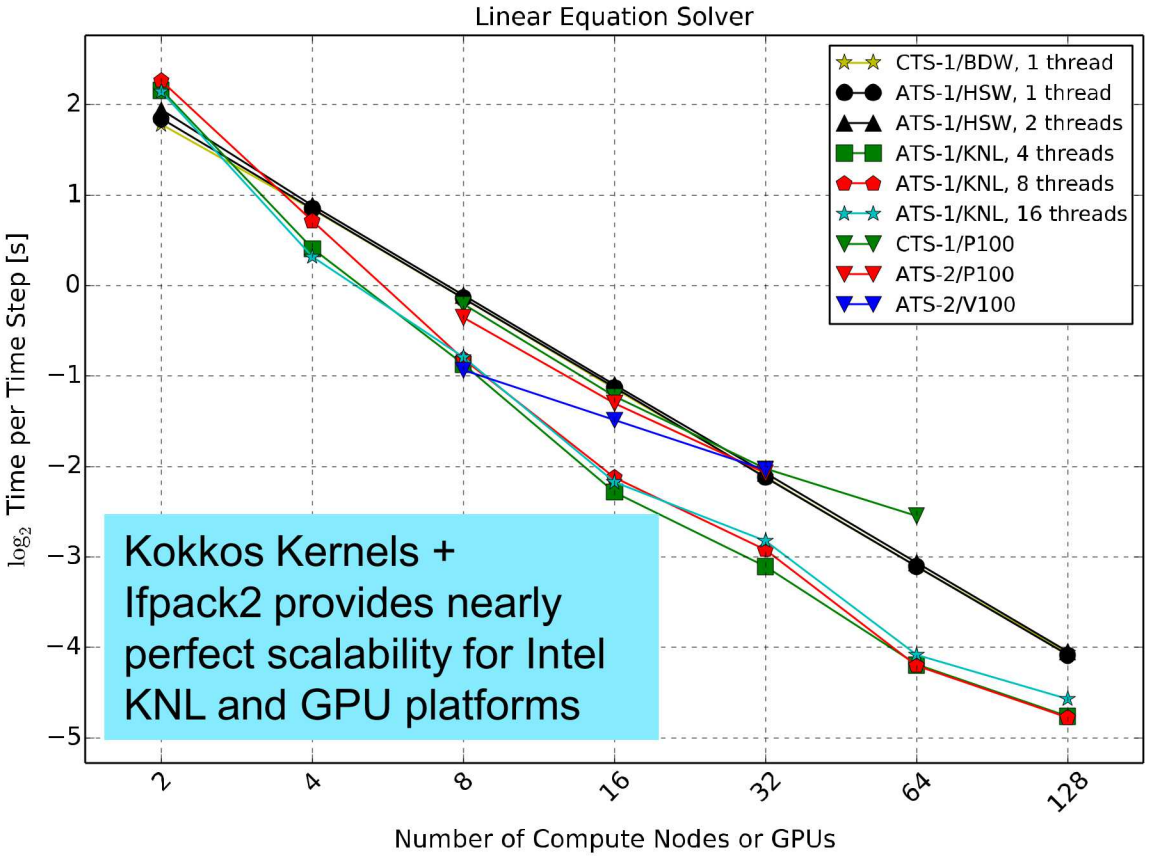
PRESENTED BY

Siva Rajamanickam

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SAND2019-XXXXXX

Developing line solvers for SPARC (ATDM)



POC: Siva Rajamanickam (1465); Micah Howard (1515)

- Develop Compact Batch Kernels needed by BLAS
  - Different from community developed standards for Batched BLAS at the device level
  - Proposed as part of the community standard and being developed as part of multiple implementations
- Optimized, vectorized implementation in Kokkos Kernels for Intel CPU, KNL and GPU platforms
  - New implementations for Astra platform developed.
- Collaboration with Intel to develop assembly level kernels into Intel MKL (released as part of MKL 2018)
- Developed line solvers based on compact kernels and integrated compact BLAS based preconditioners in SPARC
  - Up to 2x speedup in total SPARC simulation time
  - Up to 8-20x speedup in solver time

- **Developed preconditioners using compact batched kernels and demonstrated improved application performance on multiple architectures**
- **Contributed to community standards and optimized vendor implementations**

Team level Kernels Needed by Kokkos Kernels DOE users

SPARC CFD code : Team level dtrsm, dgemm, dgetrf

Support Eigen Solvers within larger parallel kernels of an Chemistry application

- New team level functionality in Kokkos Kernels functionality for Householder transformations, Givens rotations, QR, Hessenberg, Schur decomposition, and Eigen Value decomposition (somewhat larger problems O(100)

Compadre Toolkit

- Support team level variable sized Eigen solver and SVD

QMCPACK

- Support team level complex kernels (several ones)

ExaAM

- Support team level variable sized eigen solvers

Several users in optimization (team level non-linear solves)

Umbrella issue (some LANL, ORNL requirements are documented here as well)

https://github.com/kokkos/kokkos-kernels/issues/9

Multi GPU Support

Complex LU solver

- Boundary Element Method – dense, complex matrices
- Full system run on Trinity (limited usually by memory)
- Pivoting : Use cases available for both pivoting and no pivoting
- We would like a full system run on Sierra
- Current solver used
  - Pliris package in Trilinos – Scalapack functionality, hand rolled decades ago, MPI only, works well on Trinity
- GPU status
  - Using MAGMA for single GPU runs – ~4TFlops
  - Work on Kokkos version of Pliris
- An optimized MultiGPU, full system level, complex LU solver will impact the application right away.

Preconditioners

Common DOE Sparse Solver Usage

- Multigrid methods
  - Setup (can be amortized in some apps): Need sparse matrix * sparse matrix, sparse ILU(k), Gauss-Seidel, Chebyshev, SPAI
  - Solve (can not be amortized): Sparse matrix * (multiple) vectors, triangular solve or other preconditioner apply
  - Applications: Exawind (ECP), EMPIRE (ECP/ATDM), Ice sheets (ECP + Climate programs), several others
- Domain decomposition methods
  - Typically two-level or three-level domain decomposition
  - Setup (can be amortized in some apps): Direct factorization LL, LDL
  - Solve (cannot be amortized): Triangular solve (usually the primary problem for GPUs)
  - Applications: Solid Mechanics, Structural Dynamics, several others
- Direct Solvers
  - Unsymmetric and very sparse problems
  - Cannot amortize LU or the triangular solve (usually very problematic for GPUs)
  - Applications: Circuit simulation, Optimization