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Performance Portable Assembly For Plasma Fluid Equations

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Sandia National Laboratories

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National Nuclear Security Administration

Problem Description

Prediction of plasma processes at moderate to high densities

- Multifluid plasma equations – Electrons, ions and neutrals
  - Six-dimensional Boltzmann equations too high of dimensionality
  - Particle methods too expensive due to plasma frequency
  - Sets of 5 or 13 coupled PDEs with stiff source terms need to be solved
- Equations need to be composible and maintainable

Analysis Beyond Forward Simulation

- Forward solves are not enough – we want to explore complex solution spaces:
  - Simultaneous analysis and design adds requirements (typically sensitivities)
  - Do not burden analysts/physics experts with analysis algorithm requirements: i.e. programming sensitivities for implicit solvers, optimization, stability, bifurcation analysis and UQ

Engine must be flexible, extensible, maintainable and EFFICIENT!

Problem Description

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Directed Acyclic Graph-based Assembly

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Analysis Beyond Forward Simulation

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Template-based Generic Programming

Engine must be flexible, extensible, maintainable and EFFICIENT!

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Drekar/Panzer: Algorithms and Software

Drekar: Algorithms research application

- Targets coupled multi-physics
- Large scale simulation (>100k cores)
- Advanced algorithm demonstration

A co-dependent development relationship

Panzer: Multi-physics assembly engine

- Finite element focused (currently)
- Embedded analysis (AD, Sensitivities)
- Technology sharing and deployment

Drekar drives **Panzer** requirements and design goals

Panzer provides **Drekar** flexible infrastructure and core technologies

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Roger Pawlowski
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David Sondak
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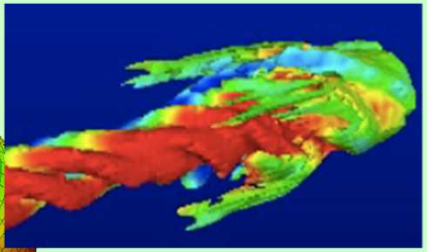
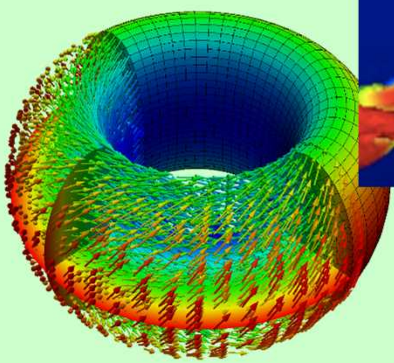
Drekar/Panzer: Capabilities

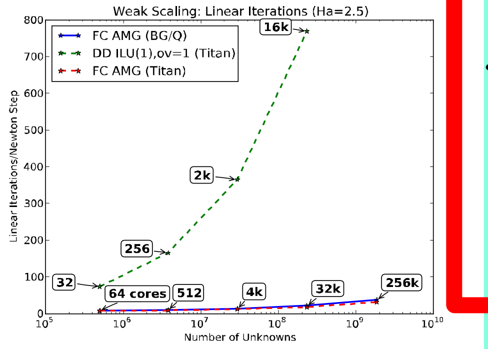
Applications



Turbulent CFD



Magnetohydrodynamics



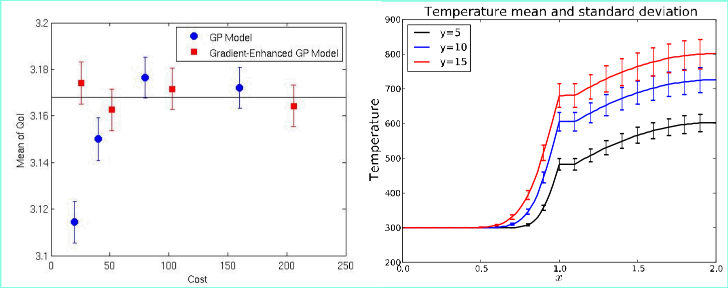
Algebraic Multigrid (>100k cores)

$$\mathcal{A} = \begin{bmatrix} I & \\ BF^{-1} & I \end{bmatrix} \begin{bmatrix} F & B^T \\ & S \end{bmatrix}$$

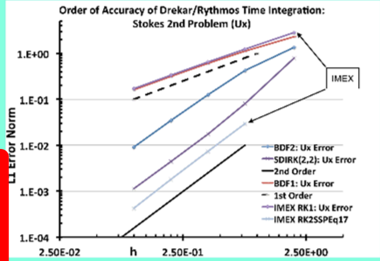
$$S = C - BF^{-1}B^T$$

Block Preconditioning

Discretizations & Algorithms

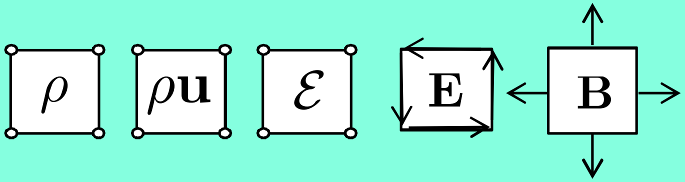


Uncertainty Quantification



IMEX

PDE Constrained Optimization

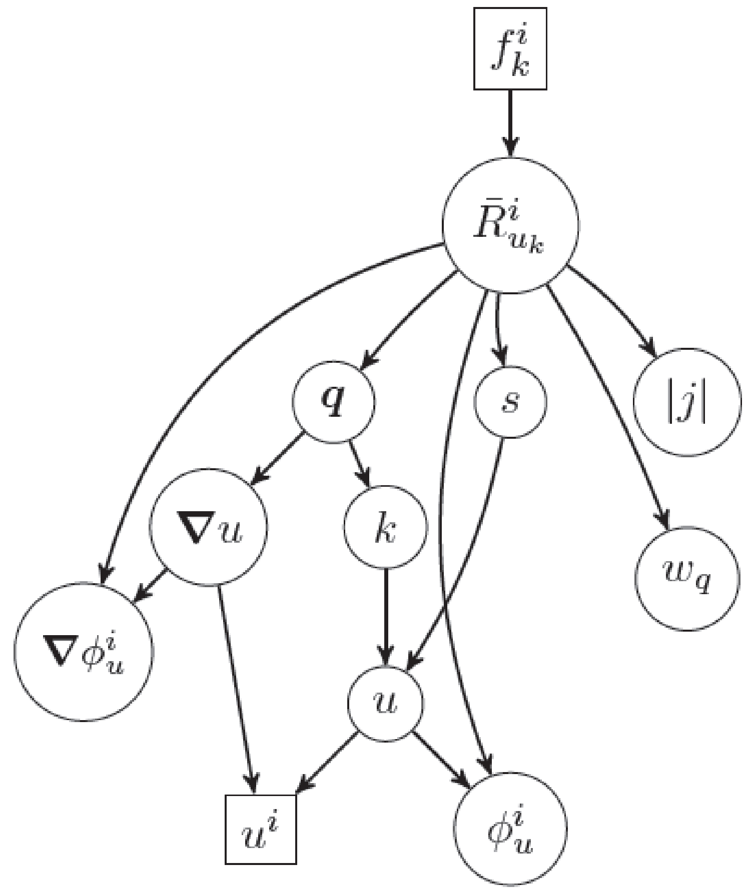


Compatible Discretizations

Lightweight DAG-based Expression Evaluation

- Decompose a complex model into a graph of simple kernels (functors)
  - Decomposition is NOT unique

$$R_u^i = \int_\Omega \left[\phi_u^i \dot{u} - \boldsymbol{\nabla} \phi_u^i \cdot \boldsymbol{q} + \phi_u^i s \right] \mathrm{d}\Omega$$



- Supports rapid development, separation of concerns and extensibility.

- A node in the graph evaluates one or more **fields**:
  - Declare fields to evaluate
  - Declare dependent fields
  - Function to perform evaluation

- Separation of data (Fields) and kernels (Expressions) that operate on the data
  - Fields are accessed via multidimensional array interface (shards or kokkos)

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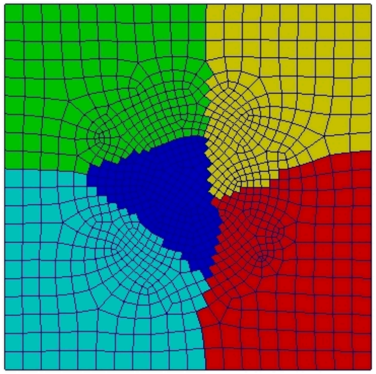
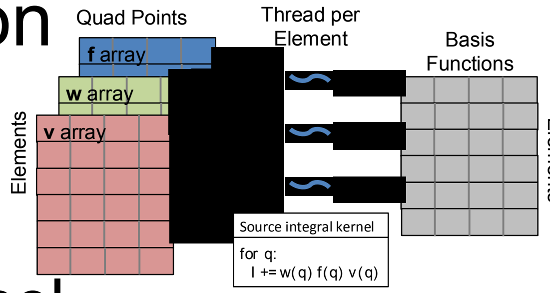
DAG Evaluation

- The problem domain is broken into worksets
  - Smaller number of elements which fit into cache or other memory structures
  - The entire DAG is evaluated for a single workset
  - Each math kernel can be threaded over the workset elements
- Worksets are filled with a gather operation
- The workset’s contributions are accrued in a matrix with a scatter operation
- All intermediate calculations are independent of if they are computing a Jacobian or residual or sensitivity

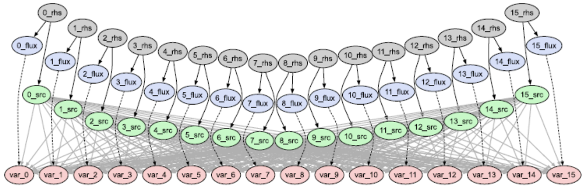
Parallelization Strategies



- MPI – Domain decomposition
  - This is the traditional approach
  - Not covered in this talk
- Threading – On node parallelization
  - More scalable for local cores
  - Extensible to GPUs/Cuda
  - Threads team up to accelerate a kernel



- Kernel parallelization
  - Different kernels at the same time
  - Asynchronous Many Tasking (AMT)



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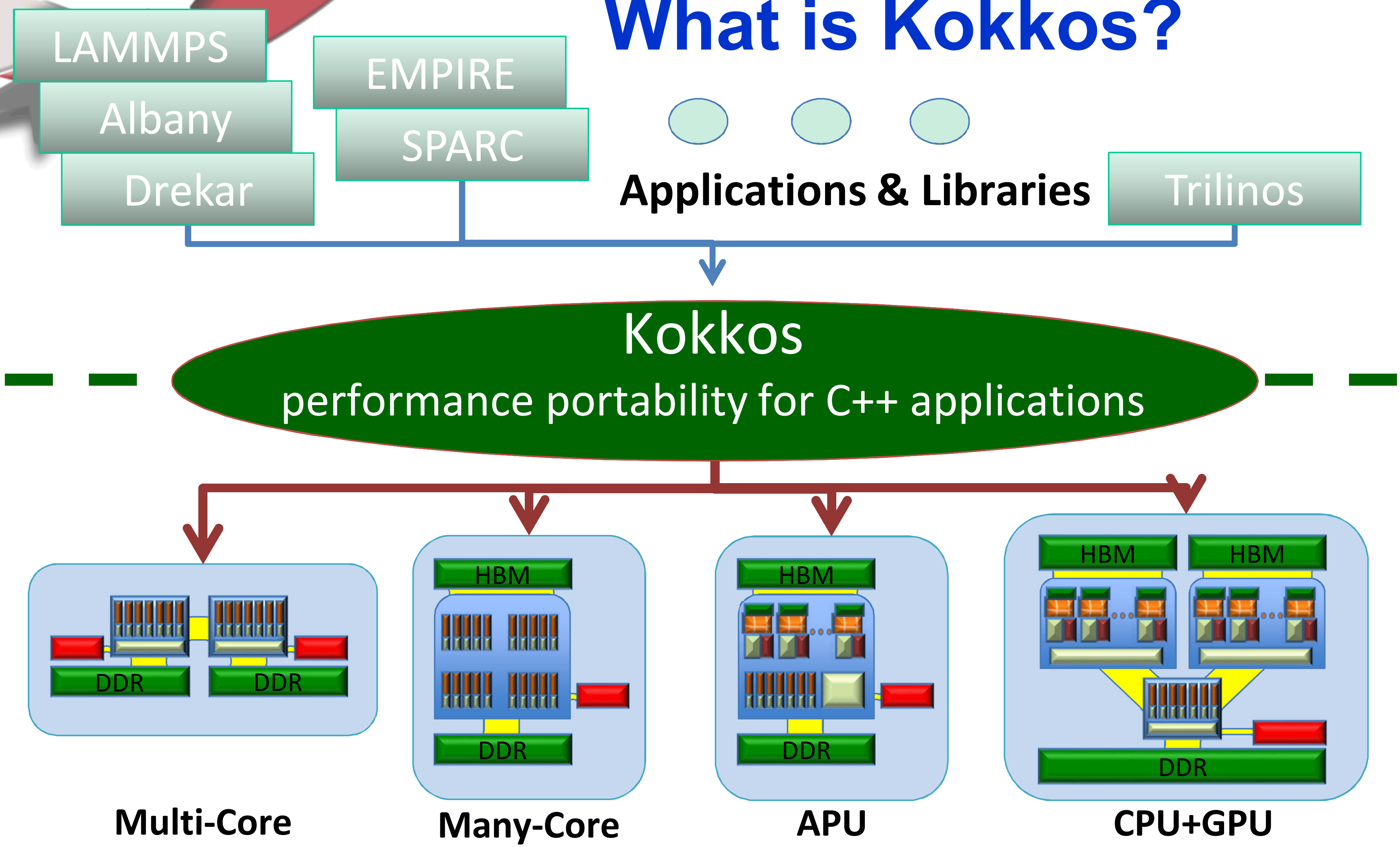
What is Kokkos?



Cornerstone for performance portability across next generation HPC architectures at multiple DOE laboratories, and other organizations.

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Abstractions
Patterns, Policies, and Spaces

- **Parallel Pattern** of user's computations
  - parallel_for, parallel_reduce, parallel_scan, task-graph, ... *(extensible)*
- **Execution Policy** tells *how* user computation will execute
  - Static scheduling, dynamic scheduling, thread-teams, ... *(extensible)*
- **Execution Space** tells *where* computations will execute
  - Which cores, numa region, GPU, ... *(extensible)*
- **Memory Space** tells *where* user data resides
  - Host memory, GPU memory, high bandwidth memory, ... *(extensible)*
- **Layout** (policy) tells *how* user array data is laid out
  - Row-major, column-major, array-of-struct, struct-of-array … *(extensible)*
- Differentiating: Layout and Memory Space
  - Versus other programming models (OpenMP, OpenACC, …)
  - Critical for performance portability …

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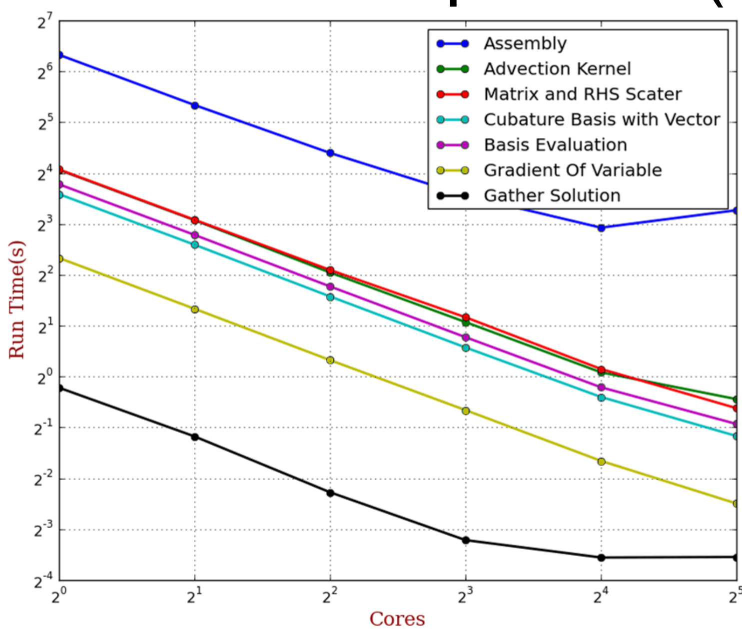
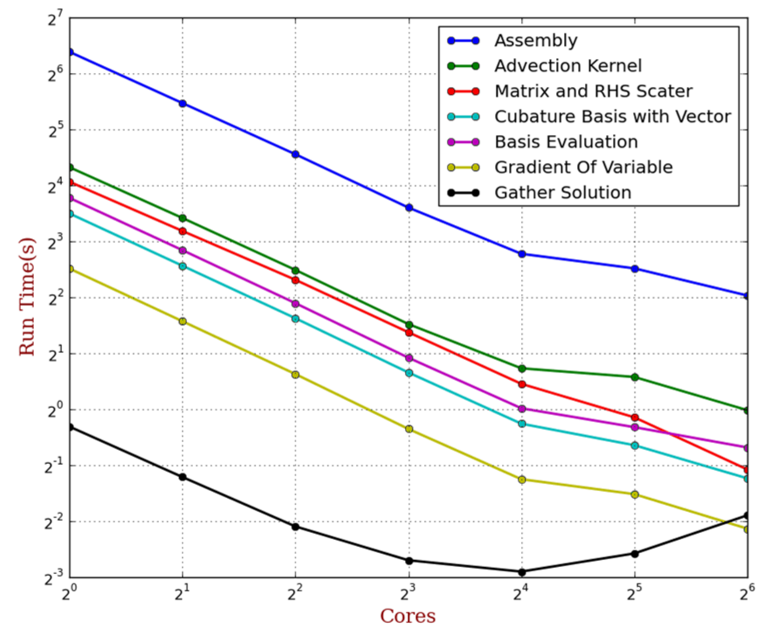
Threading
Traditional Architectures

- The gather, math routines and scatter operations were all threaded
- MPI only (left) was compared to Kokkos::OpenMP (right) on 16000 elements





Run on a dual 16 core Haswell with hyperthreading. Left result uses one socket for 1 to 32 cores and MPI across sockets. MPI results show the average time across MPI ranks. 156k total degrees of freedom. Time is for Jacobian assembly only.

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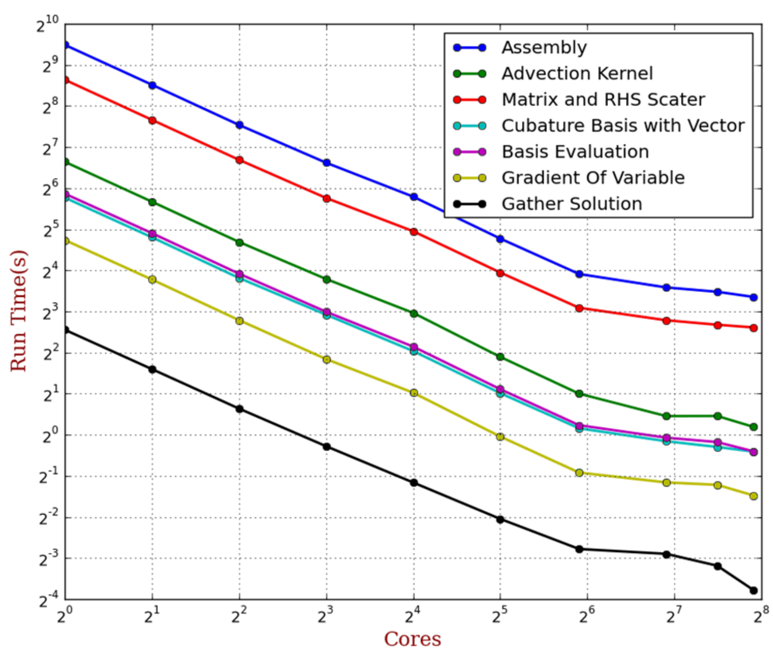
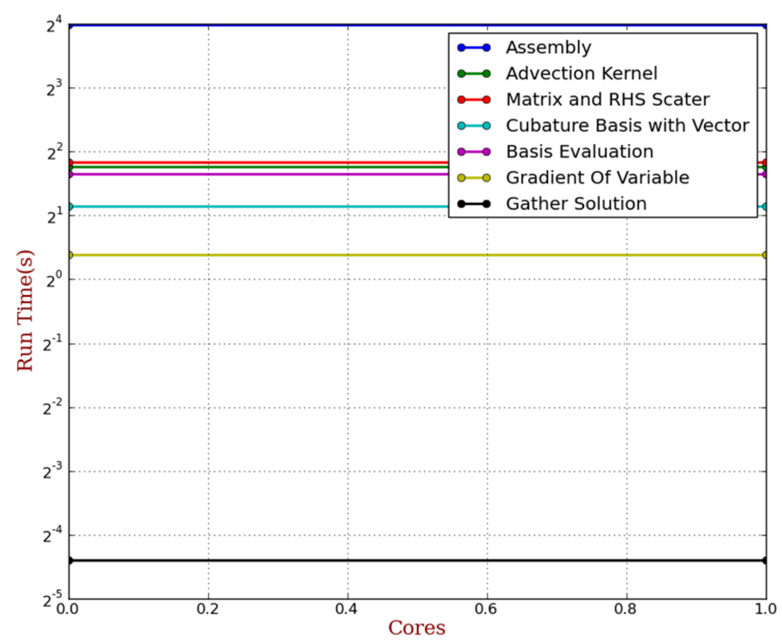
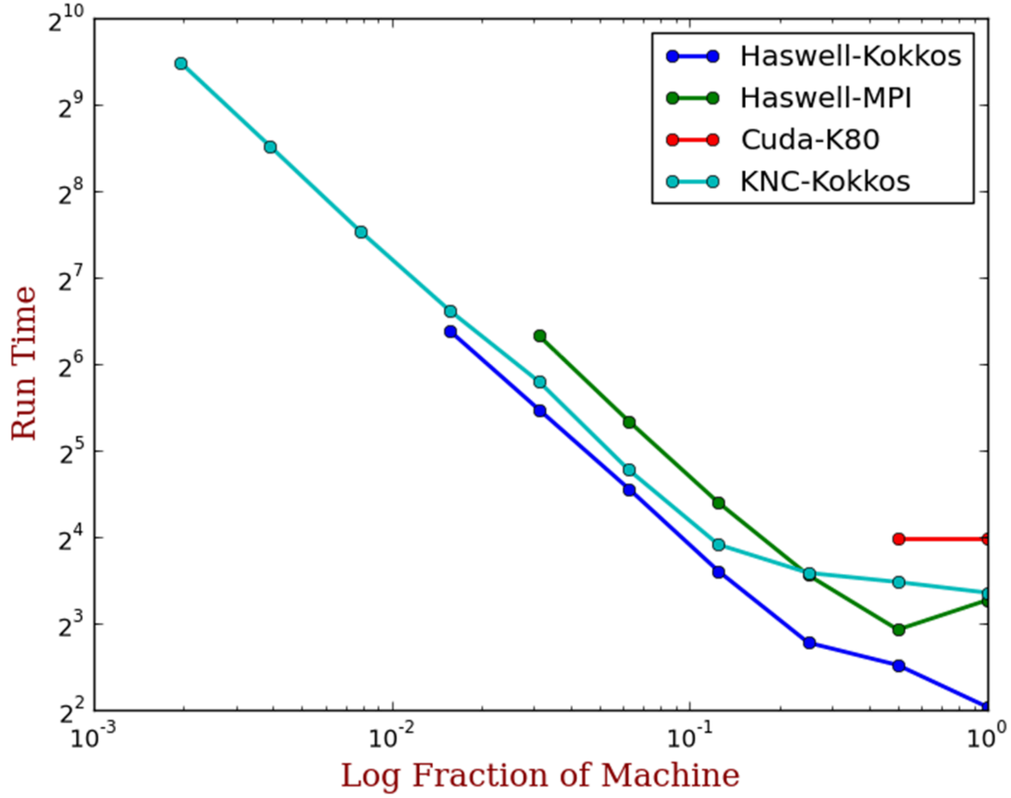
Threading
Modern Architectures

- Kokkos allows one to migrate to new machines and backends
  - Only recompilation is required to move to Intel's Knights Corner (left) or Nvidia K80 via Cuda (right)





Summary
Threading Results

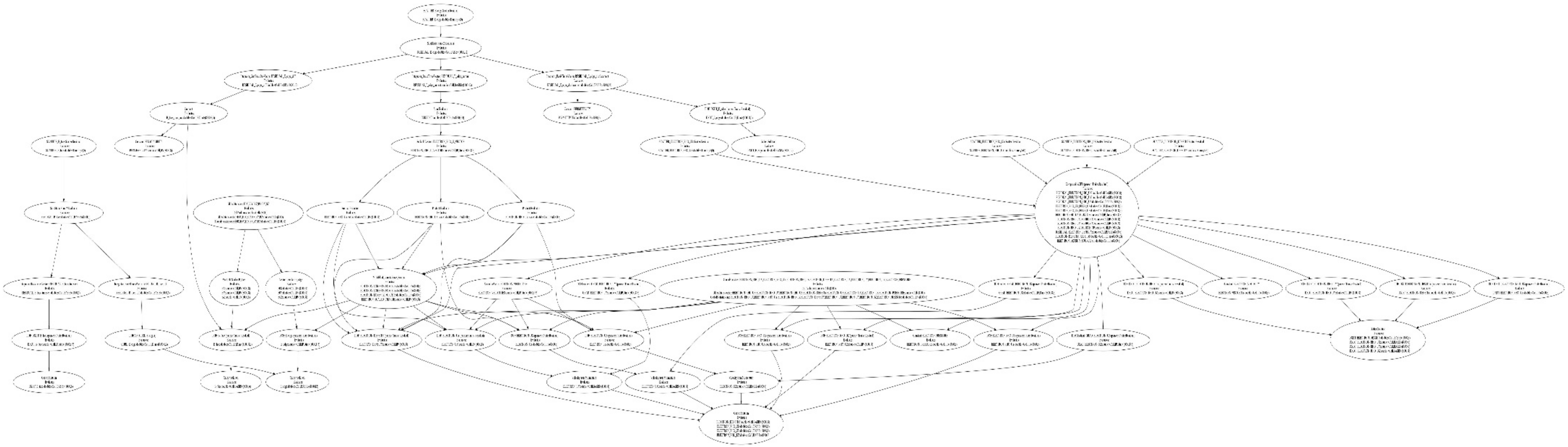


Beyond Threading

- Threading accelerates each individual math kernel
  - Eventually there is insufficient work in a single kernel to use all the threads efficiently
- Task parallelism
  - Chunks of threads solve different kernels
  - The wider the graph, the more task parallelism
  - Asynchronous Many Task (AMT) is an active research area in scheduling these tasks
    - HPX, DHARMA, Charm++, Legion, …

Task Parallelism
Single Fluid

Real DAG much more complex than the previous toy example



Theoretical speed up for this DAG

	1 Thread/Kernel	8 Threads/Kernel	16 Threads/Kernel
Jacobian	3.5	4.5	4.9
Residual	3.4	3.4	3.5

Summary
Next Steps

- Assembly performance can be improved with both threading and task parallelism
  - Threading shows up-to 64x speed up
  - Need to demonstrate these two approaches together
- Cuda parallelism performance lower than expected
  - Not enough parallelism per workset
    - Need bigger workset, however, limited memory
  - Need to implement hierarchical parallelism
- Kokkos makes thread parallelism easier
  - Need to incorporate Kokkos further