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SAND2014-4608C

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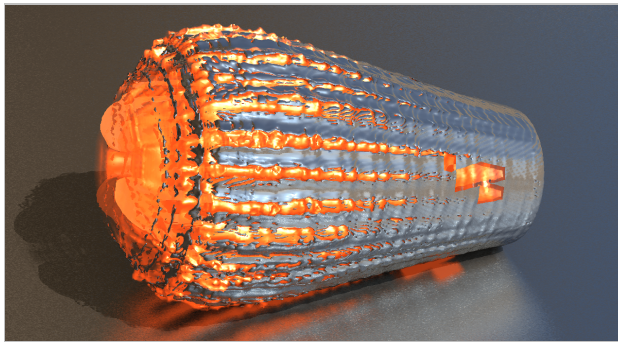
CATALYST
scalable in-situ analysis



Evaluation of Methods to Integrate Analysis into a Large-Scale Shock Physics Code

Ron A. Oldfield, Ken Moreland, Nathan Fabian
Sandia National Laboratories

David Rogers
Los Alamos National Laboratory

Approved for Public Release: SAND2014-XXXX

U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

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Extreme-Scale Computing

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- Trends: More FLOPS with comparatively less storage, I/O bandwidth
  - Consequence: A smaller fraction of data can be captured on disk

Oak Ridge National Laboratory

	System Peak	I/O BW
Jaguar (2008)	263 TFLOPS	44 GB/s
Jaguar PF (2009)	1.75 PFLOPS	240 GB/s
Titan (2012)	20 PFLOPS	240 GB/s
Factor Change	76×	5.5×

Bland, Kendall, Kothe, Rogers, and Shipman. "Jaguar: The World's Most Powerful Computer"
http://archive.hpcwire.com/hpcwire/2012-10-29/titan_sets_high-water_mark_for_gpu_supercomputing.html?featured=top

Argonne National Laboratory

	System Peak	I/O BW
Intrepid (2003)	560 TFLOPS	88 GB/s
Mira (2011)	10 PFLOPS	240 GB/s
Factor Change	17.8×	2.7×

https://www.alcf.anl.gov/intrepid
https://www.alcf.anl.gov/mira

Lawrence Livermore National Laboratory

	System Peak	I/O BW
ASC Purple (2005)	100 TFLOPS	106 GB/s
Sequoia (2012)	20 PFLOPS	1 TB/s
Factor Change	200×	9.4×

http://www.sandia.gov/supercomp/sc2002/flyers/SC02ASCIPurplev4.pdf
https://asc.llnl.gov/publications/Sequoia2012.pdf

Sandia National Laboratories

	System Peak	I/O BW
Red Storm (2003)	180 TFLOPS	100 GB/s
Cielo (2011)	1.4 PFLOPS	160 GB/s
Factor Change	7.8×	1.6×

https://cfwebprod.sandia.gov/cfdocs/CCIM/docs/033768p.pdf
http://www.lanl.gov/orgs/hpc/cielo/

Usage Models Conflict with Trends

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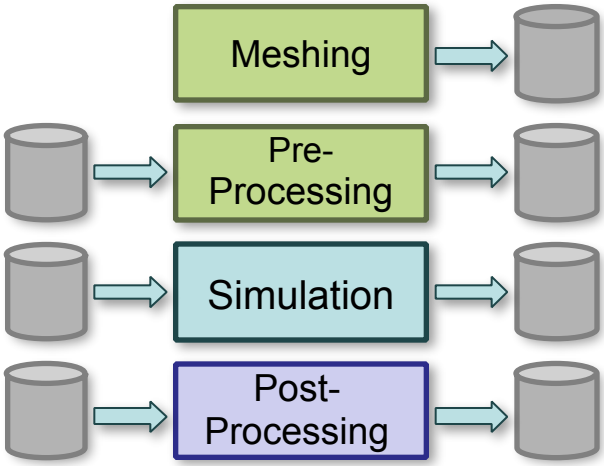
Application Workflows historically use storage system for communication



- One way to relieve I/O pressure is to integrate simulation and analysis
  1. ***In-situ processing*** provides "tightly coupled" analysis through libraries linked directly with the simulation.
  2. ***In-transit processing*** provides "loosely coupled" analysis by performing analysis on separate processing resources.

This talk presents a detailed comparison of these approaches.

Pros/Cons for In Situ and In Transit

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- In situ
  - + Most common approach for integrating analysis
  - + Straight forward to use (just function calls)
  - + If implemented right, could reuse application data structures
  - – Synchronous (app must wait for viz to complete)
  - – May add significant memory, computation, comm requirements
  - – May cause concerns for stability, scalability, resilience.
- In transit
  - + Minimal client overhead (addresses resilience, scalability, …)
  - + Asynchronous (overlap computation and analysis)
  - + Analysis can execute in different environment (e.g., linux vs lwk)
  - – Requires additional compute resources
  - – New use case: more complicated to schedule, load balance, …

Our *In situ* and *in transit* workflows

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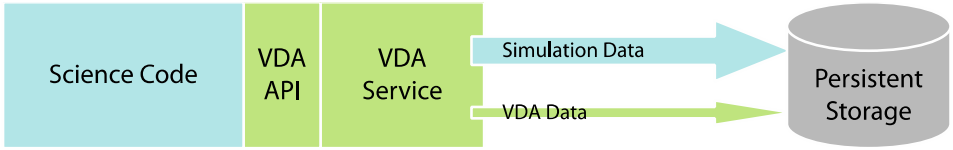
- Our ***In situ*** workflows uses *Catalyst*, an open source, VTK-based analysis library derived from ParaView.



- Our ***In transit*** workflows use the Network Scalable Service Interface (*Nessie*) to communicate with analysis services allocated on separate compute resources. Nessie is an open source data services library that is part of the Trilinos I/O Support package.

The science code uses the same API for both approaches, making comparison between the two approaches trivial.

Customer Driven Use Case

Characterize fragments in an explosion simulation

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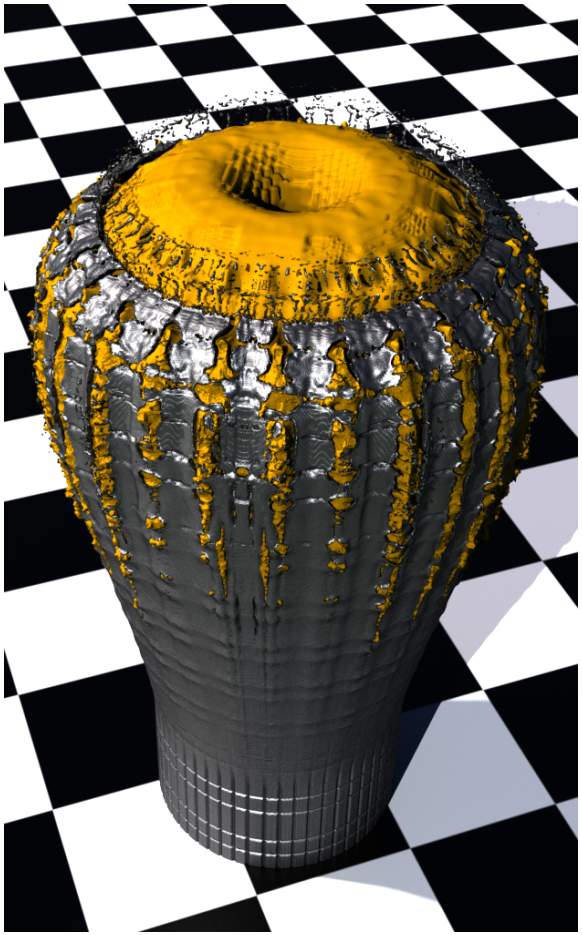
- An analysis step critical for understanding shock physics
- Partner: Jason Wilke – SNL Analyst
- Critical steps
  - Fragment detection (multiple operations required)
  - Characterize fragments (mass, velocity, etc.)
  - Extract useful information

Our e*xperiments focused on identifying the fragments*. This operation is a significantly complex part the analysis, so it serves as a useful way to characterize the operations in the driver use case.



Fragment detection

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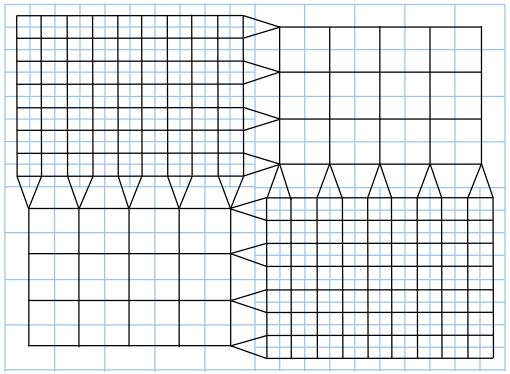
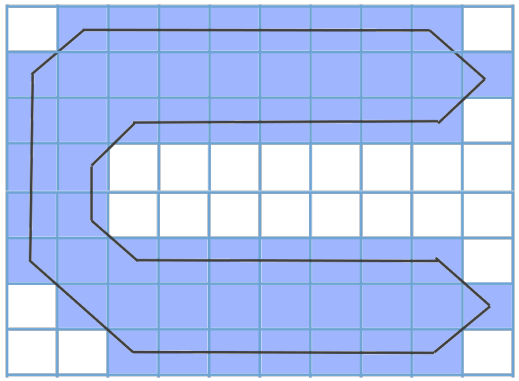
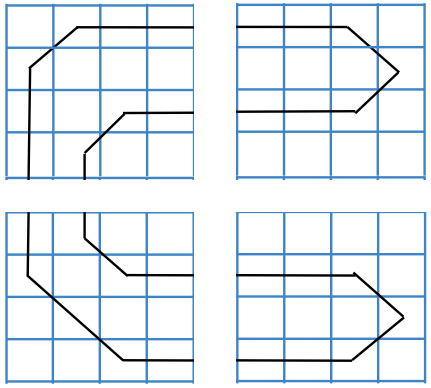
- Operations required for fragment detection (requires a watertight surface)
  1. Find block neighbors
  2. Build a conforming mesh over AMR boundaries
  3. Identify boundaries of fragments
  4. Find fragment components that are connected *(not in these experiments — **Now Complete!**)*



Step 2



Step 3



Step 4

Application Workflows

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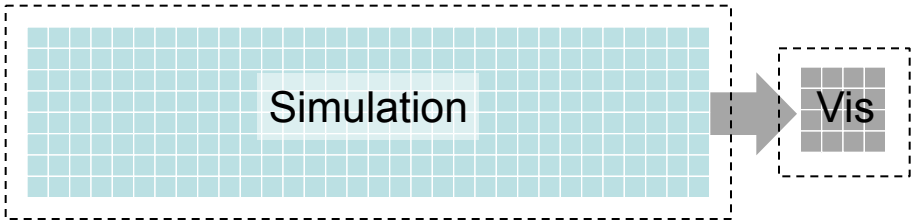
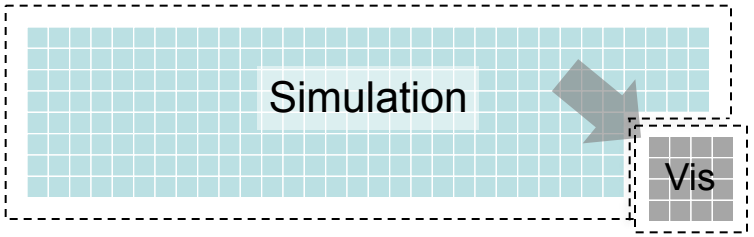
1. ***In situ baseline***: Global comm to find AMR block neighbors
2. ***In situ refined***: Gets AMR block neighbors from CTH.
3. ***In transit extra***: Extra nodes used for analysis
4. ***In transit internal***: Carve out nodes for analysis (less cores for CTH)
5. ***Disk-based post processing***: Traditional approach



In transit extra



In transit internal

In transit and post-processing workflows use baseline algorithm.

Experimental Setup

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- System: Cielo supercomputer at LANL
  - 8,944 node Cray XE6 (1.37 Petaflops peak)
  - Node: 2 AMD Opteron 6136 (Magny-Cours) 8-way processor chips
  - 32 GB memory/node
- Application: CTH (AMR) + Catalyst
  - 500 time steps of CTH
  - 51 analysis steps (approximately once every 10 time steps)
  - Five application workflows from previous slide
- Experiments
  - Strong scaling for three datasets: 33k blocks, 218k blocks, 1.5m blocks
  - Five runs for variance data
  - Data captured from instrumented code and HPCToolkit
  - Over 10m node hours for development, debugging, experiments.

Choosing the Number of Service Nodes

Memory Requirements for In Transit Service

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- Constraints given 32 GiB/node
  - Based on “trial and error” we found that one node can manage/process ~16K AMR blocks from CTH.
- Number of service nodes required for In Transit
  - 33k blocks: 2 nodes
  - 129k blocks: 16 nodes
  - 1.5m blocks: 100 nodes

Choosing the Number of Service Nodes

Computing Requirements for In Transit Service

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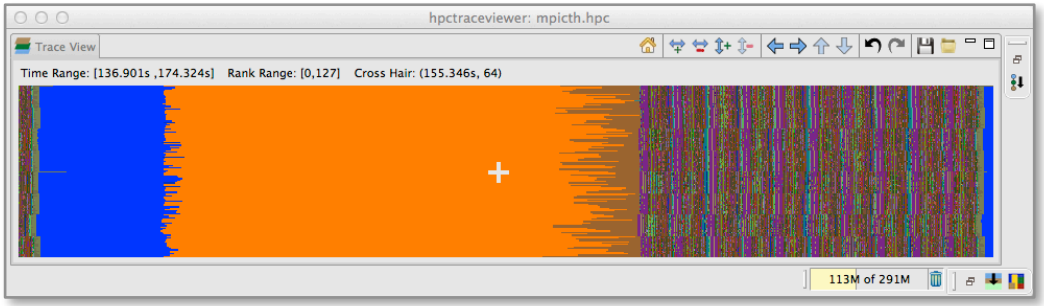
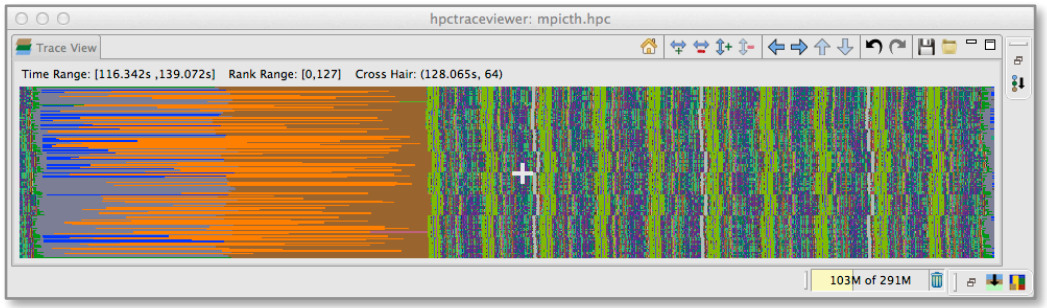
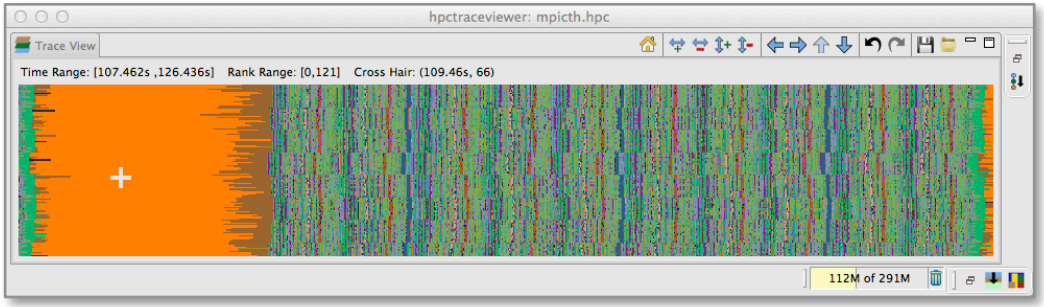
Wait for Server Transfer Data



2 server cores: 64:1
- 10 cycles in 37 secs
- Client idle waiting for servers (also affects xfers)



4 server cores: 32:1
- 10 cycles in 23 secs



8 server cores: 16:1
- 10 cycles in 19 secs
- Less than 1% time waiting

Total Runtime for All Experiments

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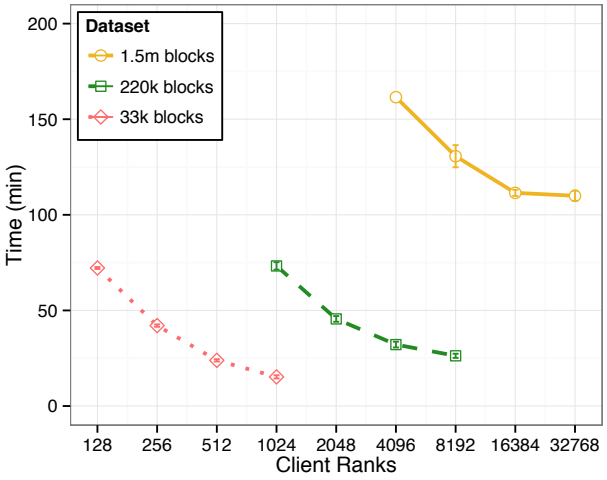
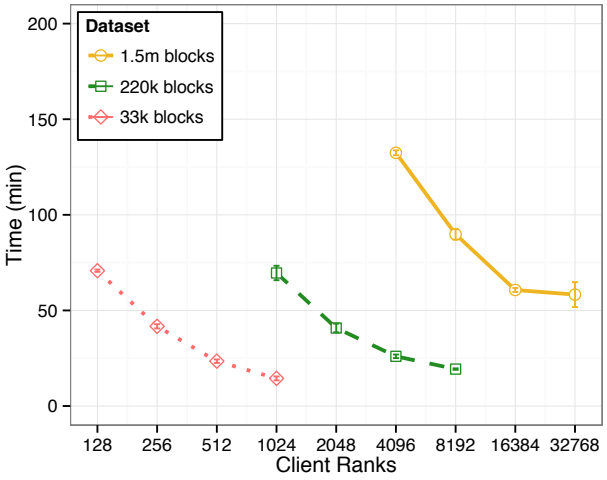
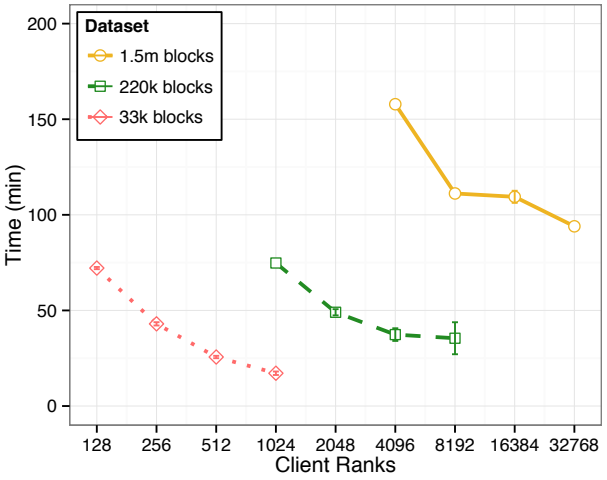


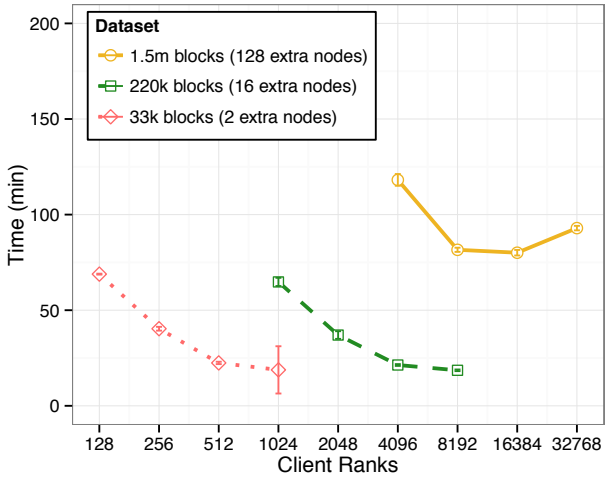
In situ baseline



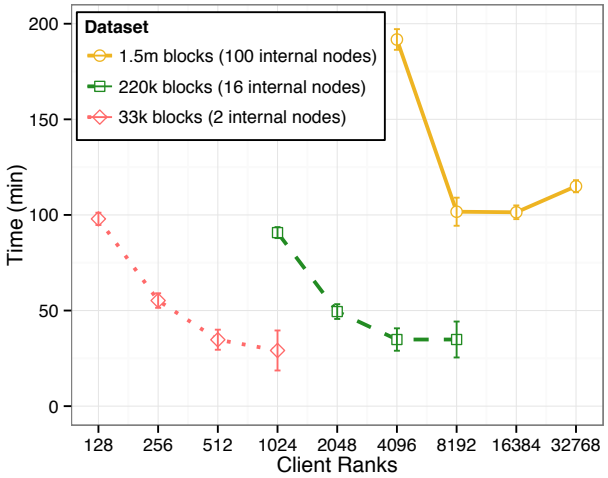
In situ refined



Disk-based post processing



In transit extra nodes



In transit internal nodes

5 applications
3 datasets

Strong scaling for each dataset

Error bars show variance

Summary Timing (1.5m blocks)

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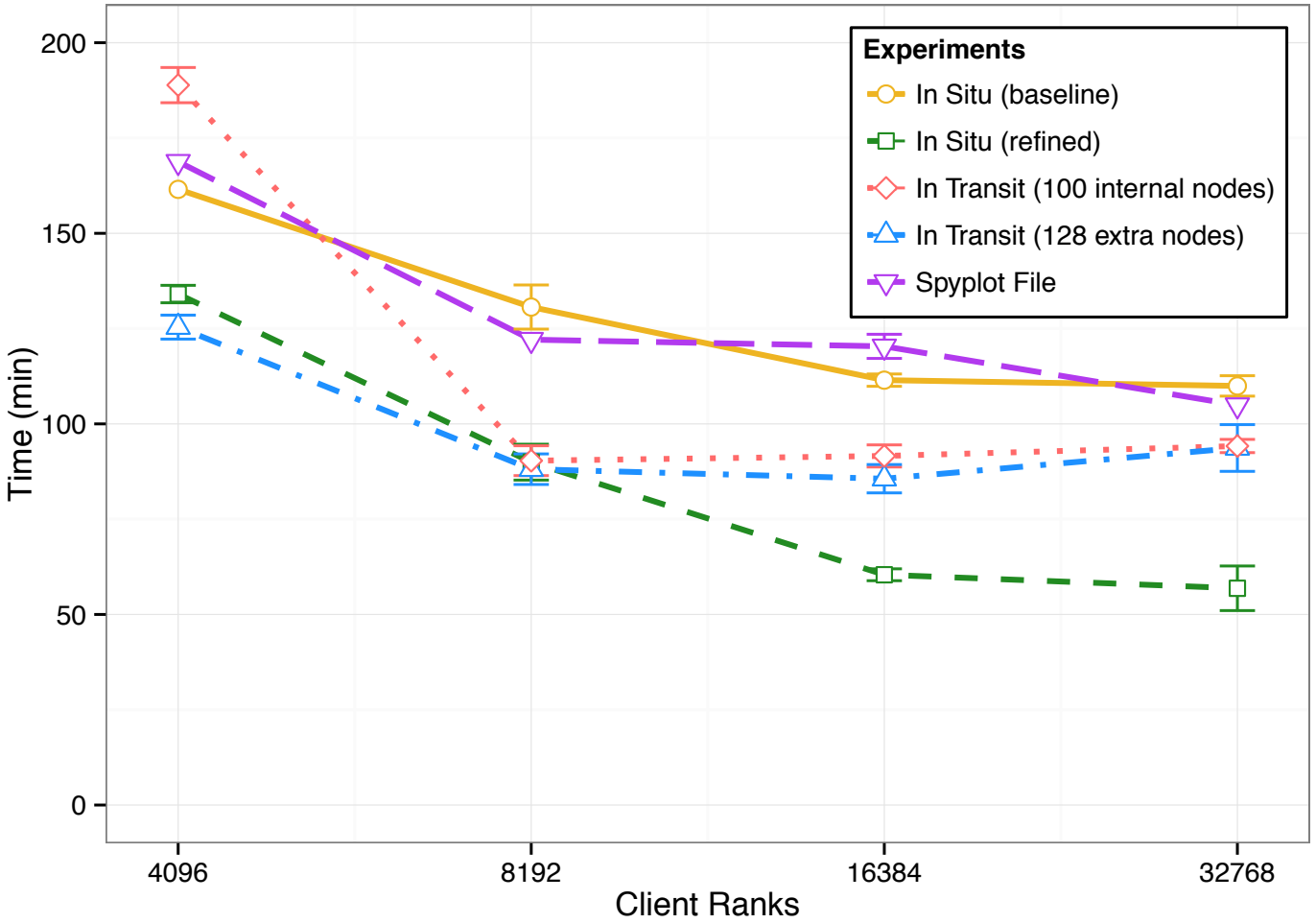
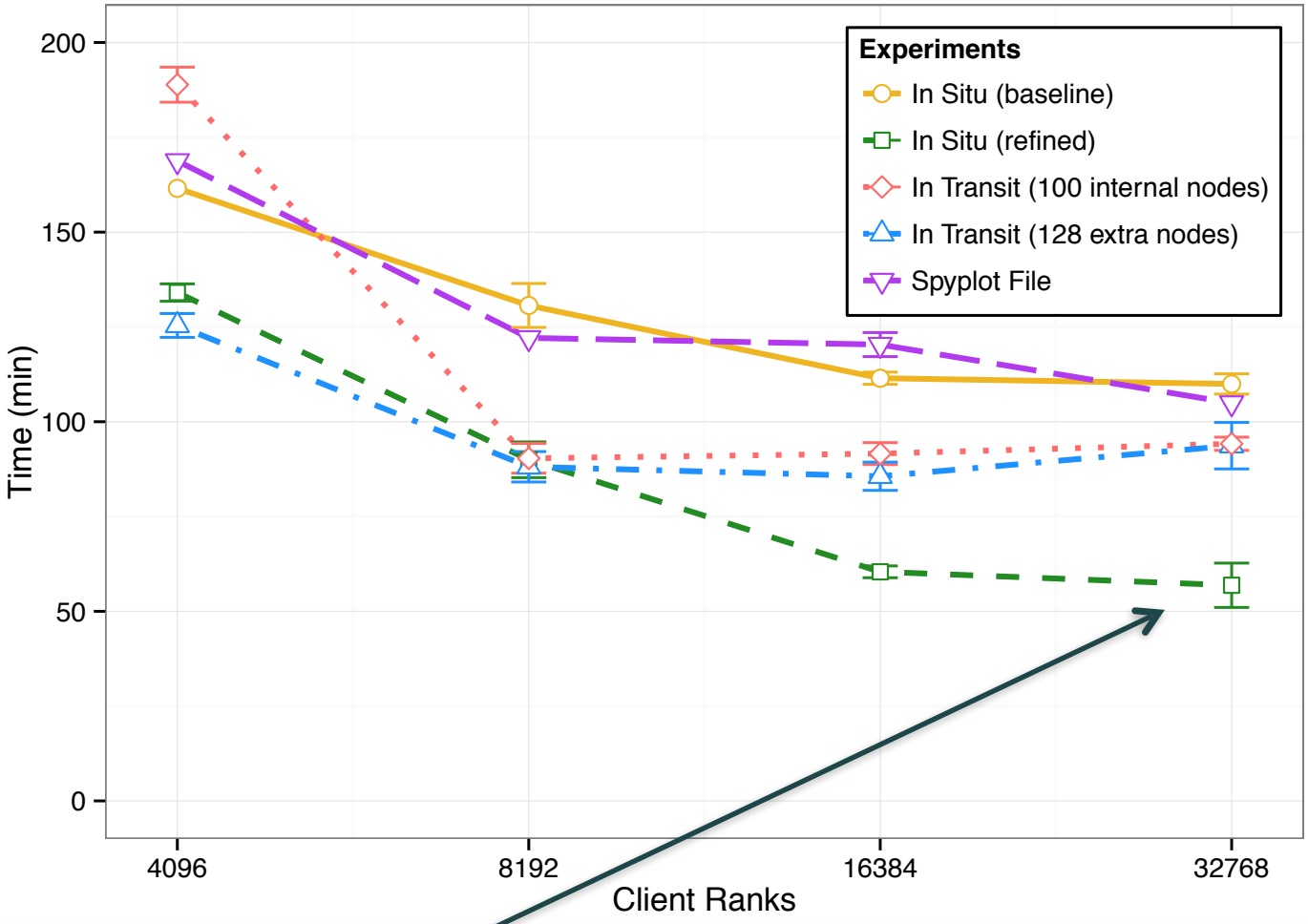


Summary Timing (1.5m blocks)

Sandia National Laboratories



No significant improvement at 32K cores. Probably insufficient work for analysis (only 45 blocks per process).

Summary Timing (1.5m blocks)

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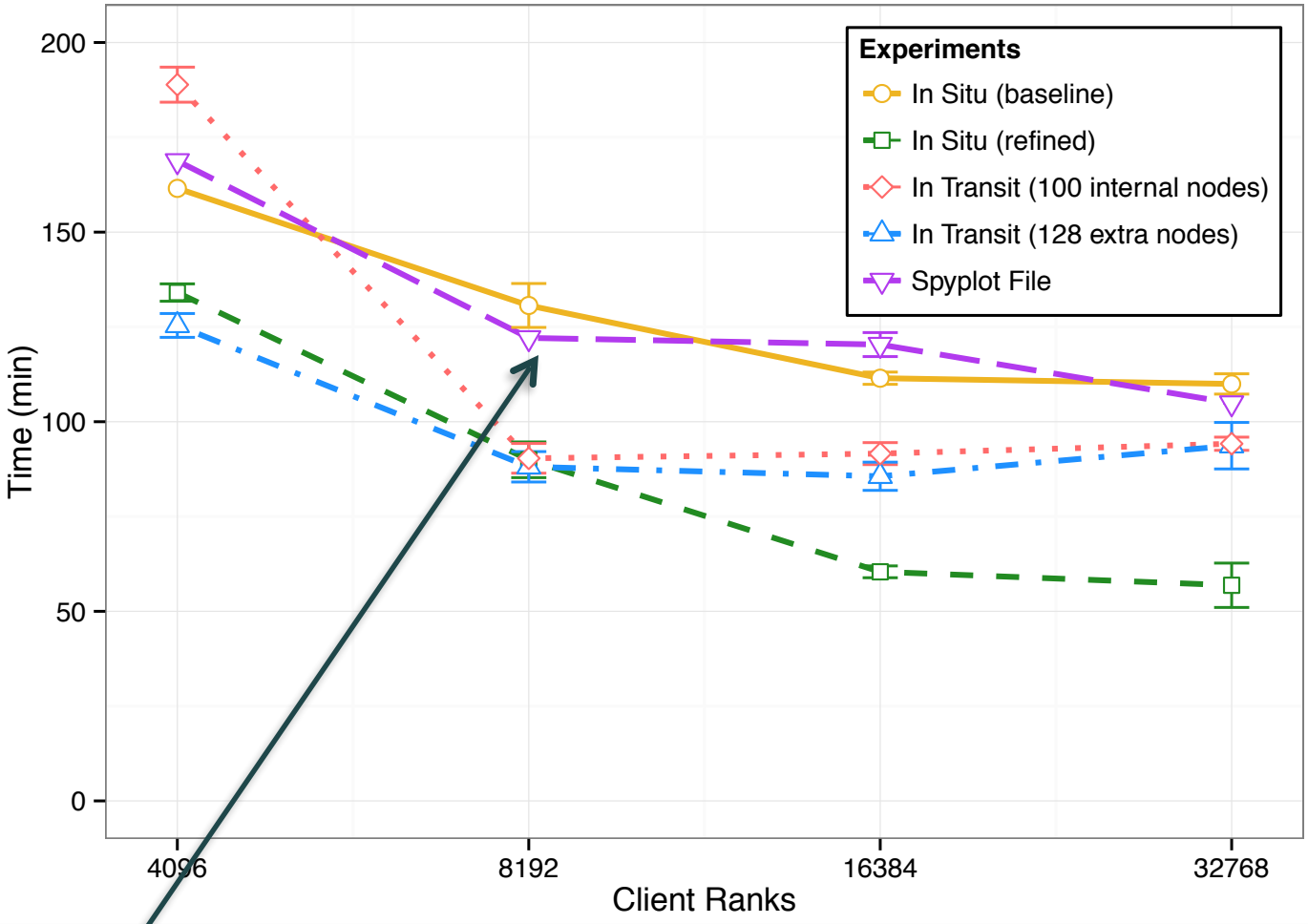

Writing files surprisingly fast. Although slower than most alternatives, still a viable option.

Summary Timing (1.5m blocks)

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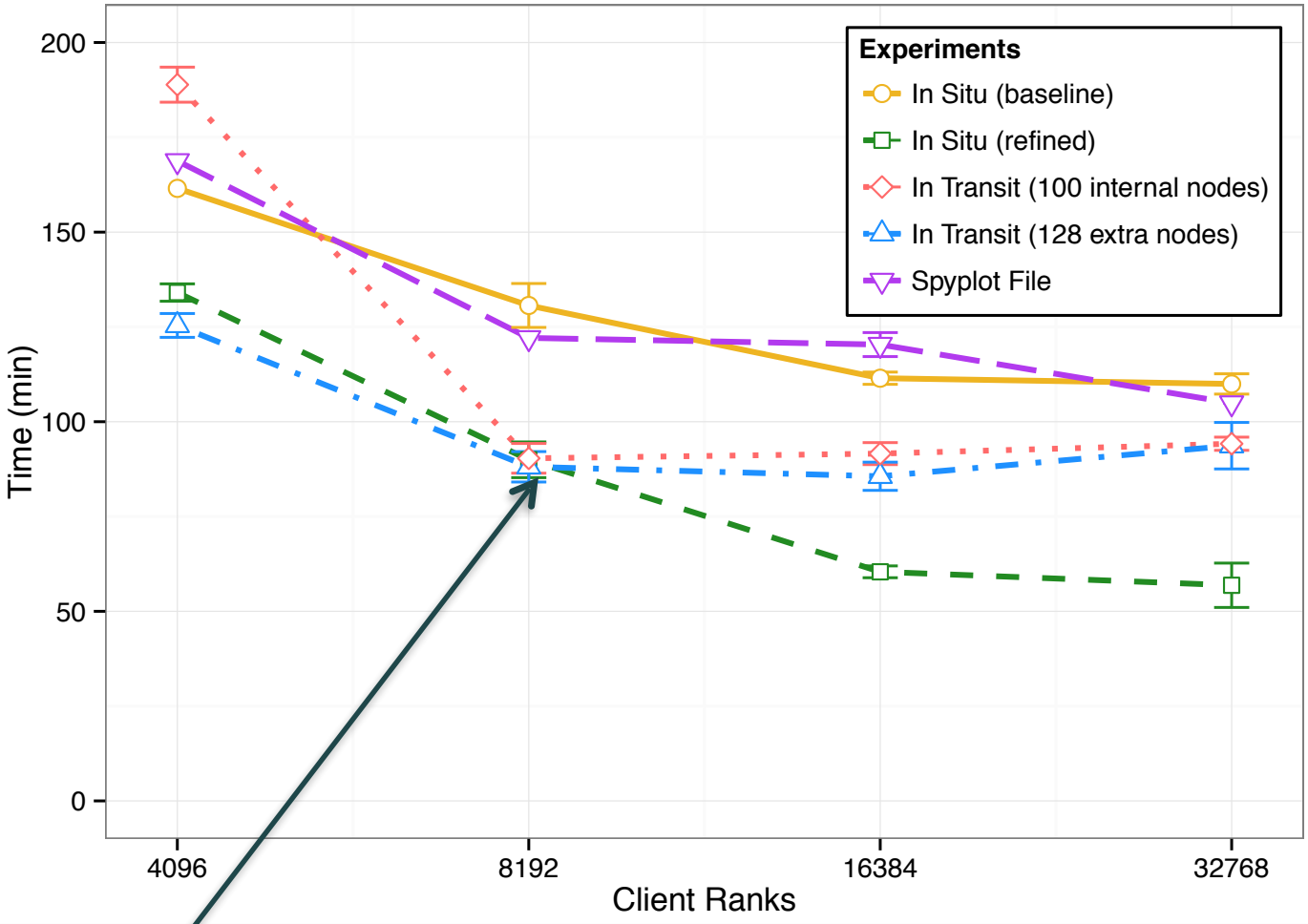
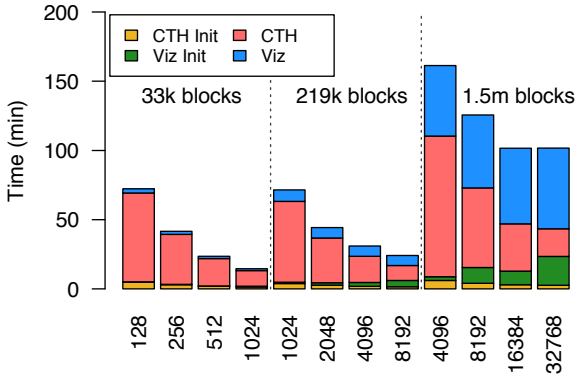
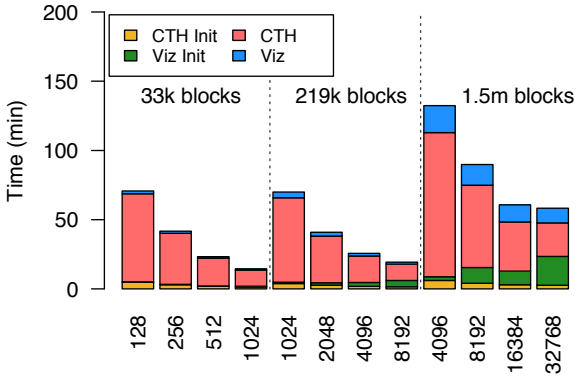


"Sweet spot" at 8K cores: *in transit* with unrefined algorithm equal to *in situ* with refined algorithm.

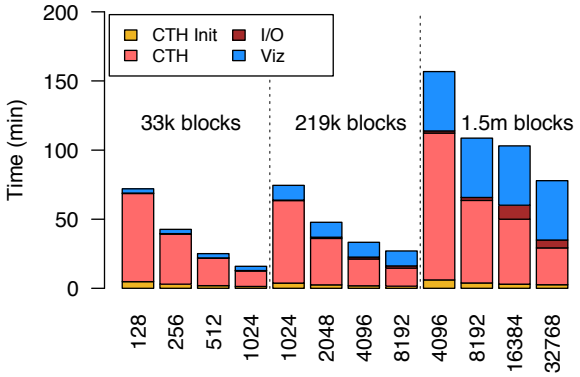
Timing Per Task



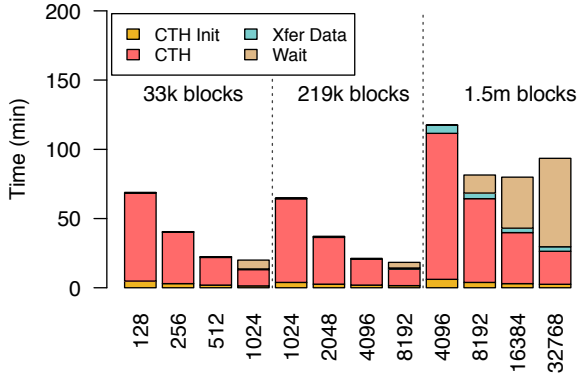
In situ baseline



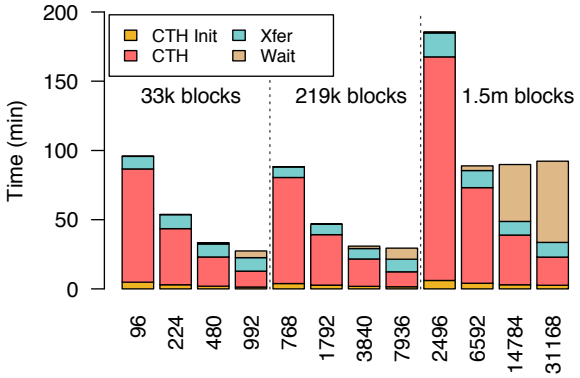
In situ refined



Disk-based post processing



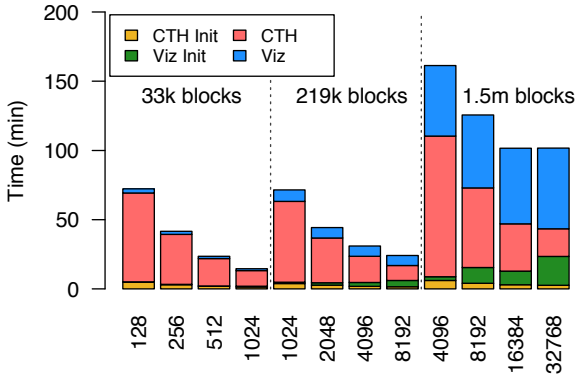
In transit extra nodes



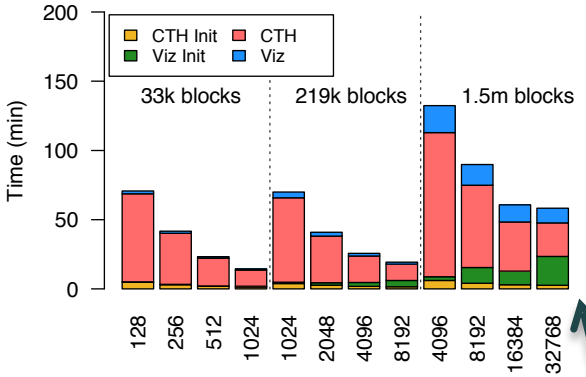
In transit internal nodes

- CTH scales well.
- Baseline algorithm does not scale
- Spyplot I/O not bad

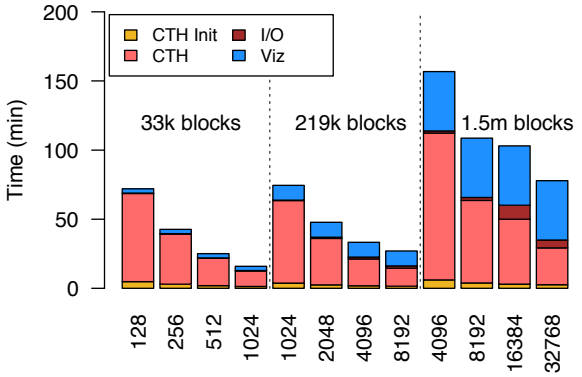
Timing Per Task



In situ baseline



In situ refined



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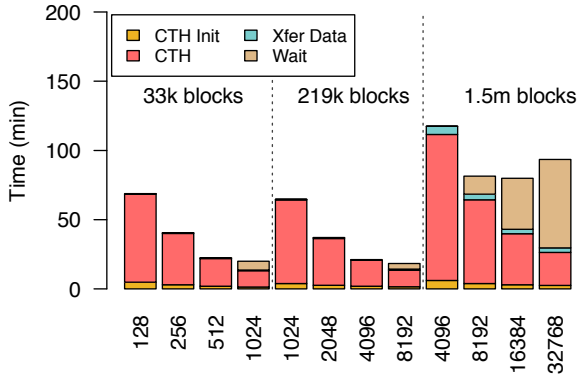
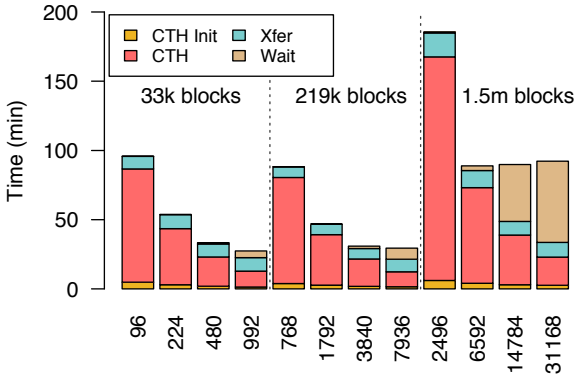


In transit extra nodes

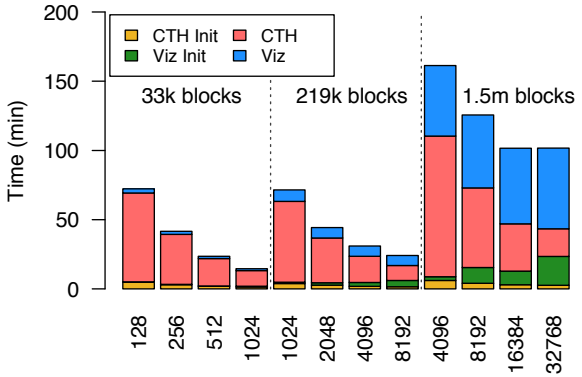


In transit internal nodes

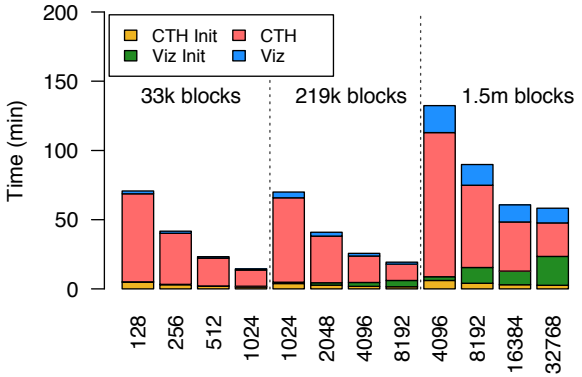
Refined analysis has lower overhead, but initialization cost is problematic.

Refined algorithm requires additional data to be passed. Not done for *in transit* experiments.

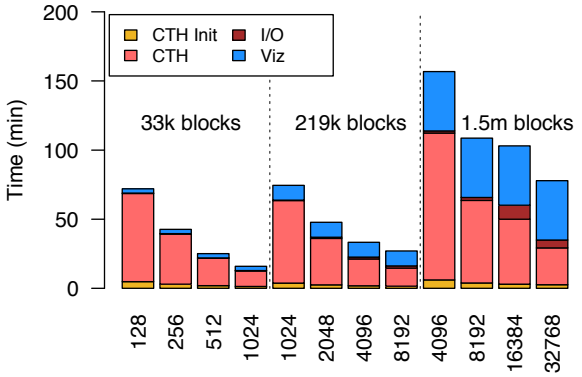
Timing Per Task



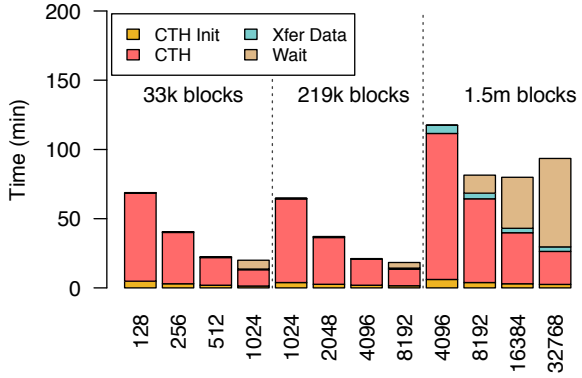
In situ baseline



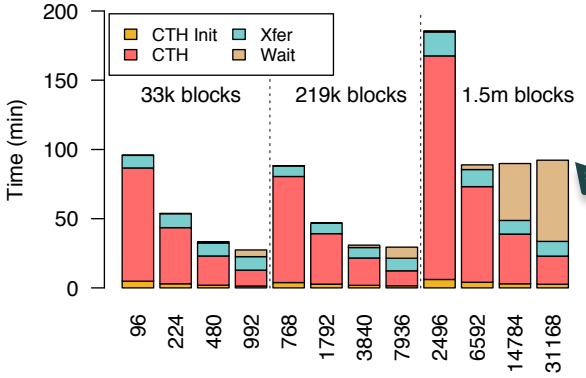
In situ refined



Disk-based post processing



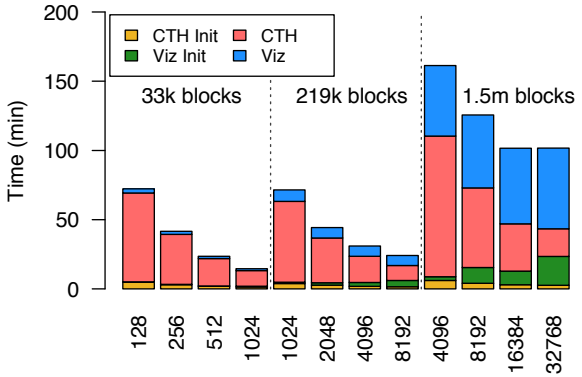
In transit extra nodes



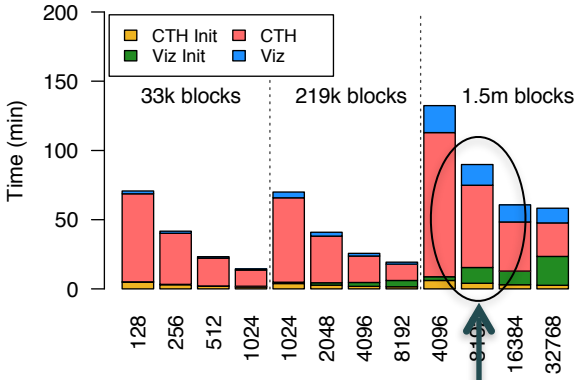
In transit internal nodes

Service is a fixed size (100 nodes), the wait time should be independent of the number of cores on the client.

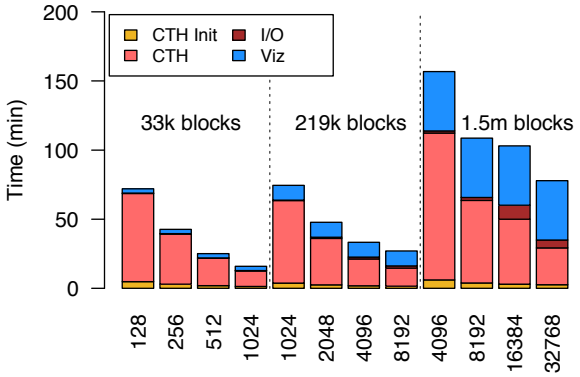
Timing Per Task



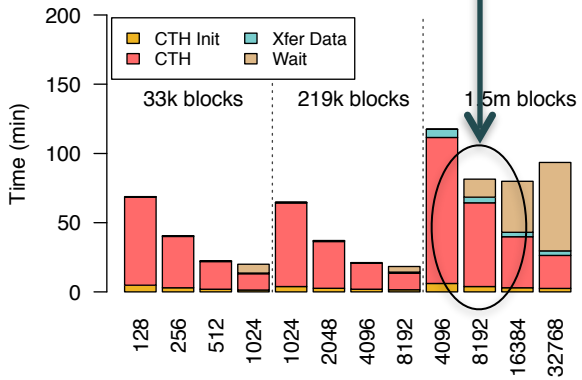
In situ baseline



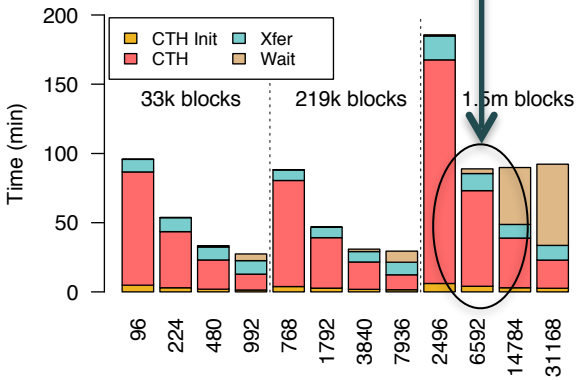
In situ refined



Disk-based post processing



In transit extra nodes



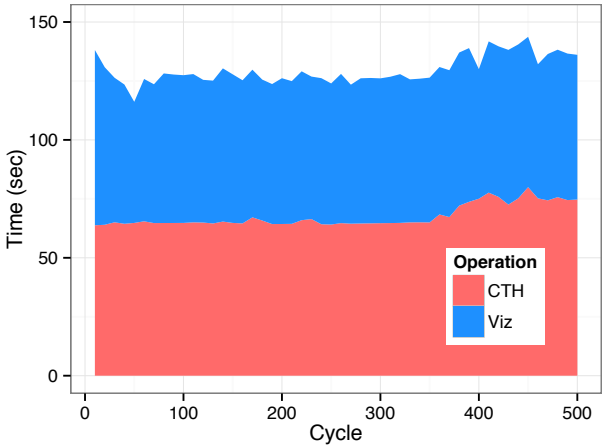
In transit internal nodes

"sweet spot"

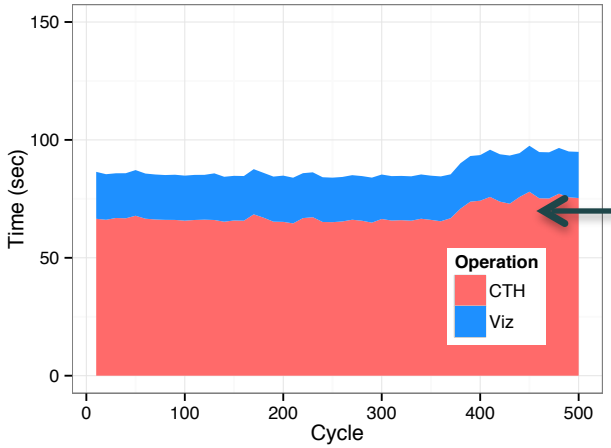
In transit internal shows balanced simulation and analysis

Time-Series Analysis (8k cores)

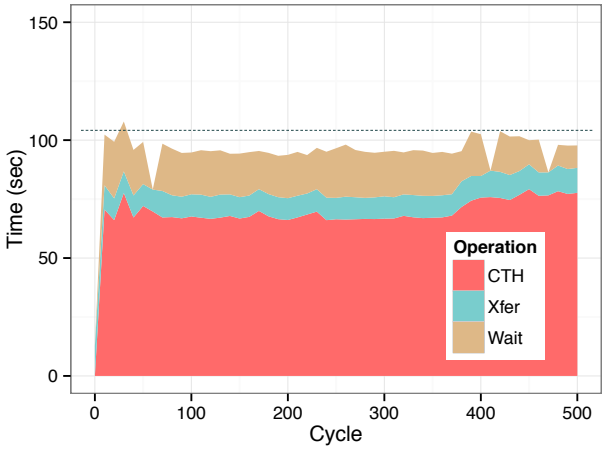
10-cycle increments



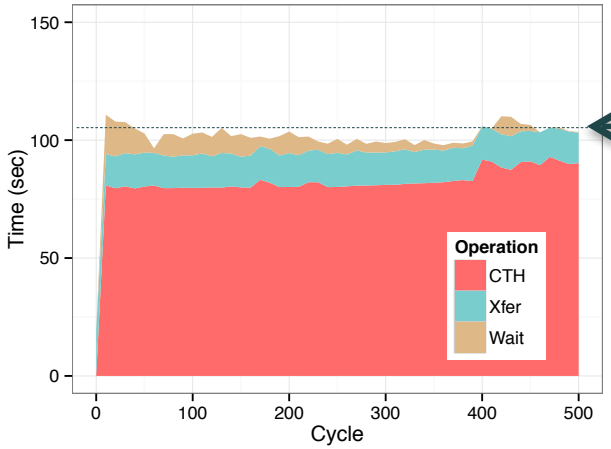
In situ baseline



In situ refined



In transit extra nodes



In transit internal nodes

Although number of blocks changes very little, CTH runtime gets longer as simulation progresses.

Vis time is roughly constant.

In transit "wins" when xfer +wait is less than viz.

In transit can flatten the runtime as long as extra simulation time consumes only wait time.

In Transit Service-Node Core Scaling

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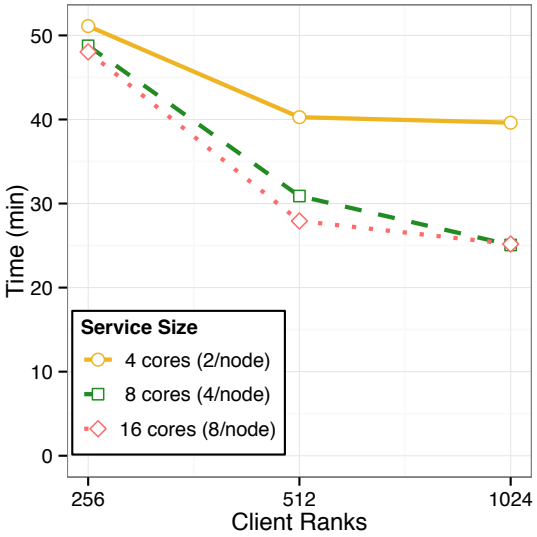
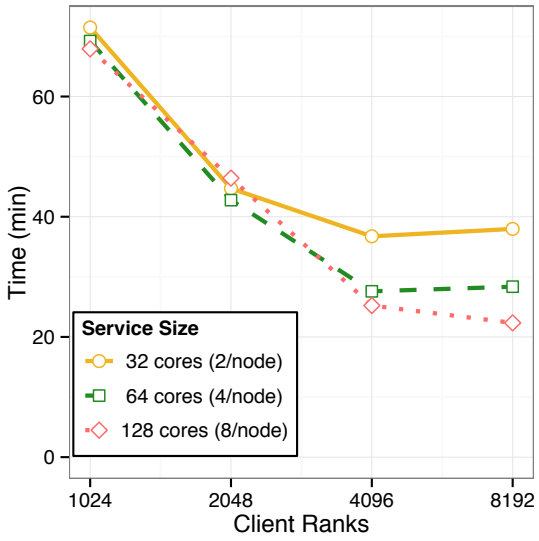
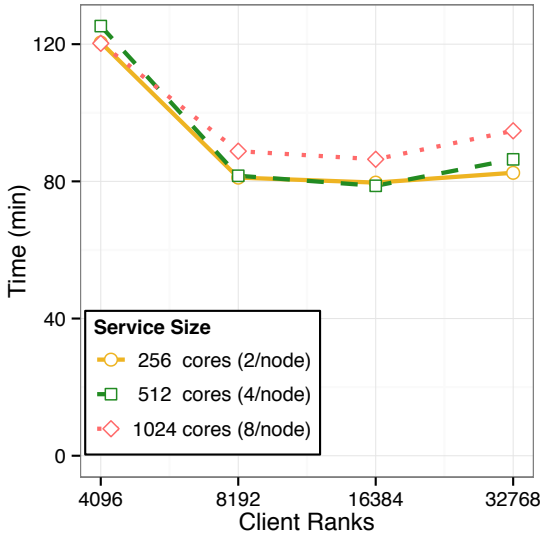
33k blocks



218k blocks



1.5m blocks



For small datasets, there is clear benefit to using 4 and 8 cores/node (agreement from preliminary tests)

For the 1.5m blocks dataset (at large scale), the opposite appears to be true. Needs further study.

Conclusions

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- In situ is extremely effective when analysis algorithm scales with the simulation code.
- In transit is beneficial for complex cases, where data-transfer (and wait) costs less than analysis.
- Balance is the key. Efficient use of resources requires careful consideration of memory, compute, and network requirements of both simulation and analysis codes.
- Traditional disk-based post-processing approaches are not dead… yet.
- Better system support is needed for in-transit approaches. Scheduling is a challenge and node sharing is not possible.

Summary and Future Work

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- Trends in hardware, data volumes, power, and desire for high-resolution analysis are motivating the integration of workflows
- Tightly coupled and loosely coupled approaches will co-exist
- Gaps remain before these approaches become “productive”
  - System software is inadequate (being addressed in Hobbes)
    - Scheduling, load balancing, node and data placement
    - Runtime requirements may differ for coupled components
  - Need portable, memory efficient mechanisms for sharing data
    - Data structure mismatches
    - Multi-resolution/Multi-scale issues
  - Need new definitions for “persistence” of transient data
    - E.g., time windows, data set versioning, …