The Kokkos Lectures

Module 5: Kokkos Kernels Math Library

August 27, 2020

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Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series:
  - Slides, recording and Q&A for the Lectures
- https://github.com/kokkos/kokkos/wiki:
  - Wiki including API reference
- https://kokkosteam.slack.com:
  - Slack channel for Kokkos.
  - Please join: fastest way to get your questions answered.
  - Can whitelist domains, or invite individual people.

Lecture Series Outline

- 07/17 Module 1: Introduction, Building and Parallel Dispatch
- 07/24 Module 2: Views and Spaces
- 07/31 Module 3: Data Structures + MultiDimensional Loops
- 08/07 Module 4: Hierarchical Parallelism
- 08/14 Module 5: Tasking, Streams and SIMD
- 08/21 Module 6: Internode: MPI and PGAS
- 08/28 Module 7: Tools: Profiling, Tuning and Debugging
- **09/04 Module 8: Kernels: Sparse and Dense Linear Algebra**
- 09/11 Reserve Day

Tools Stuff

Dense Linear Algebra (BLAS)

- BLAH.
- More BLAH.

Sparse Linear Algebra

- Sparse BLAH.
- Sparse BLAH2.

Graph Functions

- Graph BLAH.

Dense Linear Algebra (BLAS)

Kokkos Kernels dense linear algebra capabilities.

Learning objectives:

- Calling BLAS functions with Views
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Why do we need this?

HPC world owns many Fortran LOC!

- We generally cannot port it all at once.
- We need an incremental porting strategy
  - Keep our e.g. Fortran mains, drivers, physics packages
  - But port relevant infrastructure, or hotspot kernels to C++ and Kokkos

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How do we make Kokkos and Fortran talk with each other?

Fortran Language Compatibility Layer (FLCL)

- Pass multidimensional arrays accross the C++/Fortran boundary
  - See Fortran arrays as Kokkos Views and vice versa
- Create Kokkos View and DualView from Fortran
  - Allows Fortran to be the memory owner but call C++ functions with Kokkos kernels for CUDA/HIP
- Initialize and Finalize Kokkos from Fortran
- FortranIndex<T> scalar type to deal with 1 vs 0 based indexing in sparse data structures

FLCL

The Fortran Language Compatibility Layer allows an incremental porting of a Fortran code to Kokkos.

nd_array_t

The compatibility glue between Fortran arrays and Kokkos Views.

Keeps Track of:

- An array's rank
- Extents of the array
- Strides of the array
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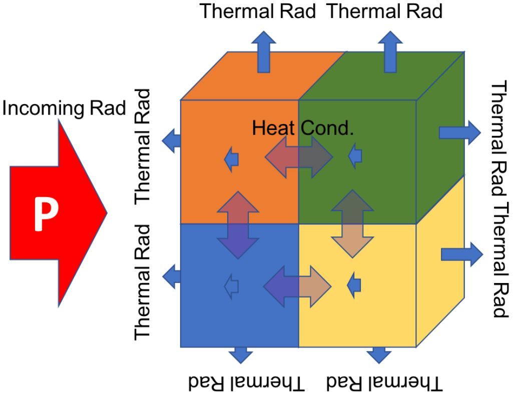
How do we create an `nd_array_t`?

- Explicit routines like `to_nd_array_i64_6`
- Simple interface taking a fortran array as argument

```
array = to_nd_array(foo);
```

3D Heat Conduction

- Heat conduction inside the body
- Thermal radiation (Black Body) on surface
- Incoming power flow from one direction



Sparse Linear Algebra

Sparse linear algebra data structures and functions.

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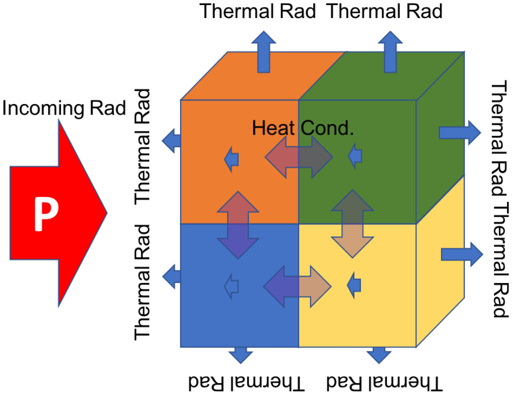

Sparse Solvers

Sparse linear algebra data structures and functions.

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- Calling BLAS functions with Views
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Sparse Solvers + Preconditioning

- Basic idea is to use the Krylov subspace method on a modified system to increase the convergence rate
- Common Krylov subspace solvers: Conjugate Gradient (CG), Biconjugate Gradient Stabilized (BiCGSTAB), Generalized Minimal Residual (GMRES)
- Common preconditioners: Jacobi (or diagonal), Sparse Approximate Inverse (SPAI), Incomplete LU factorization (ILU)

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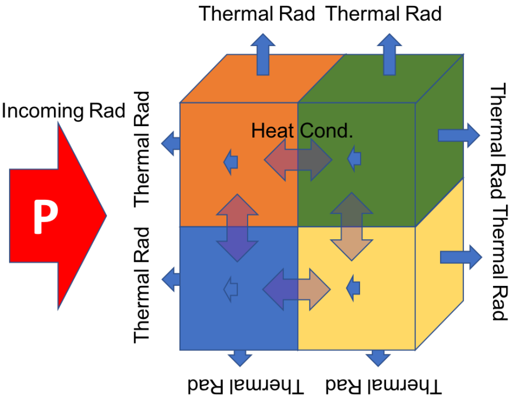

Graph Kernels

Kokkos Kernels functionality for graph computations.

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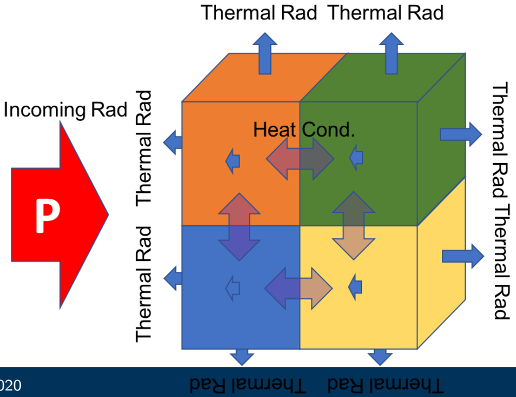
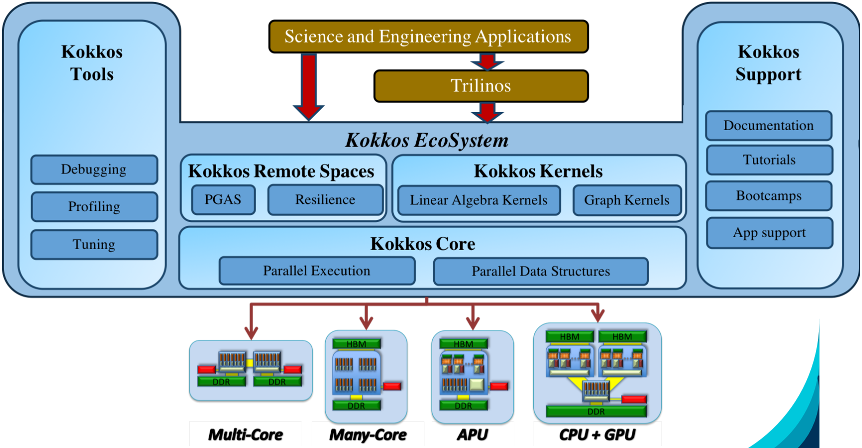


Summary

More Summary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DDR
HBM
DDR
HBM
DDR
HBM
HBM
DDR
Multi-Core
Many-Core
APU
CPU + GPU

kokkos

Los Alamos NATIONAL LABORATORY EST.1943

Sandia National Laboratories

Argonne NATIONAL LABORATORY

OAK RIDGE National Laboratory

BERKELEY LAB

CSCS

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`former:` H.C. Edwards, D. Labreche, G. Mackey, S. Bova, D. Sunderland

Kokkos Kernels: **S. Rajamanickam**, L. Berger, V. Dang, N. Ellingwood, E. Harvey, B. Kelley, K. Kim, C.R. Trott, J. Wilke, S. Acer

Kokkos Tools **D. Poliakoff**, C. Lewis, S. Hammond, D. Ibanez, J. Madsen, S. Moore, C.R. Trott

Kokkos Support **C.R. Trott**, G. Shipmann, G. Womeldorff, and all of the above
`former:` H.C. Edwards, G. Lopez, F. Foertter

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