Improving Uintah's Scalability Through the Use of Portable Kokkos-Based Data Parallel Tasks

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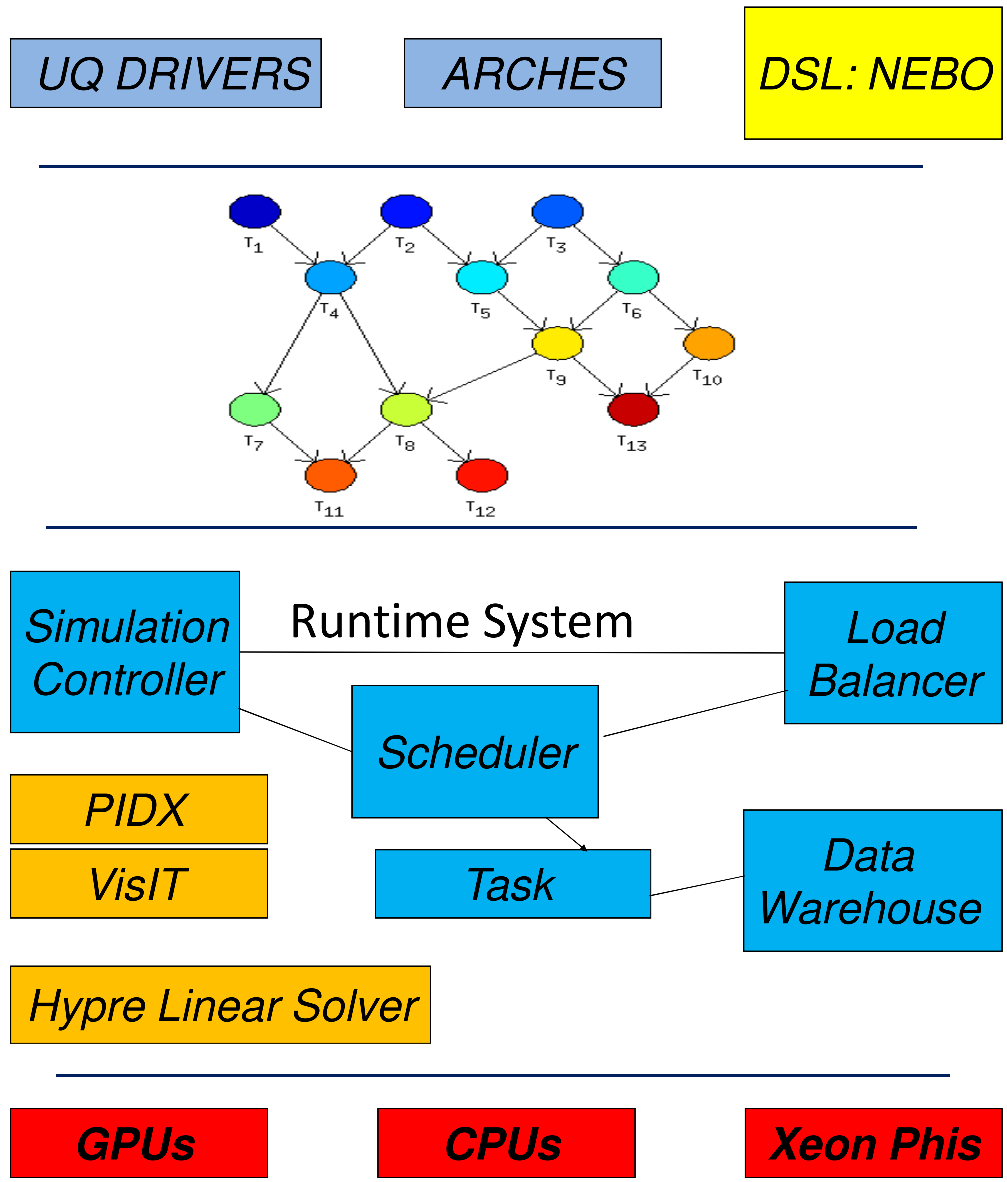
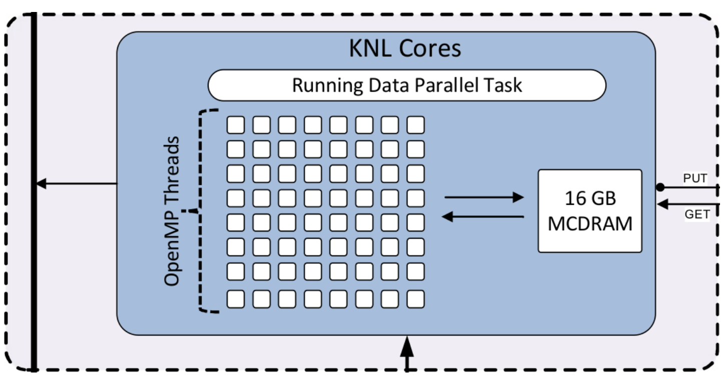
- Open source software
  - Worldwide distribution
  - Broad user base
- Applications code programming model
  - Physics routines unaware of communications
- Automatically generated abstract C++ task graph
- Adaptive execution of tasks by the runtime system
  - Asynchronous out-of-order execution,
  - work stealing,
  - overlapping of communication & computation

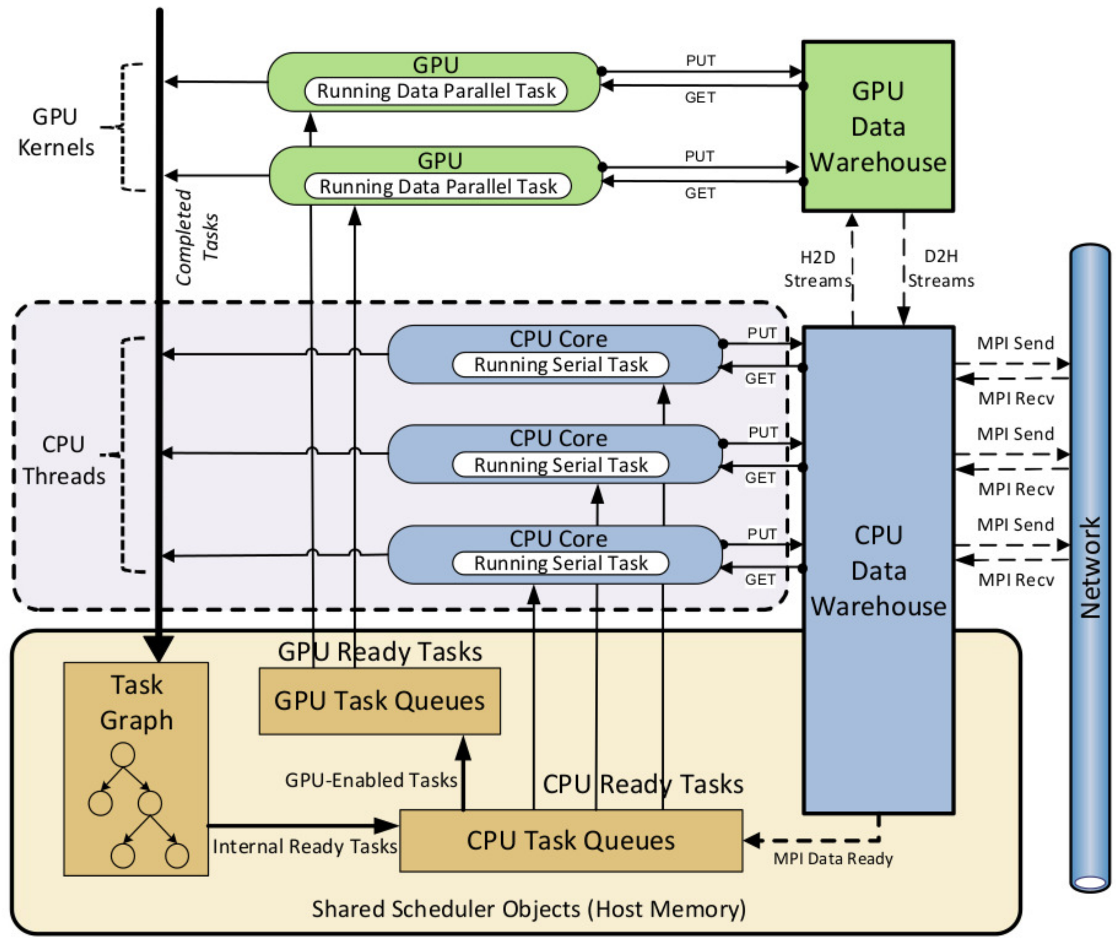
Uintah Architecture



Uintah's Heterogeneous Runtime System

- MPI+X schedulers support:
  - MPI + PThreads + CUDA
  - MPI + Kokkos
- Shared memory model on-node
  - 1 MPI process per node

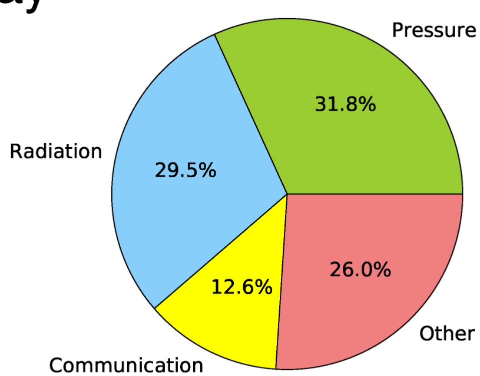


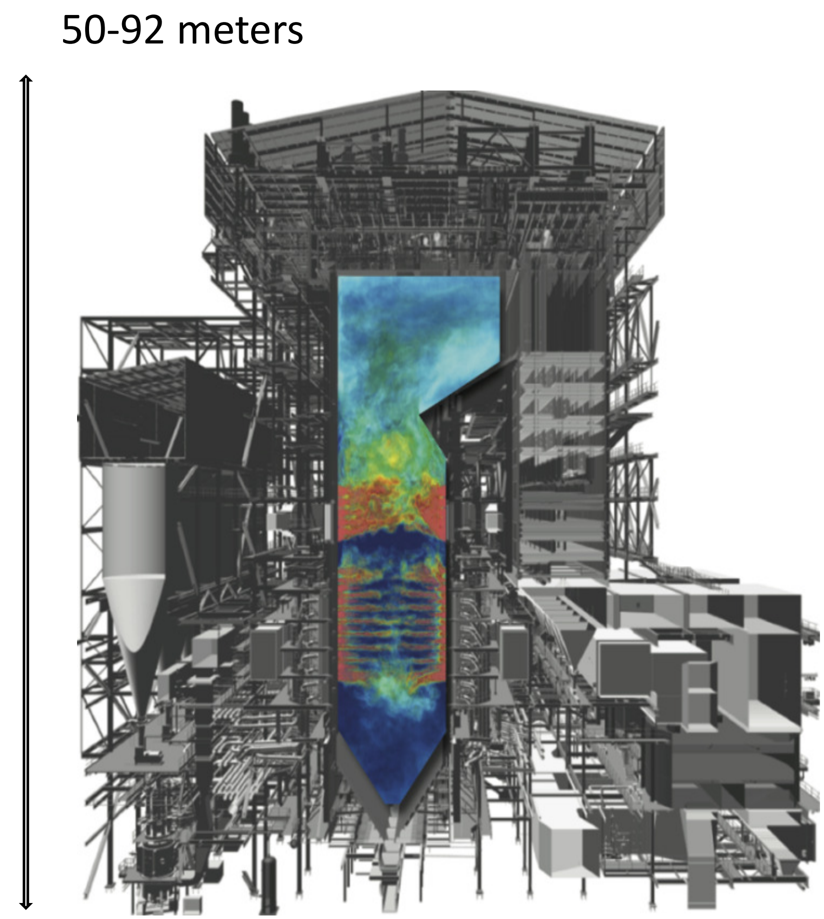


Exascale Target Problem

DOE NNSA PSAAP II Center

- Modeling an Alstom Power 1000MWe ultra, supercritical clean coal boiler at scale with Uintah
- Supply power for 1M people
- Targeted 1mm grid resolution = 9×10^{12} cells
- Significantly larger than largest problems solved today





Radiation Overview

- Solving **energy** and **radiative heat transfer** equations simultaneously

$$\frac{\partial T}{\partial t} = \text{Diffusion} - \text{Convection} + \text{Source/Sinks}$$

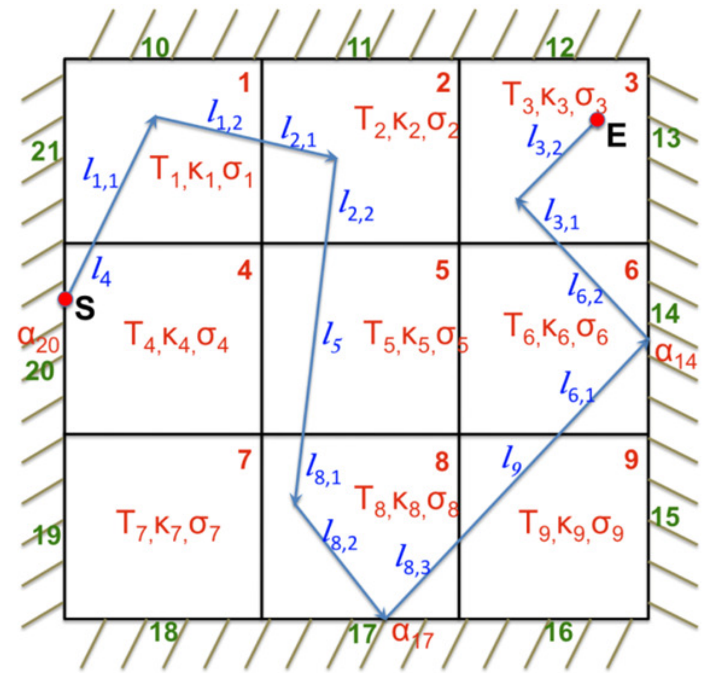
$$\nabla \cdot q$$

- Need to compute the **net radiative source term**
- The **net radiative source term** consists of *two terms*, one of which requires integration of incoming intensity about a sphere
  - RMCRT approximates the second term using Monte-Carlo methods

$$\int_{4\pi} I_{in} d\Omega \Rightarrow \sum_{ray=1}^{N} I_{ray} \frac{4\pi}{N}$$

Reverse Monte Carlo Ray Tracing

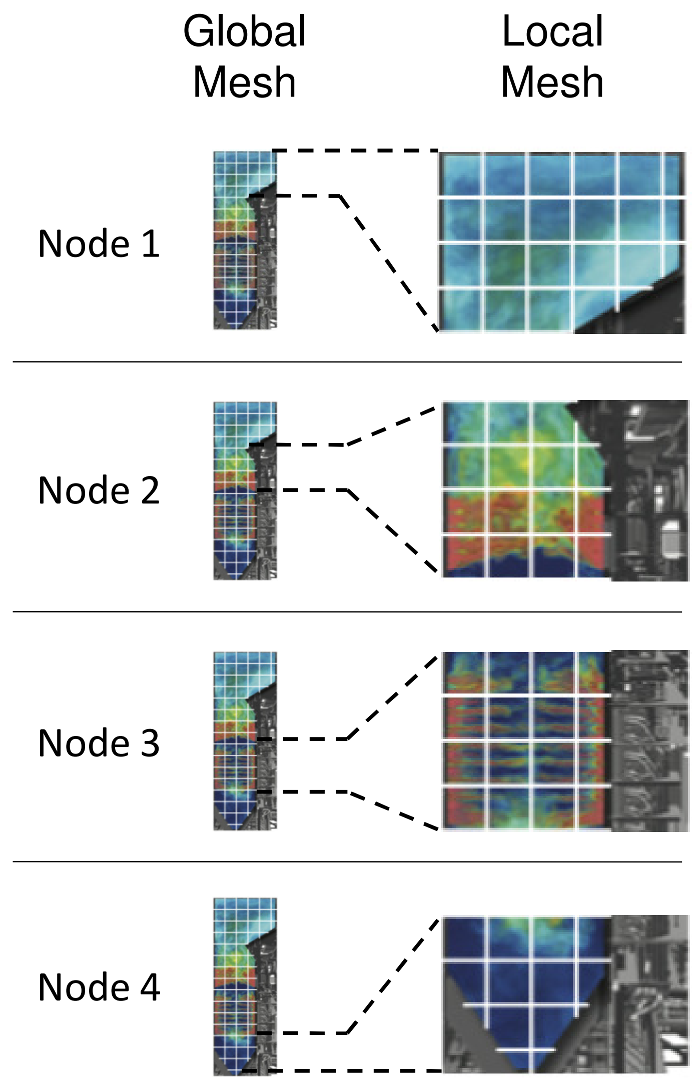
- Randomly cast rays to compute the incoming intensity absorbed by a given cell
- Rays are traced *away from* the origin cell to compute incoming intensity *backwards to* the origin cell
- When marching rays, each cell entered adds its contribution to the incoming intensity absorbed by the origin cell
- The further a ray is traced, the smaller the contribution becomes



Back path of ray from **S** to emitter **E**, 9-cell structured mesh patch

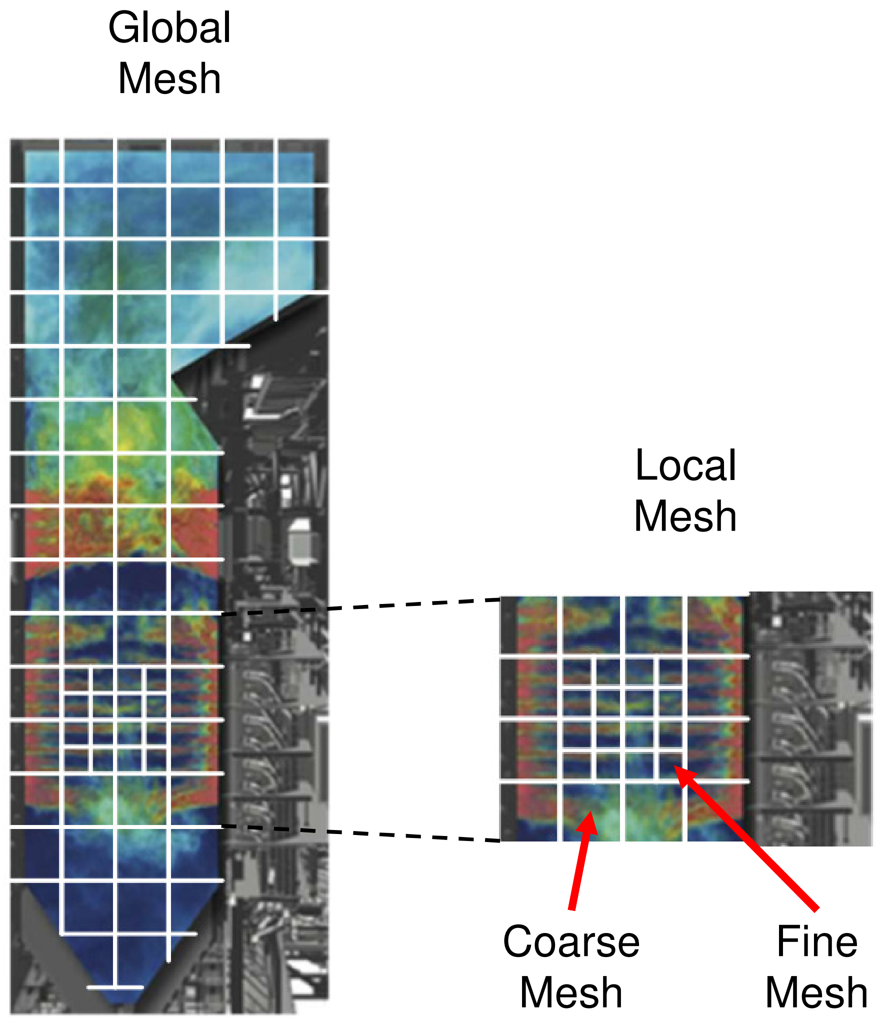
Parallel Reverse Monte Carlo Ray Tracing

- Lends itself to scalable parallelism
  - Rays are mutually exclusive
  - Multiple rays can be traced simultaneously at any given cell and/or timestep
  - Backwards approach eliminates the need to track rays that never reach an origin cell
- Parallelize by splitting the computational domain across compute nodes
- Each node is responsible for tracing rays from within each origin cell that it owns across the entire domain
- Nodes must communicate and store geometry information and physics properties for the entire domain



Multi-Level AMR RMCRT

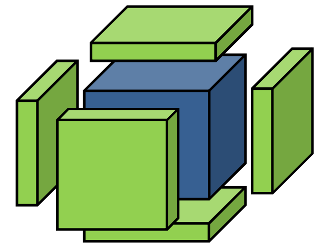
- Global approach involves too much communication
- Use a multilevel representation of computational domain
  - Reduces computational cost, memory usage, and MPI message volume
- Define Region of Interest (ROI), which is surrounded by successively coarser grids
- As rays travel away from ROI, the stride taken between cells becomes larger

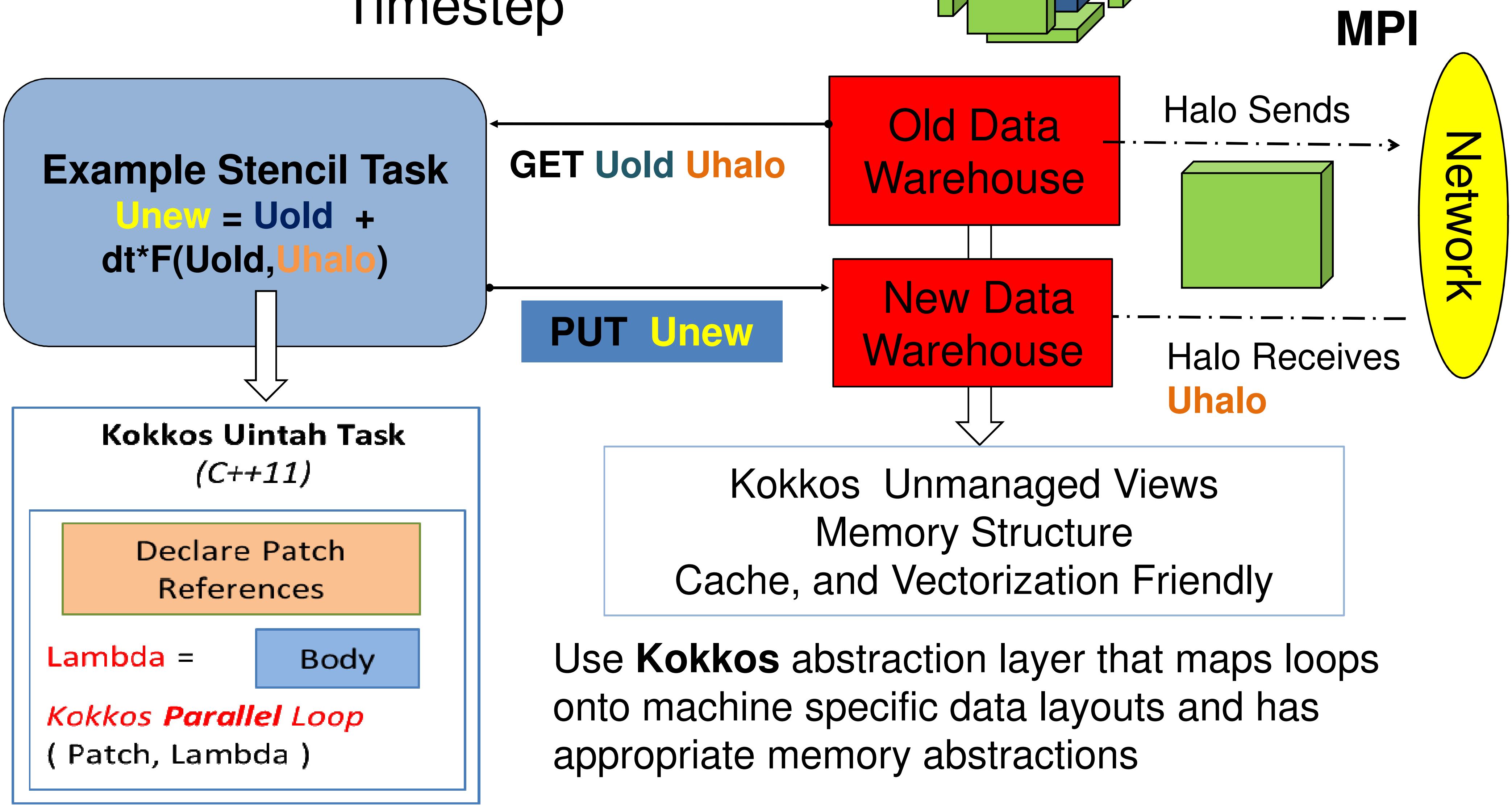


Kokkos Performance Portability Library

- C++ library allowing developers to write portable, thread-scalable code optimized for CPU-, GPU-, and MIC-based architectures
- Kokkos provides abstractions to control:
  - how/where kernels are executed,
  - where data is allocated, and
  - how data is mapped to memory
- While Kokkos enables performance portability, the user is responsible for writing performant kernels
- Source Available at: https://github.com/kokkos/kokkos

Uintah Programing Model for Stencil Timestep





Use **Kokkos** abstraction layer that maps loops onto machine specific data layouts and has appropriate memory abstractions

Kokkos-Based RMCRT

- CPU-, GPU-, and MIC-based RMCRT efforts have resulted in several different implementations

- Introduced RMCRT:Kokkos to consolidate implementations
  - Encapsulated “hot spots” within a Kokkos functor

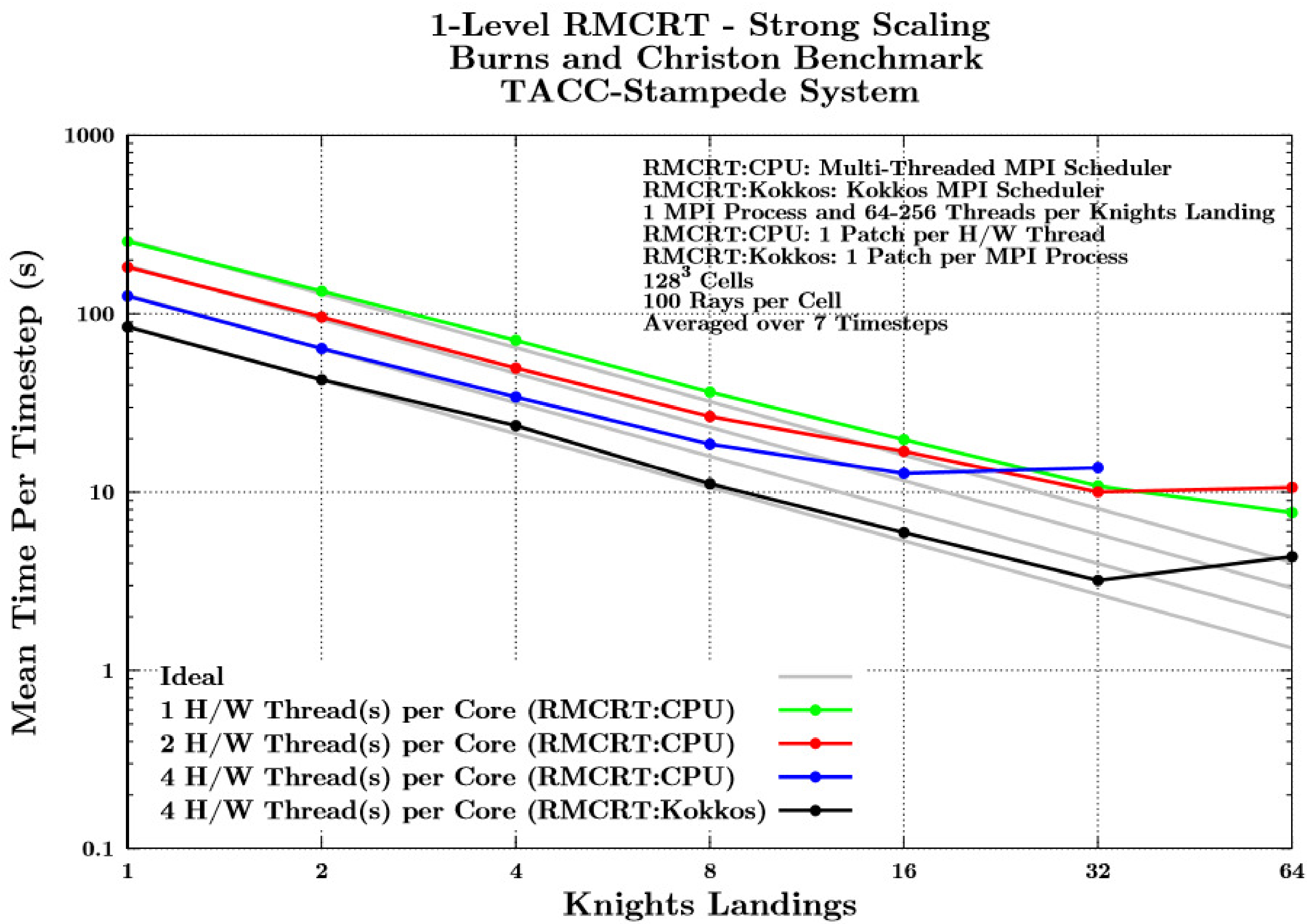
- This new implementation:
  - Required < 100 lines of new code
  - Replaces a naïve cell iterator with a Kokkos parallel loop, enabling the selection of optimal iteration schemes via Kokkos
  - Enables multi-threaded task execution via Kokkos back-ends

Node-Level Parallelism Within Uintah

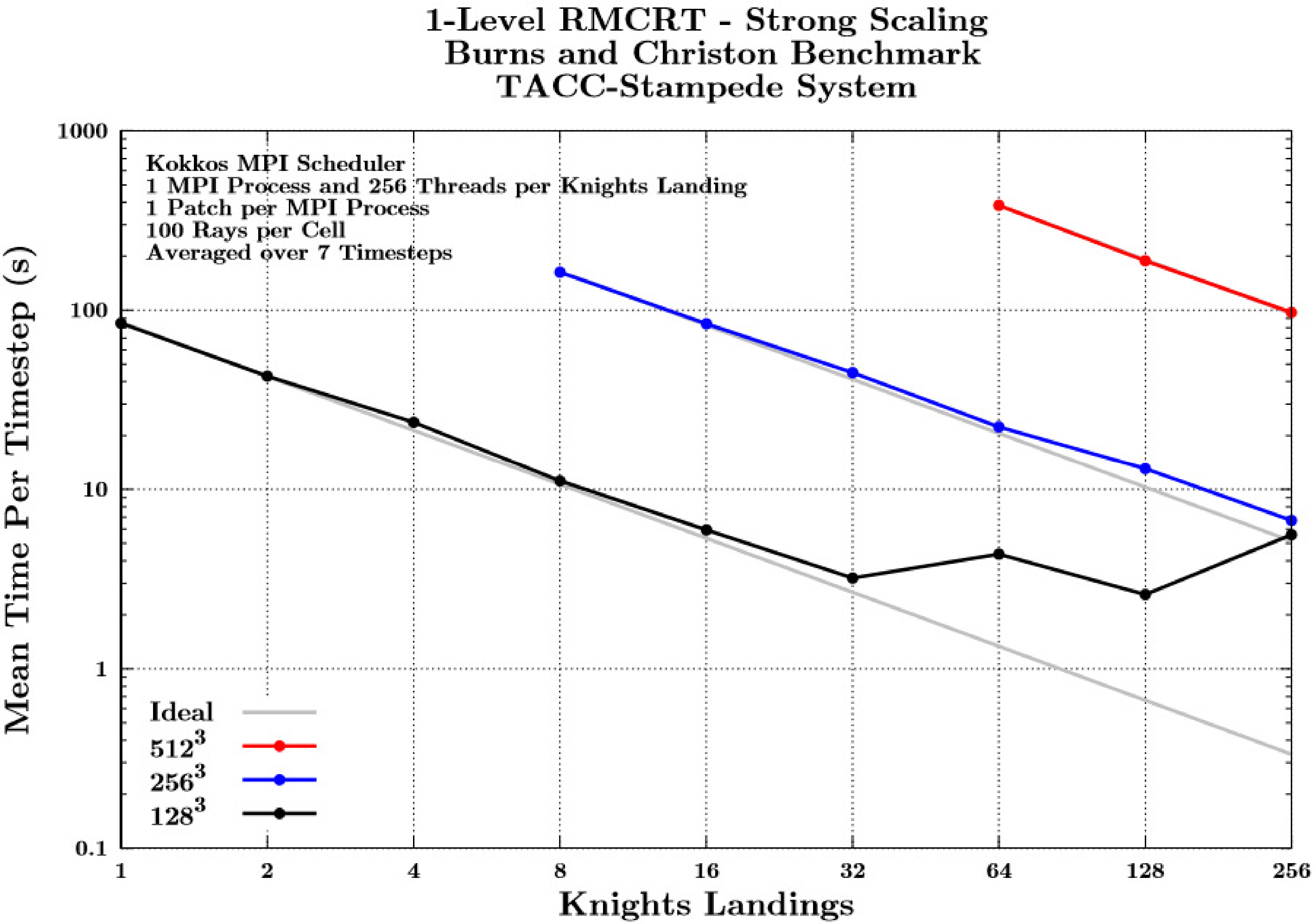
- For CPU and MIC architectures, Uintah features **parallel execution of serial tasks**
  - 1 running task per thread
  - Requires at least 1 patch per thread
  - Breaks down as patches are subdivided to support more threads/cores

- Current Kokkos-based scheduler features **serial execution of data parallel tasks**
  - 1 running task per MPI process
  - Requires at least 1 patch per MPI process
  - Eliminates the need to create a new patch to run with another thread

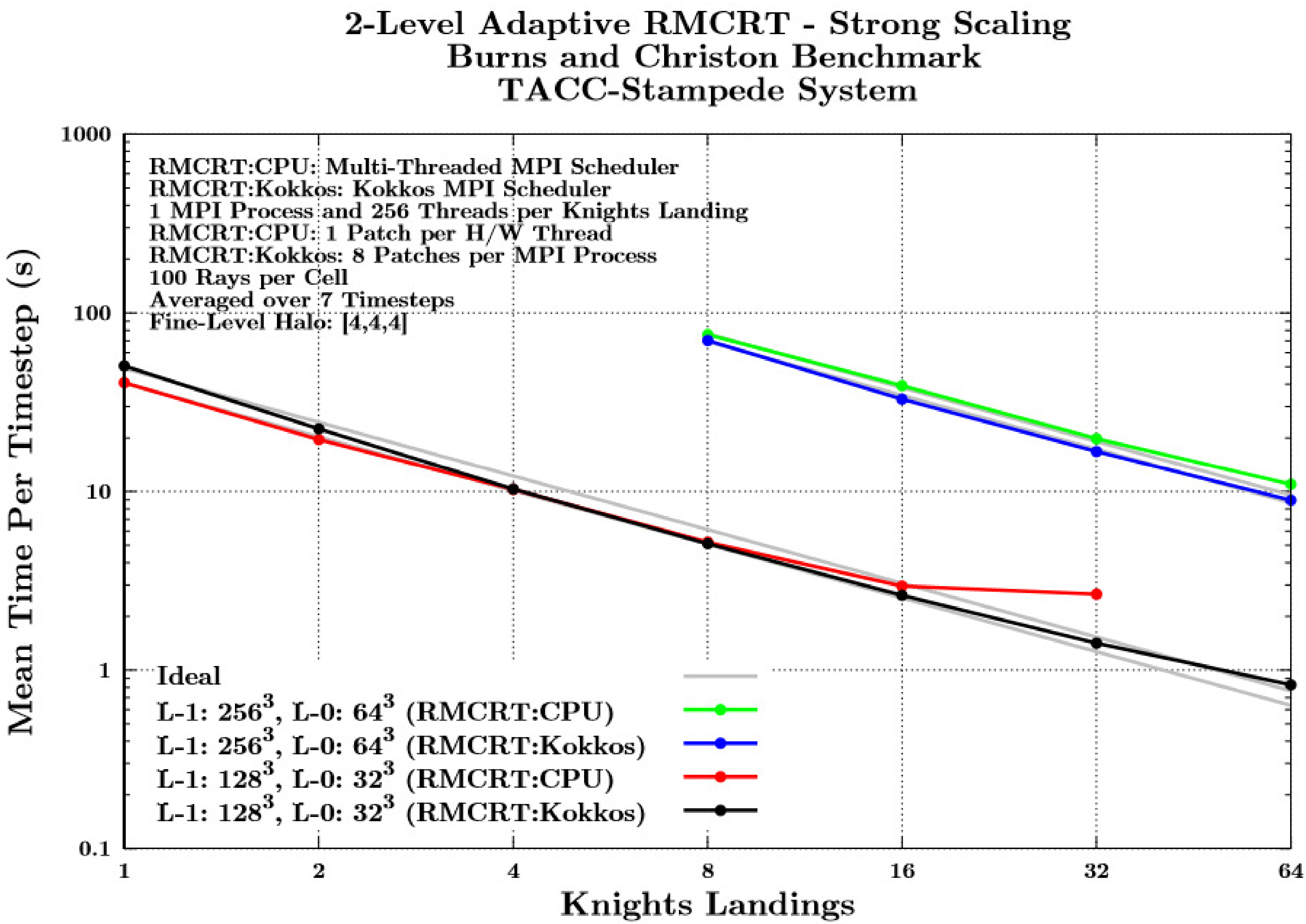
- Next step is a Kokkos-based scheduler w/ **parallel execution of data parallel tasks**
  - We already do this for GPU but not for CPU and MIC

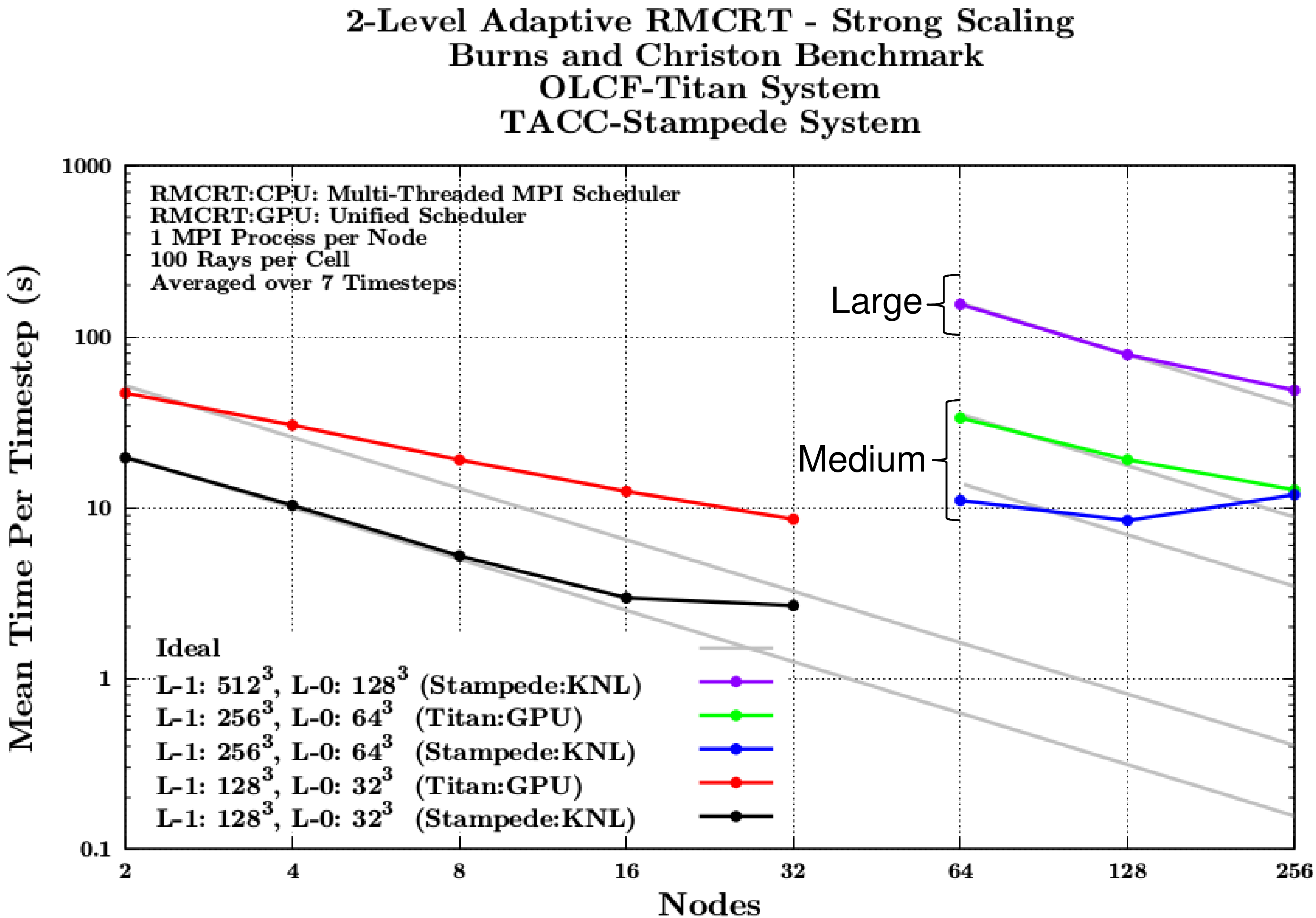


1-Level RMCRT - Strong Scaling
Burns and Christon Benchmark
TACC-Stampede System
RMCRT:CPU: Multi-Threaded MPI Scheduler
RMCRT:Kokkos: Kokkos MPI Scheduler
1 MPI Process and 64-256 Threads per Knights Landing
RMCRT:CPU: 1 Patch per H/W Thread
RMCRT:Kokkos: 1 Patch per MPI Process
128^3 Cells
100 Rays per Cell
Averaged over 7 Timesteps
Mean Time Per Timestep (s)
1000
100
10
1
0.1
1
2
4
8
16
32
64
Knights Landings
Ideal
1 H/W Thread(s) per Core (RMCRT:CPU)
2 H/W Thread(s) per Core (RMCRT:CPU)
4 H/W Thread(s) per Core (RMCRT:CPU)
4 H/W Thread(s) per Core (RMCRT:Kokkos)



1-Level RMCRT - Strong Scaling
Burns and Christon Benchmark
TACC-Stampede System
Kokkos MPI Scheduler
1 MPI Process and 256 Threads per Knights Landing
1 Patch per MPI Process
100 Rays per Cell
Averaged over 7 Timesteps
Mean Time Per Timestep (s)
1000
100
10
1
0.1
1
2
4
8
16
32
64
128
256
Knights Landings
Ideal
512^3
256^3
128^3


2-Level Adaptive RMCRT - Strong Scaling
Burns and Christon Benchmark
TACC-Stampede System
RMCRT:CPU: Multi-Threaded MPI Scheduler
RMCRT:Kokkos: Kokkos MPI Scheduler
1 MPI Process and 256 Threads per Knights Landing
RMCRT:CPU: 1 Patch per H/W Thread
RMCRT:Kokkos: 8 Patches per MPI Process
100 Rays per Cell
Averaged over 7 Timesteps
Fine-Level Halo: [4,4,4]
Ideal
L-1: 256^3, L-0: 64^3 (RMCRT:CPU)
L-1: 256^3, L-0: 64^3 (RMCRT:Kokkos)
L-1: 128^3, L-0: 32^3 (RMCRT:CPU)
L-1: 128^3, L-0: 32^3 (RMCRT:Kokkos)
Mean Time Per Timestep (s)
Knights Landings
1000
100
10
1
0.1
1
2
4
8
16
32
64


2-Level Adaptive RMCRT - Strong Scaling
Burns and Christon Benchmark
OLCF-Titan System
TACC-Stampede System
RMCRT:CPU: Multi-Threaded MPI Scheduler
RMCRT:GPU: Unified Scheduler
1 MPI Process per Node
100 Rays per Cell
Averaged over 7 Timesteps
Large
Medium
Mean Time Per Timestep (s)
Nodes
1000
100
10
1
0.1
2
4
8
16
32
64
128
256
Ideal
L-1: 512^3, L-0: 128^3 (Stampede:KNL)
L-1: 256^3, L-0: 64^3 (Titan:GPU)
L-1: 256^3, L-0: 64^3 (Stampede:KNL)
L-1: 128^3, L-0: 32^3 (Titan:GPU)
L-1: 128^3, L-0: 32^3 (Stampede:KNL)

Summary

- Data parallel tasks for CPU- and MIC-based architectures allow Uintah to support larger thread/core counts per node
- Data parallel tasks offer the potential to improve microarchitecture use (e.g. per-patch work can be computed cooperatively by multiple threads sharing a cache)
- Use of Kokkos allows data parallel tasks to be introduced in a portable manner
  - Helps avoid code divergence and architecture-specific implementations
  - Reduces the gap between development time and our ability to run on newly introduced machines
- Titan comparisons offer encouragement as we prepare for the Aurora Early Science Program

Questions?

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Uintah Download: **http://www.uintah.utah.edu**

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