This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

SAND2020-10955C

Enhancing the Performance and Scalability of Third-Party Libraries in the Sandia I/O Software Stack

COMPSIM

HDF5 User Group Meeting 2020, October 14-16, 2020

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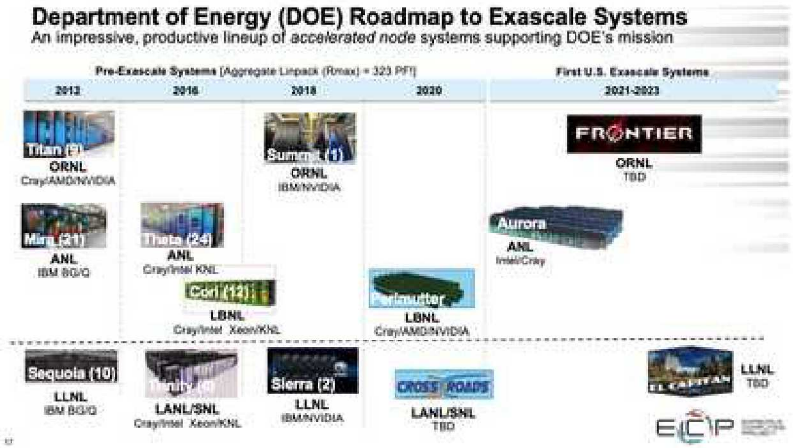
Sandia National Laboratories, Albuquerque NM



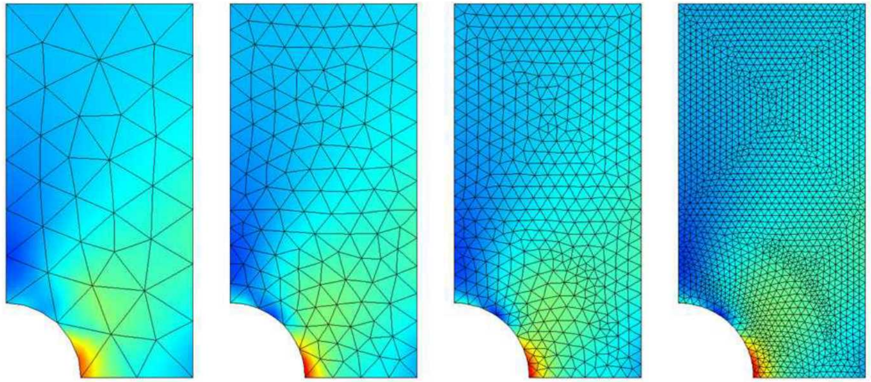
Department of Energy (DOE) Roadmap to Exascale Systems

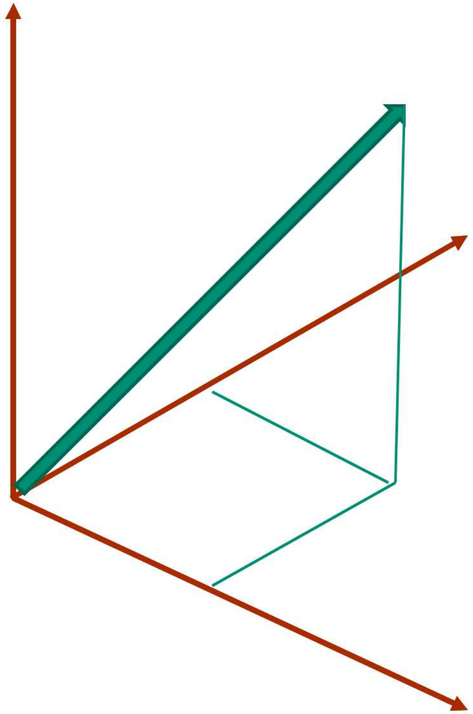
An impressive, productive lineup of *accelerated node* systems supporting DOE's mission

Pre-Exascale Systems [Aggregate Linpack (Rmax) = 323 PF!]

First U.S. Exascale Systems

2012	2016	2018	2020	2021-2023
Titan (7) ORNL Cray/AMD/NVIDIA		Summit (1) ORNL IBM/NVIDIA		FRONTIER ORNL TBD
Mira (21) ANL IBM BG/Q	Theta (24) ANL Cray/Intel KNL Cori (12) LBNL Cray/Intel Xeon/KNL		Perlmutter LBNL Cray/AMD/NVIDIA	Aurora ANL Intel/Cray
Sequoia (10) LLNL IBM BG/Q	Trinity (6) LANL/SNL Cray/Intel Xeon/KNL	Sierra (2) LLNL IBM/NVIDIA	CROSSROADS LANL/SNL TBD	EL CAPITAN LLNL TBD

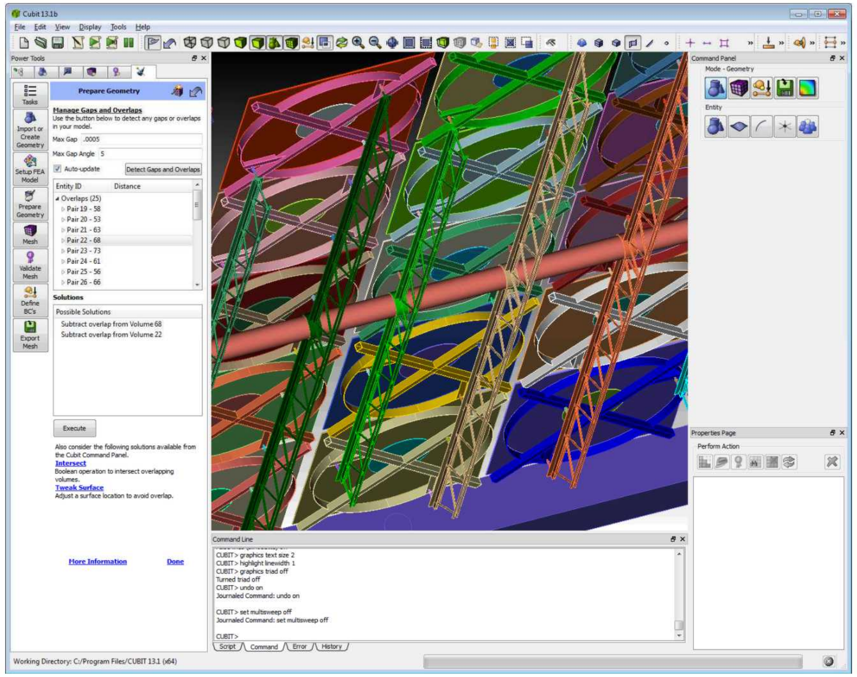




Scalability

Capacity

Complexity



Prepare Geometry

Manage Gaps and Overlaps

Use the button below to detect any gaps or overlaps in your model.

Max Gap .0005

Max Gap Angle 5

☑ Auto-update   Detect Gaps and Overlaps

Entity ID	Distance
Overlaps (25)	
Pair 19 - 58	
Pair 20 - 53	
Pair 21 - 63	
Pair 22 - 68	
Pair 23 - 73	
Pair 24 - 61	
Pair 25 - 56	
Pair 26 - 66	

Solutions

Possible Solutions

Subtract overlap from Volume 68

Subtract overlap from Volume 22

Execute

Also consider the following solutions available from the Cubit Command Panel.

Intersect

Boolean operation to intersect overlapping volumes.

Tweak Surface

Adjust a surface location to avoid overlap.

More Information   Done

Command Line

```
CUBIT> graphics text size 2
CUBIT> highlight linewidth 1
CUBIT> graphics triad off
Turned triad off
CUBIT> undo on
Journaled Command: undo on

CUBIT> set multisweep off
Journaled Command: set multisweep off

CUBIT>
```

Script Command Error History

Working Directory: C:/Program Files/CUBIT 13.1 (x64)

Exodus

Background

- Developed 1992
- Replaced old fortran-unformatted read/write files with a device-independent, random access database.
- Based on NetCDF

- Single format used by all SNL Structural and Thermal FE Codes
- Nodes, Homogenous Element Blocks, NodeSets, Sidesets
  - Transient Data on Nodes and Elements.
- A Suite of mesh generation, preprocessing, postprocessing, visualization, and translation tools developed to generate and modify exodus files. SEACAS

- Backward Compatibility Essential

Exodus Evolution

Capacity:

- 1992: CDF1 ~34 Million Nodes/Elements (~NetCDF-2.3.X)
- 2004: CDF2 ~500 Million Nodes/Elements (NetCDF-3.6.0)
  - Internal changes to exodus format to reduce dataset sizes
- 2008: NetCDF-4 (HDF5 based) 2.1 Billion Nodes/Elements
- 2012: 64-bit Integer changes (HDF5 Enabled) Multi-Billion Nodes/Elements
  - Converts integer size on the fly. Ids, indices, maps

Capability:

- Named blocks, sets, attributes, and maps
- Transient variables on all blocks and sets
- “unlimited” string size replaced fixed 32 character limit
- Full topology support (Element->Face->Edge->Node)
- Arbitrary Polyhedral element support
- Compression (via HDF5)
- File Groups (via HDF5)
- Assemblies, Entity Attributes, Discontinuous Galerkin

Exodus Evolution -- Parallel

Original workflow was file-per-processor

- External tools to split to parallel and join from parallel
- Extension library “nemesis” provided parallel data structures
- Each “processor” file is valid exodus file.

Exodus becomes “parallel-aware”

- Nemesis Embedded in Exodus (ne_? Changed to ex_?)
- PNetCDF and HDF5 provide parallel IO capabilities
- Can support auto-decomposition and auto-join

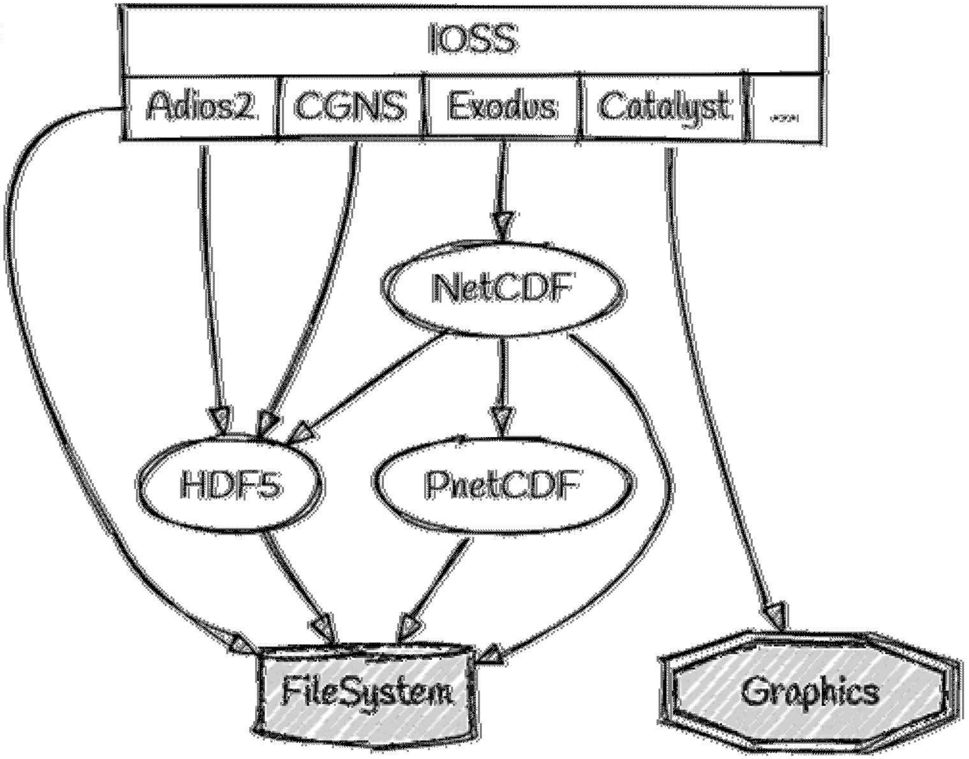
I/O Subsystem – IOSS Library

- Started as the IO component of the Sierra project – 12/1999
- Provide a database-independent interface to applications
  - (Exodus, CGNS, SAF, XDMF, ADIOS2, …)
- Also functions as a "pseudo-C++ API" for the exodus libr
- Supports Advanced HPC Capabilities:
  - Kokkos Data
  - Burst Buffer
  - Data Warehouse (FAODEL)
  - Embedded Visualization

- Auto-decomposition
  - Replaces legacy file-per-processor mode
  - Uses either HDF5 or PnetCDF for parallel input
  - Uses decomposition methods in Zoltan and ParMETIS
  - Supports Exodus and CGNS (Structured and Unstructured)

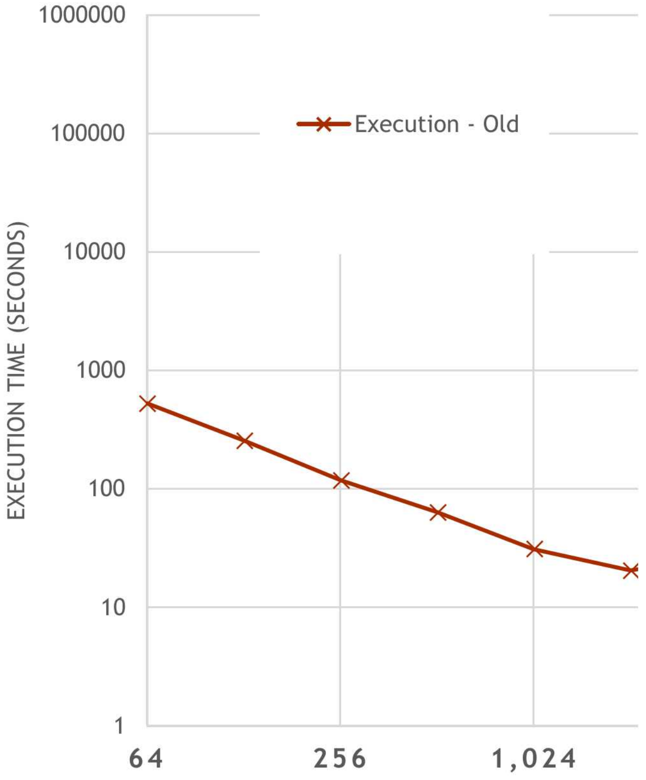
- Auto-join (single file output) option
  - Uses HDF5 or PnetCDF for parallel output
  - Scalability issues.... Being addressed.

- HDF5 is used by 3 of the supported Data types.



Parallel Scalability -- Exodus

2 Billion Elements
Sequoia
Lustre Filesystem



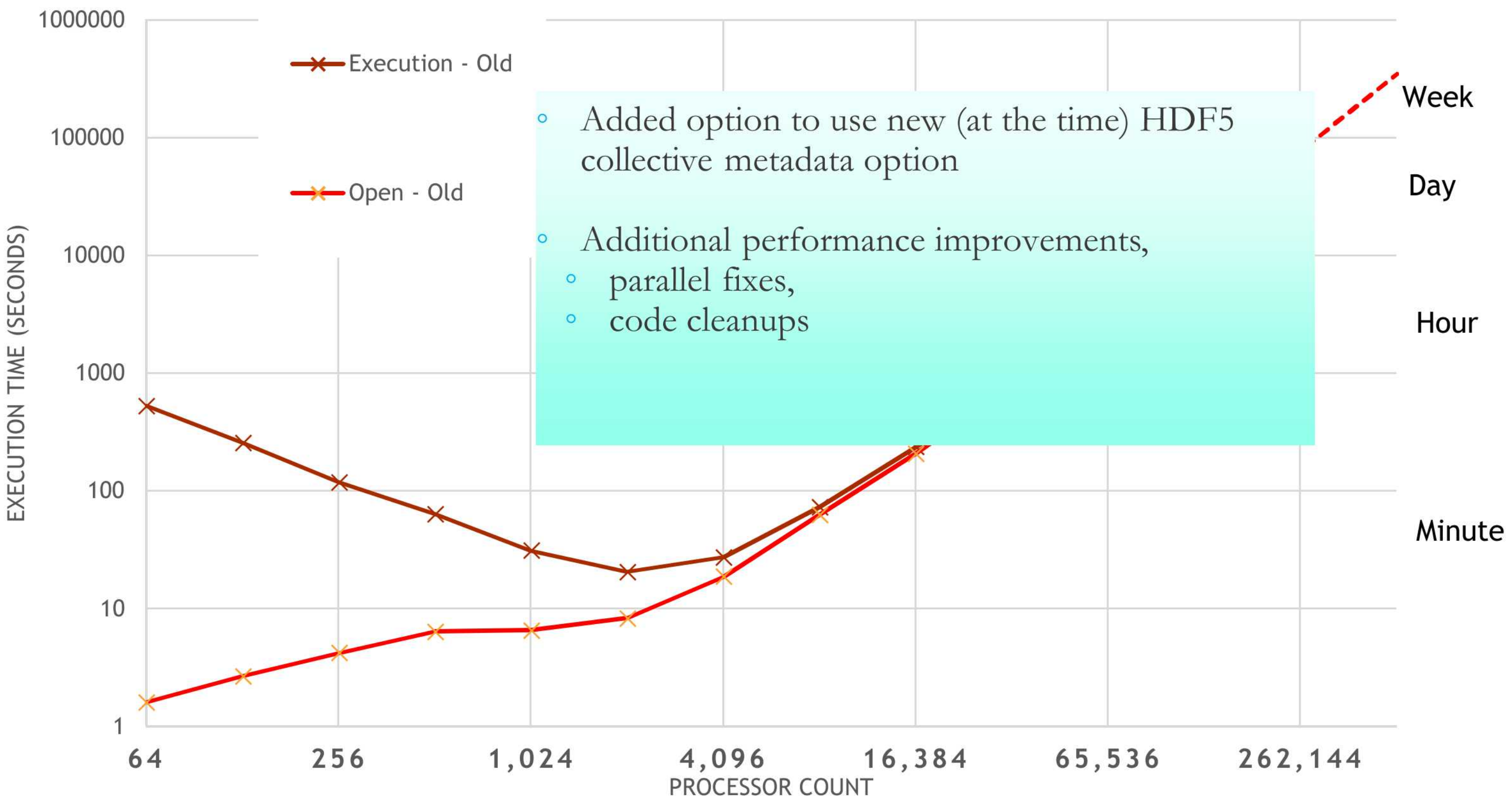
Large model being run on Sequoia
Application reported “analysis is hanging”

Ran same mesh in IOSS simulator with tracing enabled to determine what was happening

Initial results looked promising…

Parallel Scalability -- Exodus

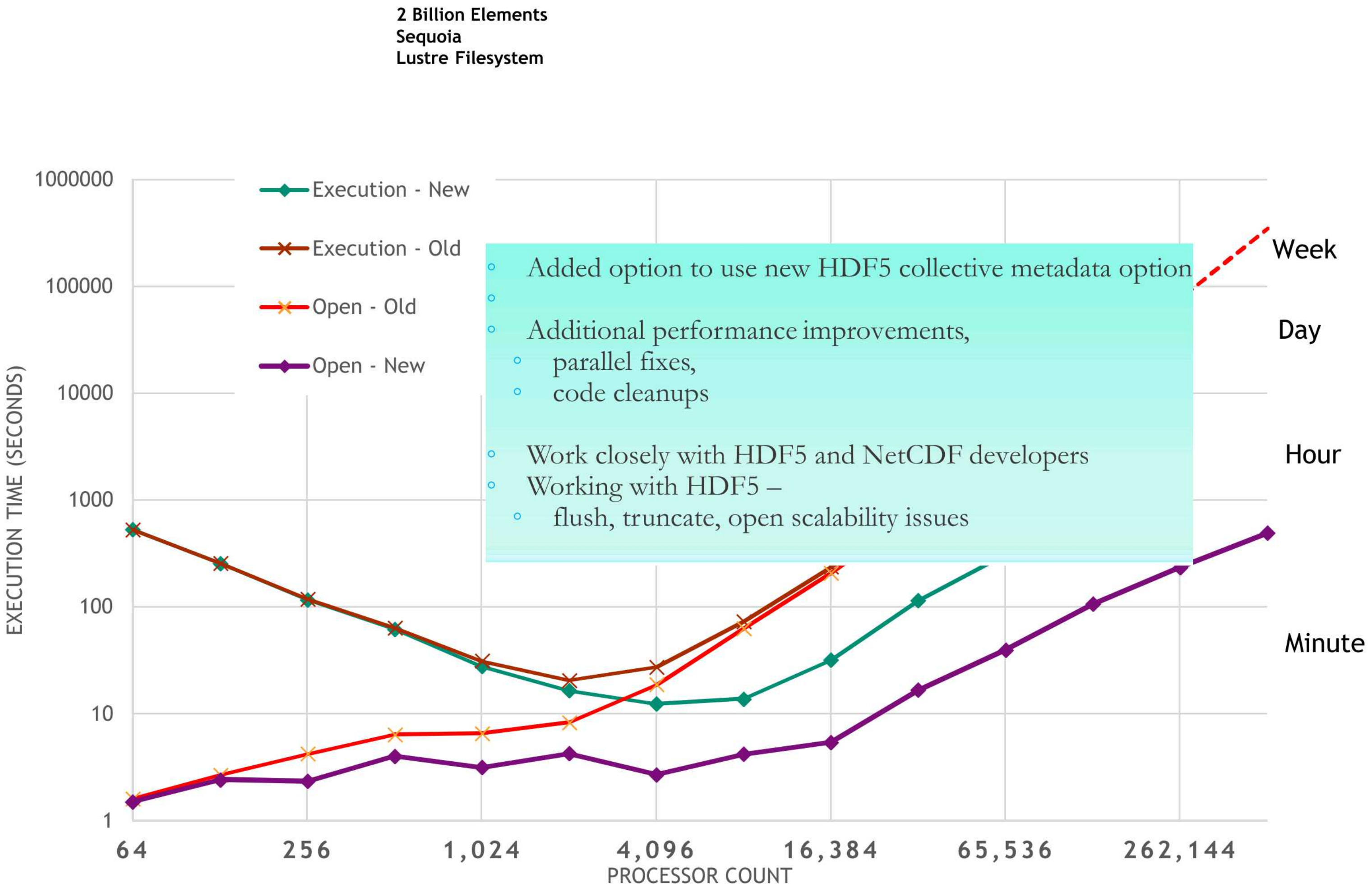
2 Billion Elements
Sequoia
Lustre Filesystem



- Added option to use new (at the time) HDF5 collective metadata option
- Additional performance improvements,
  - parallel fixes,
  - code cleanups

A supercomputer is a device for turning compute-bound problems into I/O-bound problems

Parallel Scalability -- Exodus



- Added option to use new HDF5 collective metadata option
-
- Additional performance improvements,
  - parallel fixes,
  - code cleanups

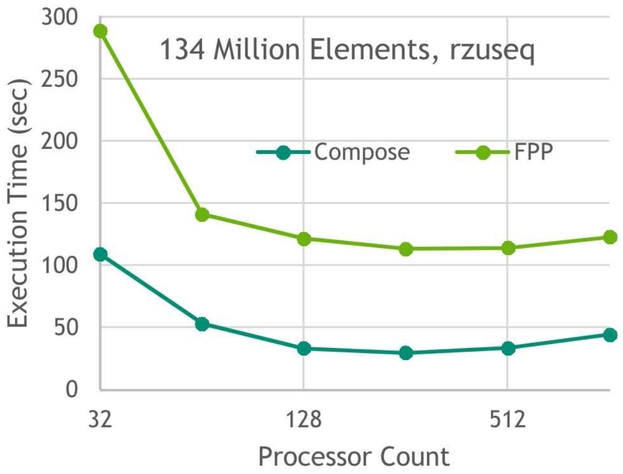
- Work closely with HDF5 and NetCDF developers
- Working with HDF5 –
  - flush, truncate, open scalability issues

A supercomputer is a device for turning compute-bound problems into I/O-bound problems

Parallel Scalability – Exodus AutoJoin

Improving parallel scalability of auto-join (single file output)

- Patch NetCDF/HDF5 to avoid unneeded data access (PR 336)
- Code review of Ioss "autojoin" routines

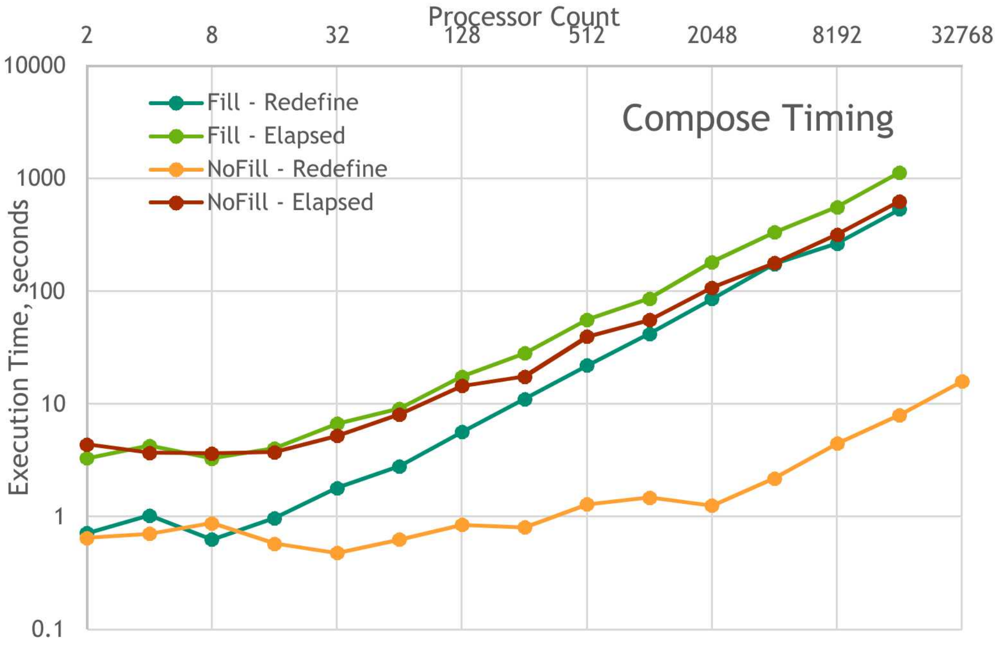


Preliminary results look promising, more to do:

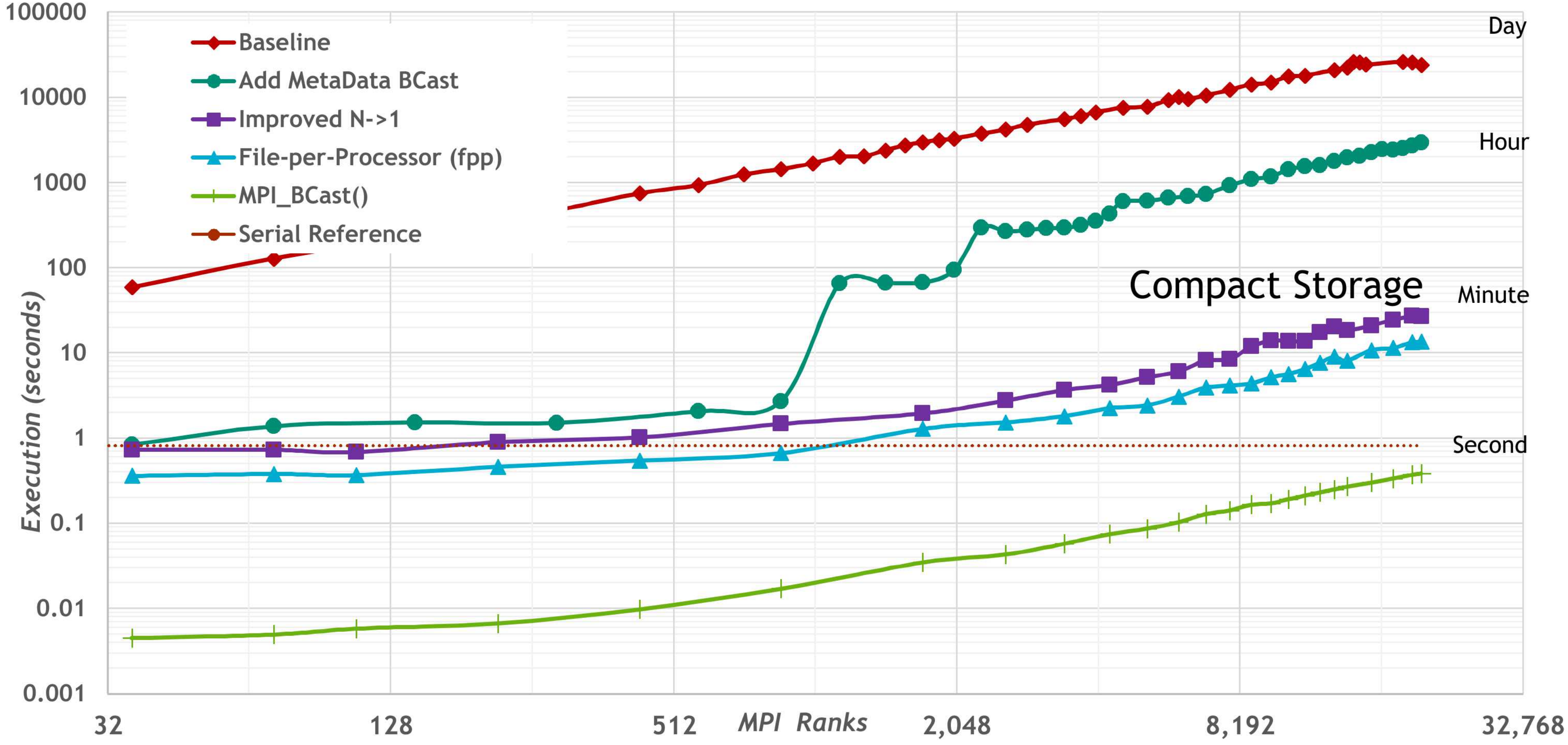
- Darshan Profiling
- MPI Profiling
- MPI-IO Tuning
- Filesystem Tuning

Working with HDF5 –

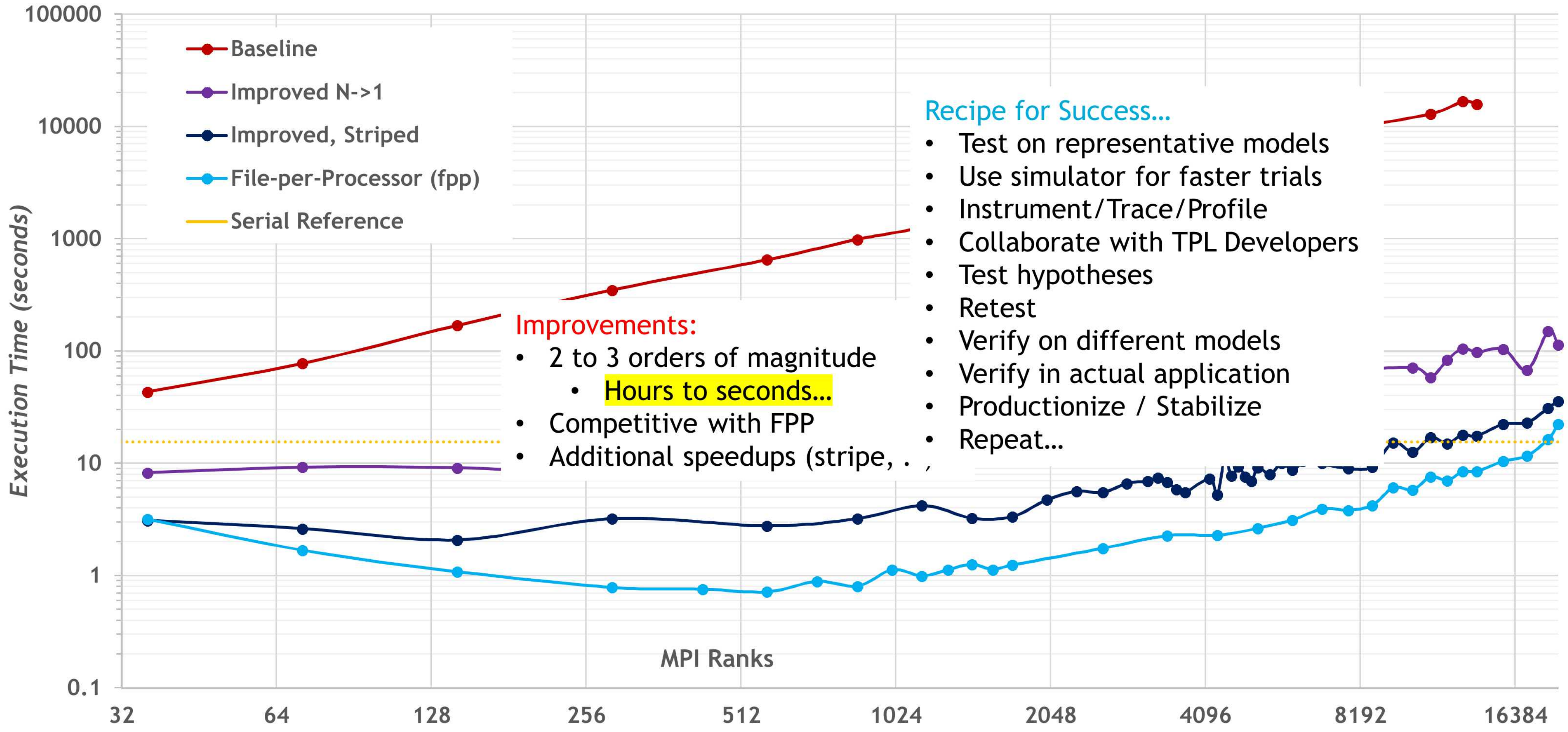
- Flush, truncate, close scalability issues



Input/Output performance improvements
CGNS Structured Mesh



Input/Output performance improvements – Large Model CGNS Structured Mesh



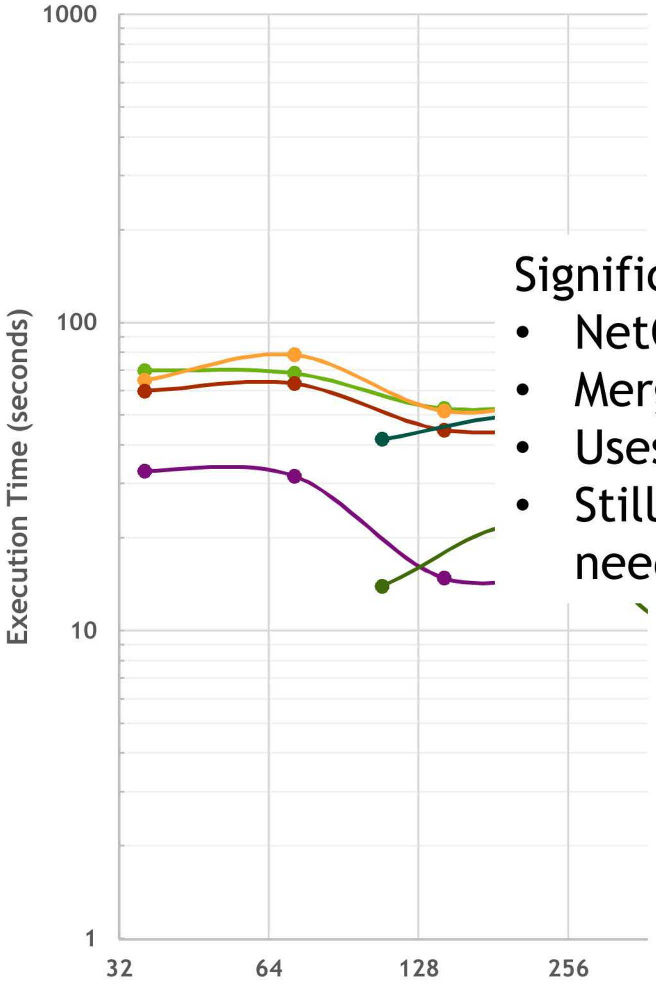
Improvements:

- 2 to 3 orders of magnitude
  - Hours to seconds…
- Competitive with FPP
- Additional speedups (stripe, .

Recipe for Success…

- Test on representative models
- Use simulator for faster trials
- Instrument/Trace/Profile
- Collaborate with TPL Developers
- Test hypotheses
- Retest
- Verify on different models
- Verify in actual application
- Productionize / Stabilize
- Repeat…

Exodus speedups…



Exodus format file in NetCDF-4 (HDF5) format

- 64-bit integers, 64-bit doubles
- 48.3 Gbyte file

- 390 Million finite element nodes
- 49 Million 27-node hexahedral elements
- 1 time step with 8 variables per node

Significant Speedup Realized

- NetCDF PR1570 (HDF5 Compact Storage).
- Merged, Released in 4.7.4.
- Uses existing API function
- Still slower than FPP by >2X; more profiling needed

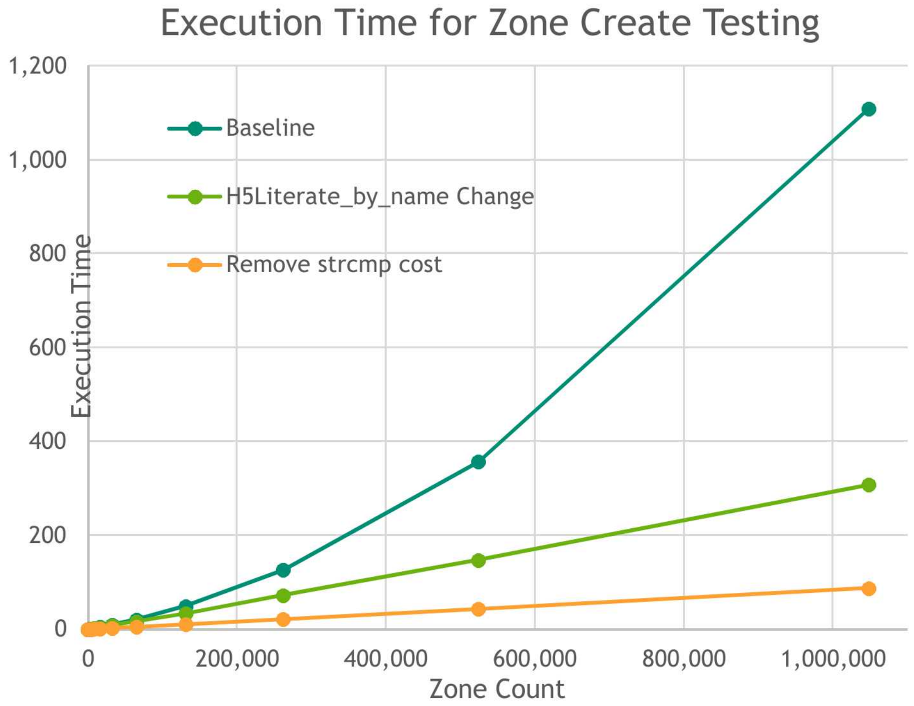
Run on “serrano” CTS-1 system

- 2.1 GHz processors
  - Dual sockets with 18 cores each
  - Intel Broadwell® E5-2695 v4
  - ~1.2 TFLOPs per node
- 128 GB RAM per node (3.55 GB per core)
- Intel Omni-Path high speed interconnect

Cgns many zone optimization

Creating a cgns file with "many" zones exposes N^2 behavior

- Metadata only being written
- Serial or Parallel



Input by Scot Breitenfeld and Mickael Philit

Profiling showed "`H5Literate_by_name`" major contributor

`H5Literate_by_name` changed to `H5Lexists`

Code calling this function no longer shows as a hot-spot

Still N^2 behavior in another part of code due to string compares.

Looking at hashing strings to avoid this cost.

With both of these fixes, behavior is near-linear performance out to a million zones.

Conclusions

Scalability, Complexity, and Capacity are very important to HPC Applications

- Measure performance in entire spectrum; verify performance
- Make sure to probe high end of range (large MPI ranks especially…)
- Timers / Diagnostics important to locate source of non-performant behavior
- Don’t guess – measure and verify.

The HDF5 library has helped Sandia I/O libraries remain performant

- **Capacity**:
  - HDF5 eliminated 32-bit limit of NetCDF, Compression
- **Complexity**:
  - HDF5 has removed several TPL limitations making it easier to store complex models
  - Use of correct function is important (H5Lexists vs H5Literate_by_name)
- **Scalability**:
  - Collective Metadata routines have reduced execution time by 2 to 3 orders of magnitude
  - Compact Storage capability has shown similar reductions
  - Burst Buffer support and other features (GPU, Threading, …) are under development and research
  - Testing of the HDF5 library at scale is being done by THG

- Thanks to Scot Breitenfeld and Elena for THG support for much of this work.