ExaIO HDF5 features and application use cases

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ExaIO - Many Team Members and Contributors

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- ANL: Venkat Vishwanath, Huihuo Zheng, Rick Zamora, Paul Coffman
- The HDF Group: Scot Breitenfeld, Elena Pourmal, John Mainzer, Richard Warren, Dana Robinson, Neil Fortner, Jerome Soumagne, Jordan Henderson, Neelam Bagha
- North Carolina State University: John Ravi, Michela Becchi

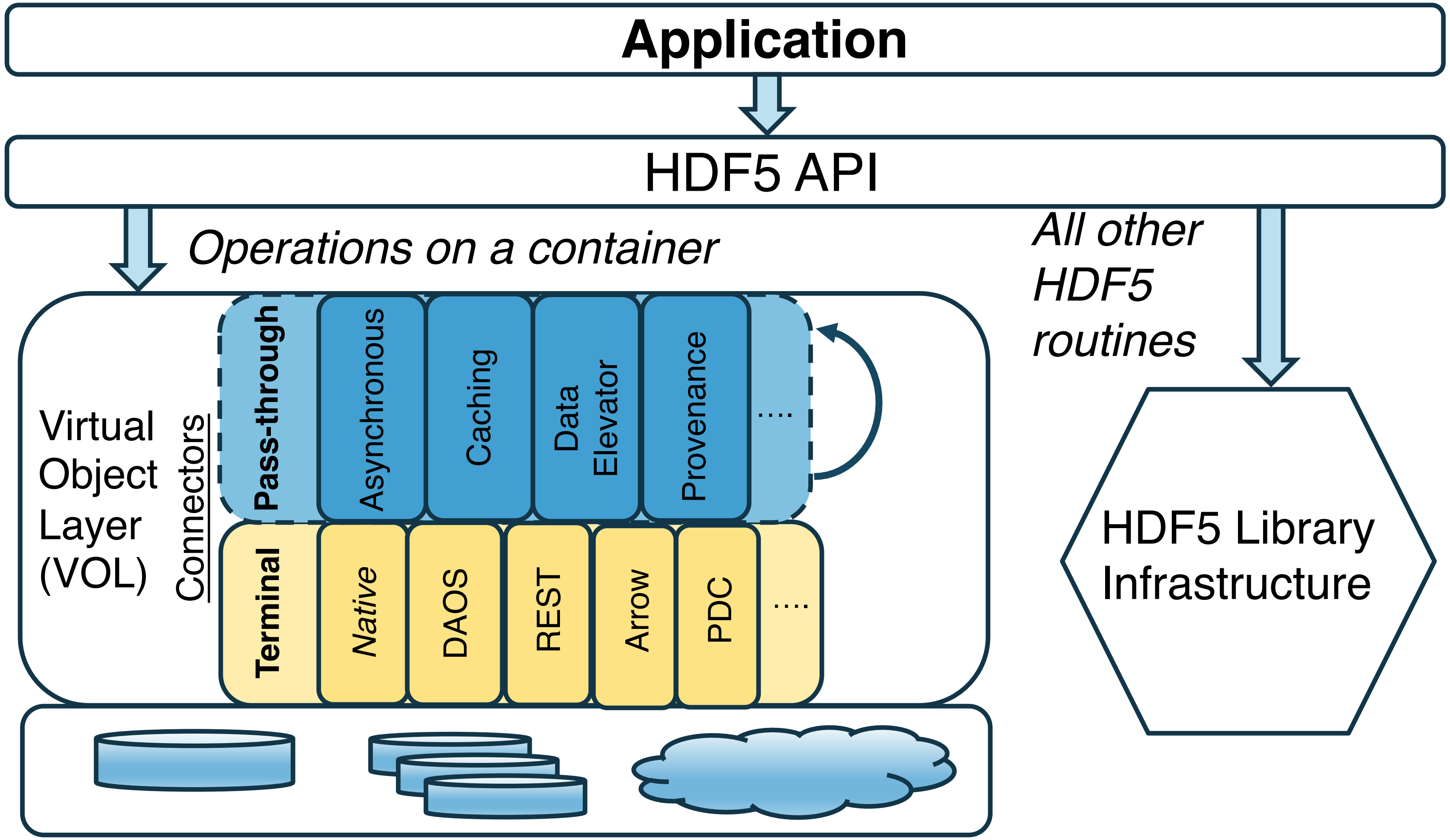
Overview

- Features
  - HDF5 Virtual Object Layer (VOL) Introduction
  - ECP VOL Connectors
    - Asynchronous I/O
    - Node-local Caching
  - Subfiling and querying
- ECP HDF5 Applications and benchmarks
  - EQSIM
  - AMReX - Nyx and Castro
  - Chombo-IO
  - h5bench

HDF5 Virtual Object Layer (VOL)

- **VOL Framework is an abstraction layer within HDF5 Library**
    - Redirects I/O operations into VOL “connector”, immediately after an API routine is invoked
    - Non-I/O operations handled with library “infrastructure”
- **VOL Connectors**
    - Implement storage for HDF5 objects, and “methods” on those objects
        - Dataset create, write / read selection, query metadata, close, …
    - Can be transparently invoked from a dynamically loaded library, without modifying application source code
        - Or even rebuilding the app binary

VOL: High-Level Overview



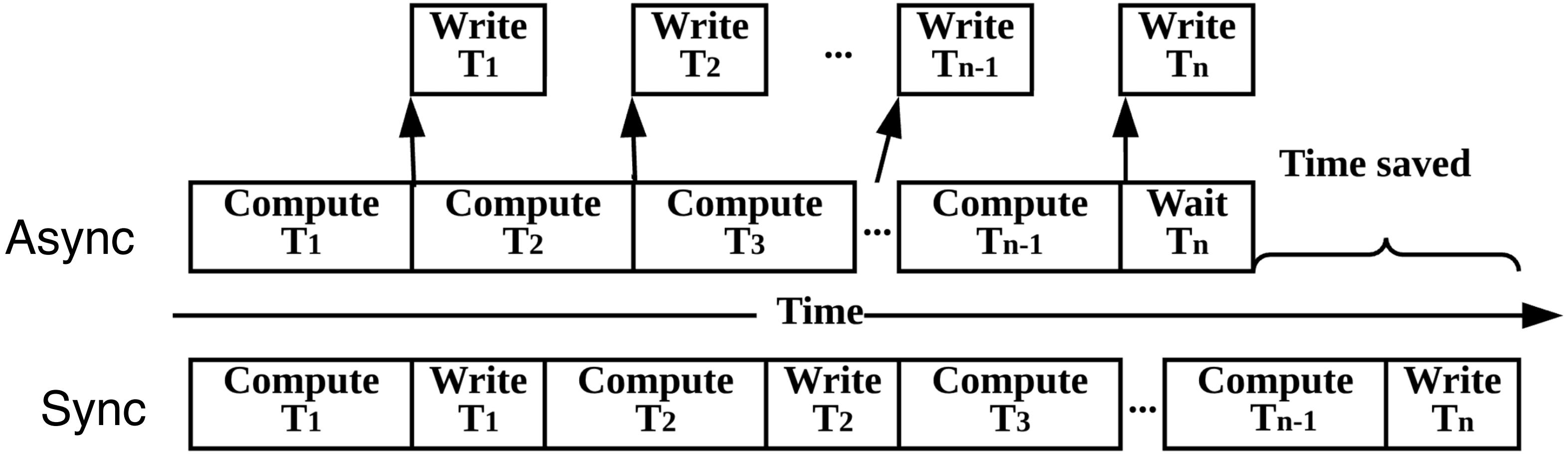
Virtual Object Layer (VOL) Connectors

- Implement callbacks for HDF5 data model operations
- “Terminates” call by performing action directly, or “passes operation through” by invoking VOL API connector interface:
  - Pass-through - can be stacked, must eventually have terminal connector
    - Examples:
      - Provenance tracking (https://github.com/hpc-io/vol-provenance)
      - Asynchronous I/O (https://github.com/hpc-io/vol-async)
      - Caching (https://github.com/hpc-io/vol-cache)
  - Terminal - non-stackable, final connector
    - Examples:
      - Remote access (e.g. cloud, streaming, etc.)
      - Non-HDF5 file access (e.g., ADIOS BP, netCDF “classic”, etc.)
      - Object stores (e.g., DAOS (https://github.com/HDFGroup/vol-daos), S3, Apache Arrow, etc.)

Async VOL Connector

Main developer: Houjun Tang

- Pass-through VOL connector
  - Can be stacked on any other connector, to provide asynchronous operations to it
- Uses an "event set" to manage async operations
  - Can extract more performance, e.g., enable async read and write:



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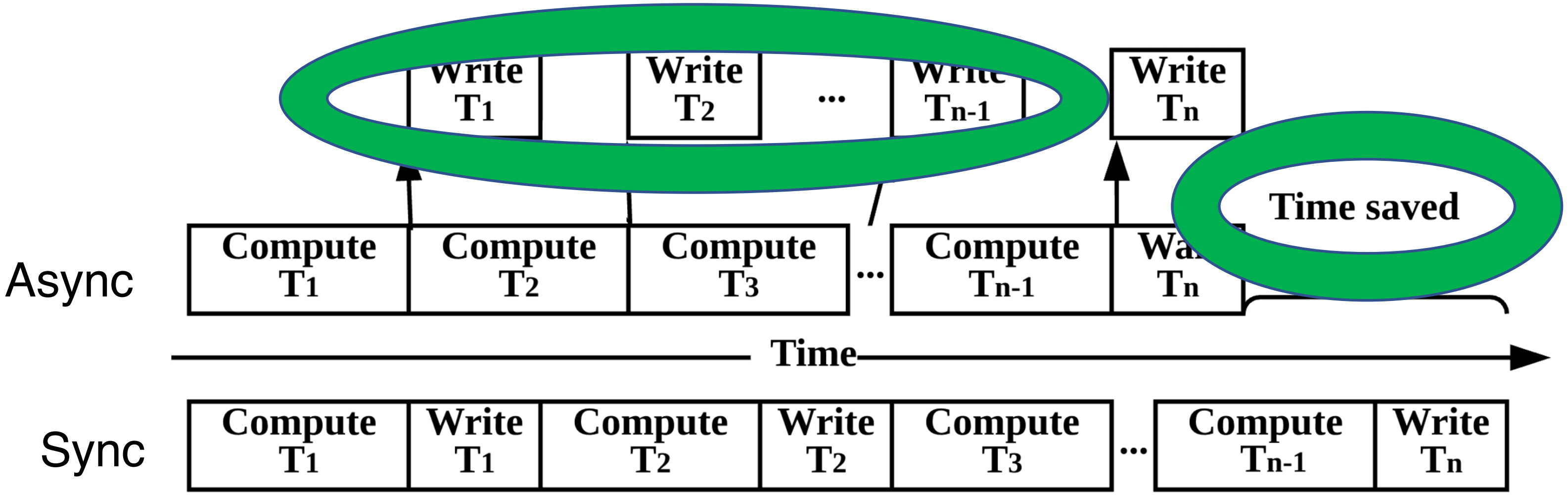

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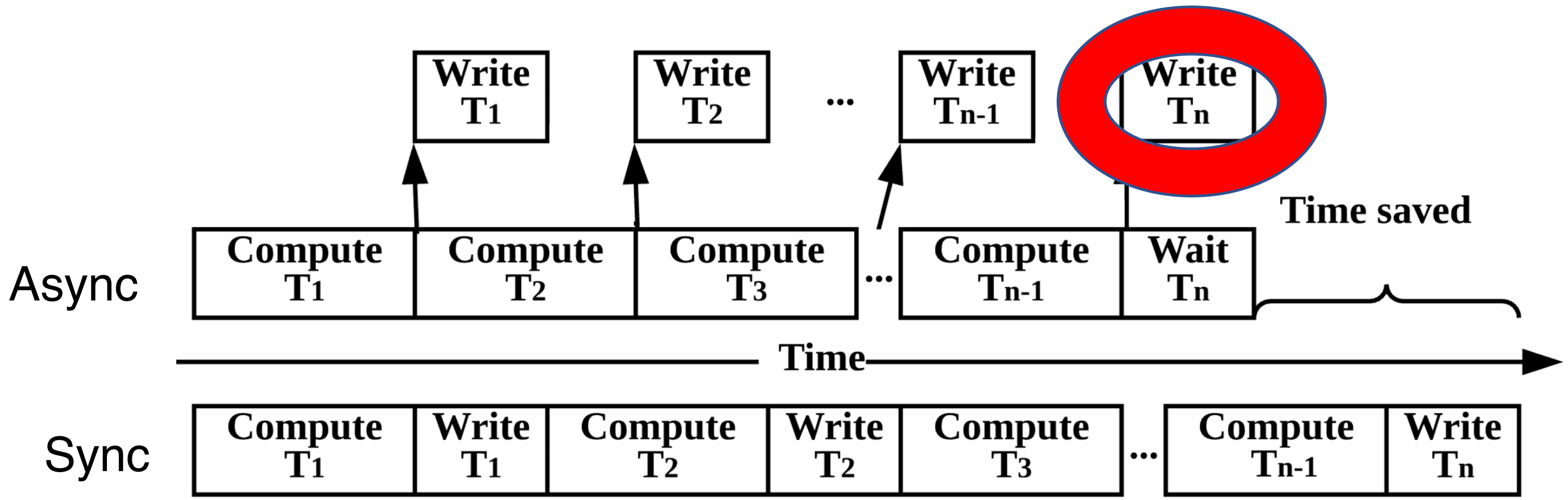
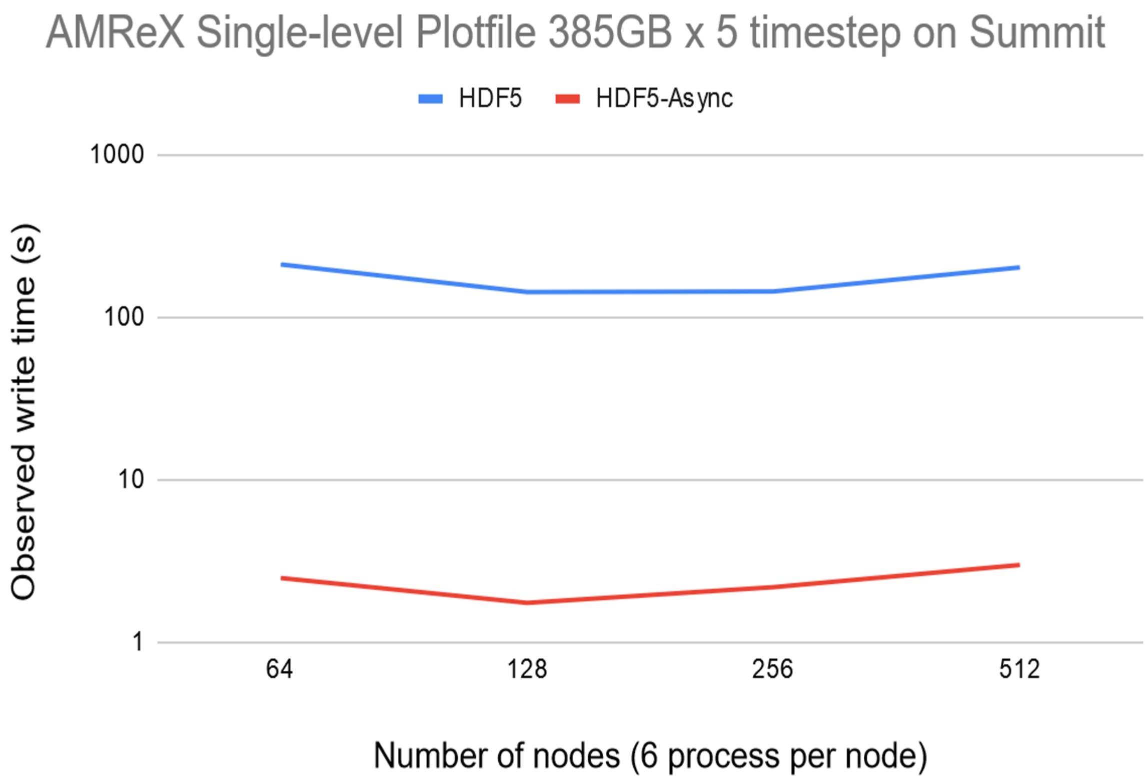
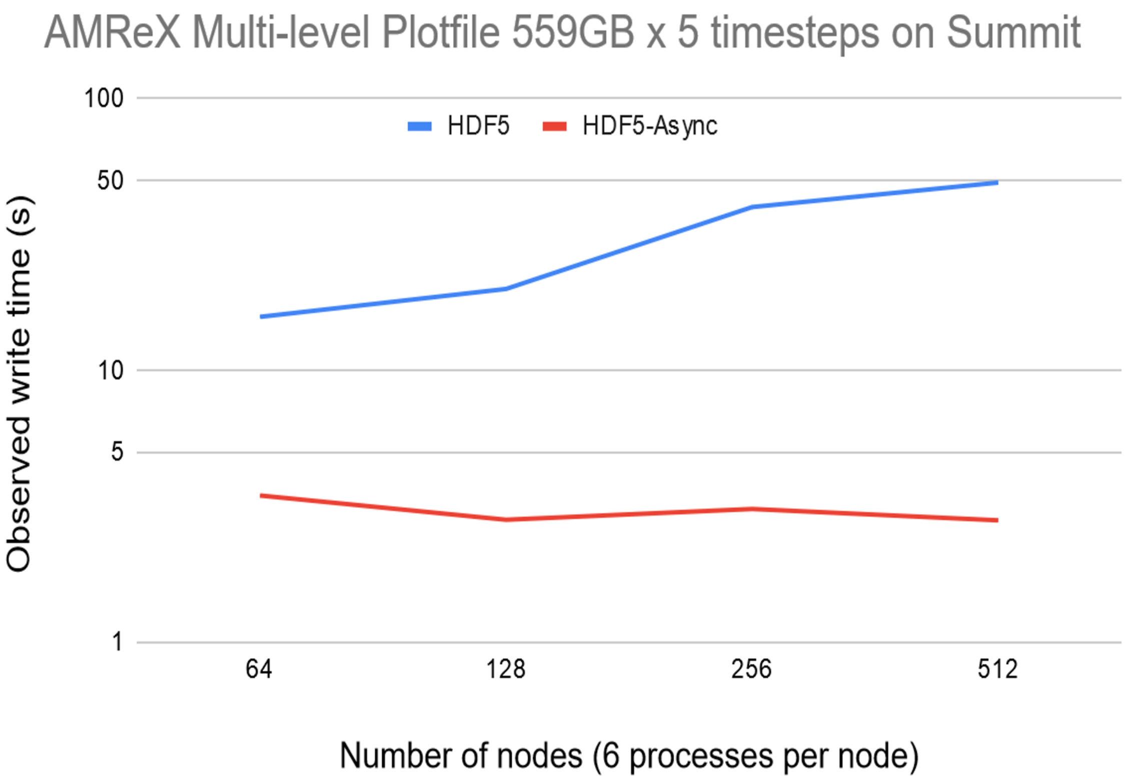


Async VOL Connector – Benefits





Async VOL Connector – Programming Example

```
fid = H5Fopen(..);
gid = H5Gopen(fid, ..);
did = H5Dopen(gid, ..);
status = H5Dwrite(did, ..);

status = H5Dwrite(did, ..);

...
<other user code>
...
```

https://github.com/hpc-io/vol-async

Async VOL Connector – Programming Example

```
es_id = H5EScreate();                            // Create event set for tracking async operations
fid = H5Fopen_async(.., es_id);                  // Asynchronous, can start immediately
gid = H5Gopen_async(fid, .., es_id);             // Asynchronous, starts when H5Fopen completes
did = H5Dopen_async(gid, .., es_id);             // Asynchronous, starts when H5Gopen completes
status = H5Dwrite_async(did, .., es_id);         // Asynchronous, starts when H5Dopen completes,
                                                 //        may run concurrently with other H5Dwrite in event set
status = H5Dwrite_async(did, .., es_id);         // Asynchronous, starts when H5Dopen completes,
                                                 //        may run concurrently with other H5Dwrite in event set
...
<other user code>
...
H5ESwait(es_id);                                 // Wait for operations in event set to complete, buffers
                                                 //   used for H5Dwrite must only be changed after wait
```

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Async VOL Connector – Programming Example

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H5ESwait(es_id);                           // Wait for operations in event set to complete, buffers
                                           //   used for H5Dwrite must only be changed after wait
```

https://github.com/hpc-io/vol-async

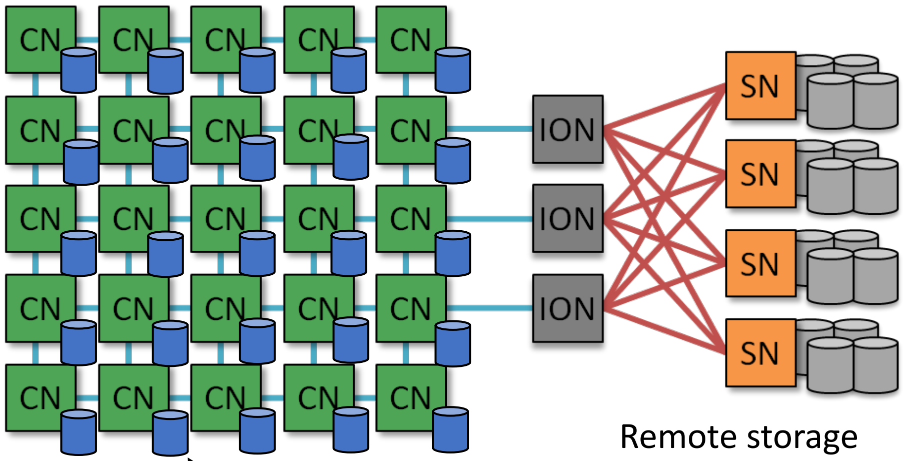
Async VOL Connector

- Available now:
  - Source: https://github.com/hpc-io/vol-async
  - Docs: https://hdf5-vol-async.readthedocs.io/en/latest
- Future work:
  - Merge compatible VOL operations
    - If two async dataset write operations are putting data into same dataset, can merge into only one call to underlying VOL connector
    - Turn multiple 'normal' group create operations into a single 'multi' group create operation
  - Use multiple background threads
    - Needs HDF5 library thread-safety work, to drop global mutex
  - Switch to TaskWorks thread engine
    - A portable, high-level, task engine designed for HPC workloads
    - Task dependency management, background thread execution.

Cache VOL Connector - Integrating node-local storage into parallel I/O

Main developer: Huihuo Zheng

Typical HPC storage hierarchy



Node-local storage (SSD, NVMe, etc)

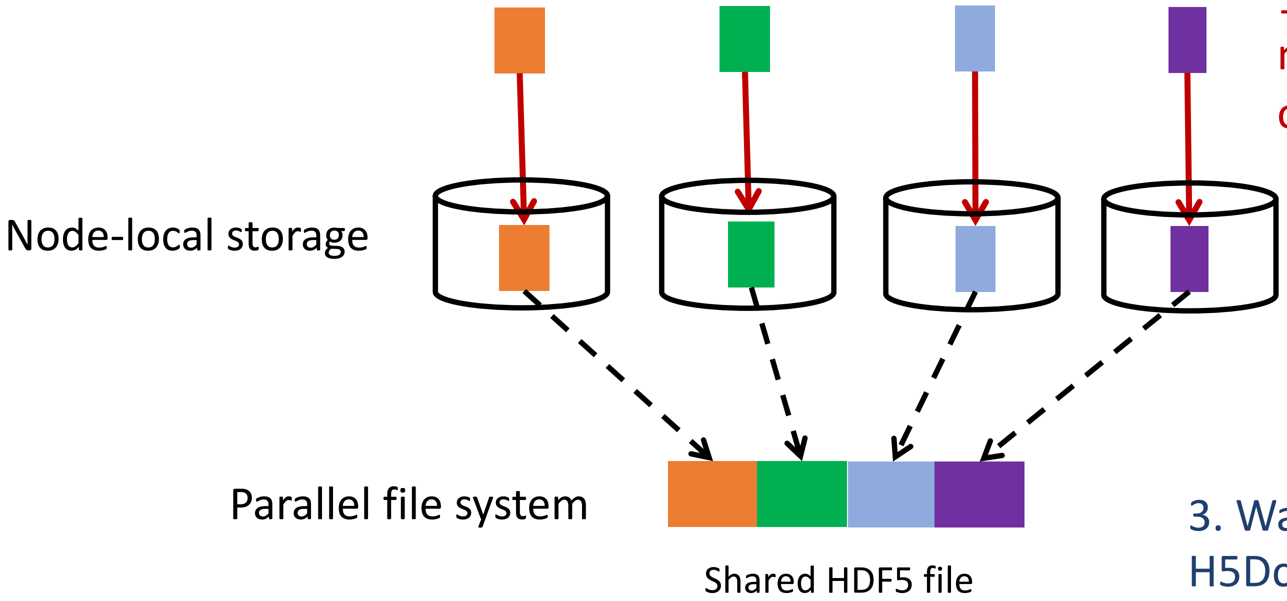
Theta @ ALCF: Lustre + SSD (128 GB / node),
ThetaGPU (DGX-3) @ ALCF: NVMe (15.4 TB / node)
Summit @ OLCF: GPFS + NVMe (1.6 TB / node)

Cache VOL

- Using node-local storage for caching / staging data for fast and scalable I/O.
- Data migration to and from the remote storage is performed in the background.
- Managing data movement in multi-tiered memory / storage through stacking multiple VOL connectors (*async -> cache -> async*)
- All complexity is hidden from the users

Repo: https://github.com/hpc-io/vol-cache.git

Parallel Write (H5Dwrite)



Node-local storage

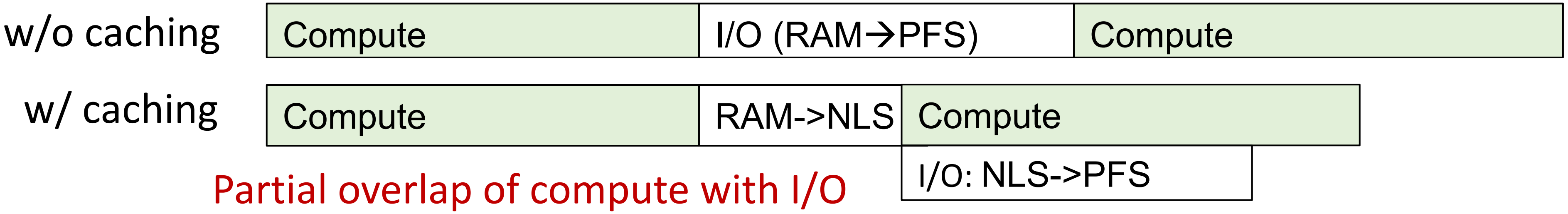
Parallel file system

Shared HDF5 file

1. Data is synchronously copied from the memory buffer to memory mapped files on the node-local storage using POSIX I/O.

2. Move data from memory mapped file to the parallel file system asynchronously by calling the dataset write function from the *Async VOL* stacked below the Cache VOL

3. Wait for all the tasks to finish in H5Dclose() / H5Fclose()



w/o caching

Compute

I/O (RAM→PFS)

Compute

w/ caching

Compute

RAM->NLS

Compute

I/O: NLS->PFS

Partial overlap of compute with I/O

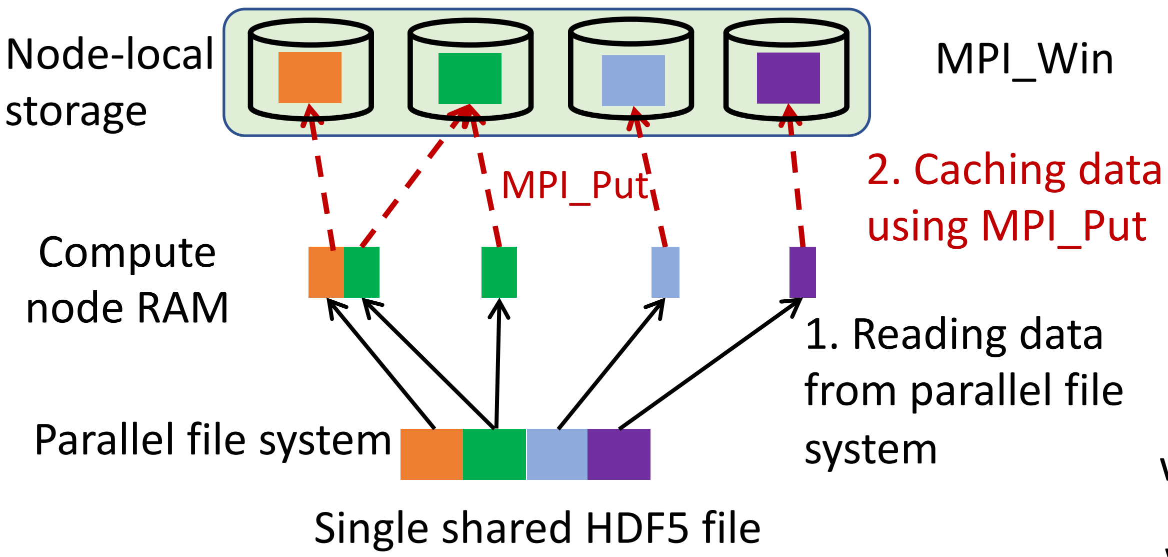
Details are hidden from the application developers.

Parallel Read (H5Dread)

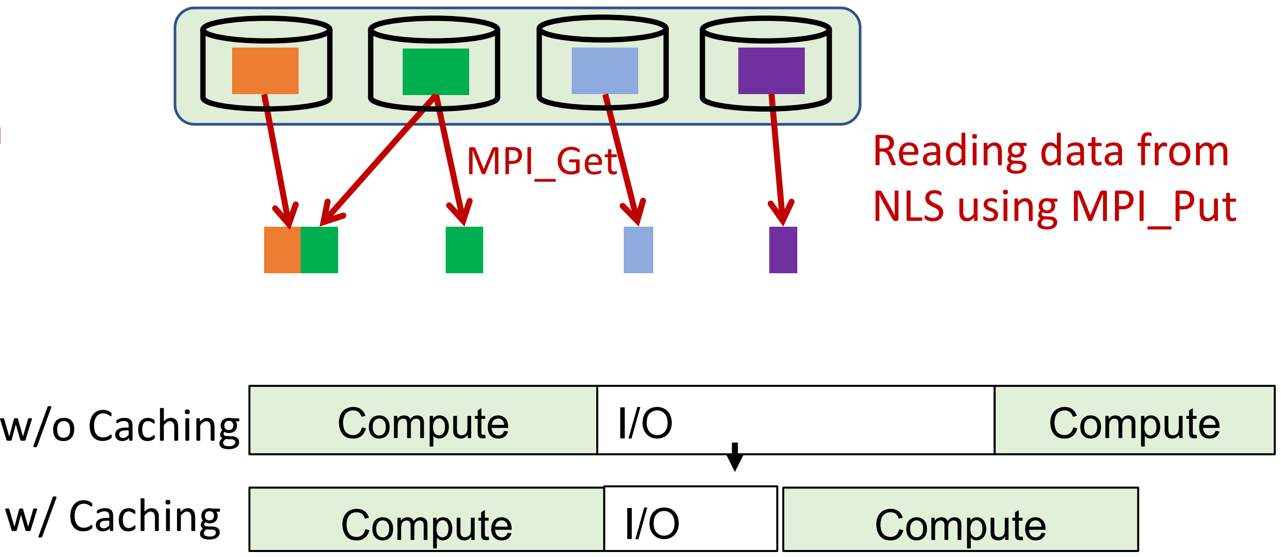
One-sided communication for accessing remote node storage.

- Each process exposes a part of its memory to other processes (MPI Window)
- Other processes can directly read from or write to this memory, without requiring that the remote process synchronize (MPI_Put, MPI_Get)

Create memory mapped files and attached them to a MPI_Win for one-sided remote access

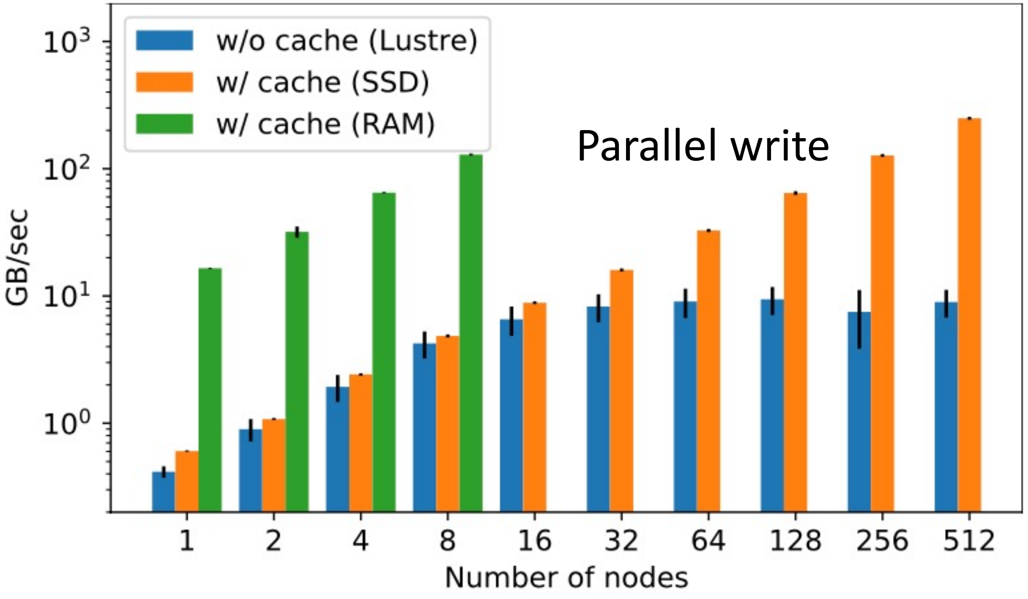


First time reading the data

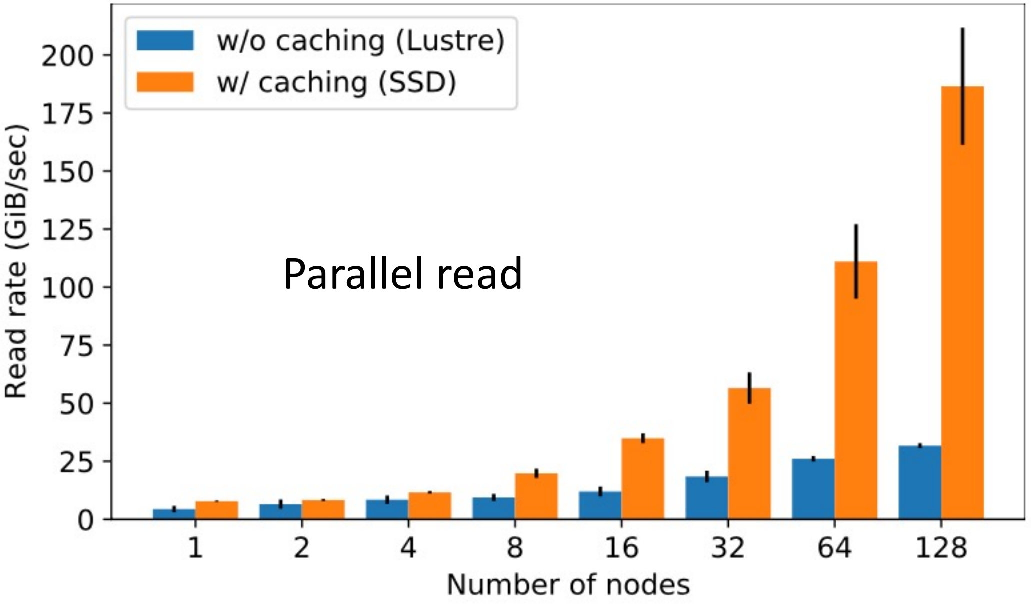


Reading the data directly from node-local storage

Performance evaluation on Theta @ ALCF



Parallel write performance on Theta w/ and w/o caching data on RAM or node-local SSDs. (Lustre stripe count is 48, and Lustre stripe size is 16MB). Each processor writes 16 MB data to a shared file.



Parallel read performance on Theta. At each step, each processor reads a random batch (32) of samples (224×224×3) from a shared HDF5 file. All the processors together read the entire dataset in one iteration. The read performance is measured after the first iteration finishes.

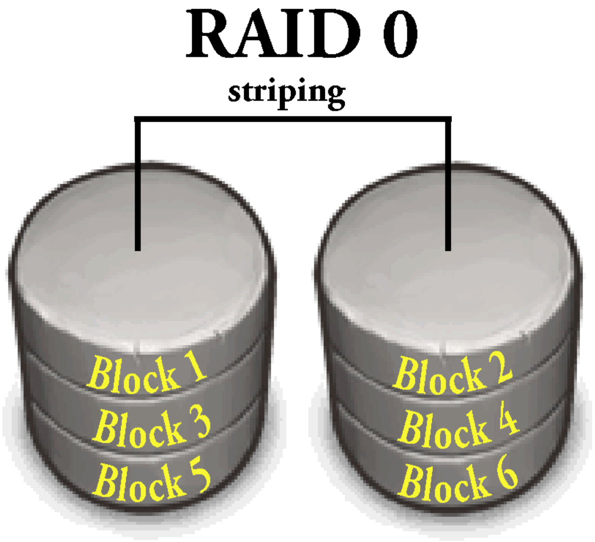
VCD100: VOL Connector Development 100

- **Subscribe to the hdf5vol mailing list:**
  - Email hdf5vol-subscribe@hdfgroup.org with “subscribe” as subject
- **Clone the “external pass-through” example VOL connector**
  - An “external” VOL connector that has all VOL callbacks implemented as transparent “no-ops”, just invoking the underlying VOL connector
    - External VOL connectors can be loaded with environment variables
  - https://bitbucket.hdfgroup.org/projects/HDF5VOL/repos/external_pass_through/browse
- **Build the external pass-through connector with logging enabled:**
  - Follow instructions in README in the git repo
  - **Modify to your purposes**

Subfiling

Main developer: THG devs

- Subfiling: a compromise between file-per-process (*fpp*) and a single shared file (*ssf*)
  - Multiple files are organized as a Software RAID-0 Implementation
    1. Configurable “stripe-depth” and “stripe-set size”
    2. A default “stripe-set” is created by using 1 file per node
    3. A default “stripe-depth” is 32MB
  - One metadata (.h5) file *stitching* the small files together

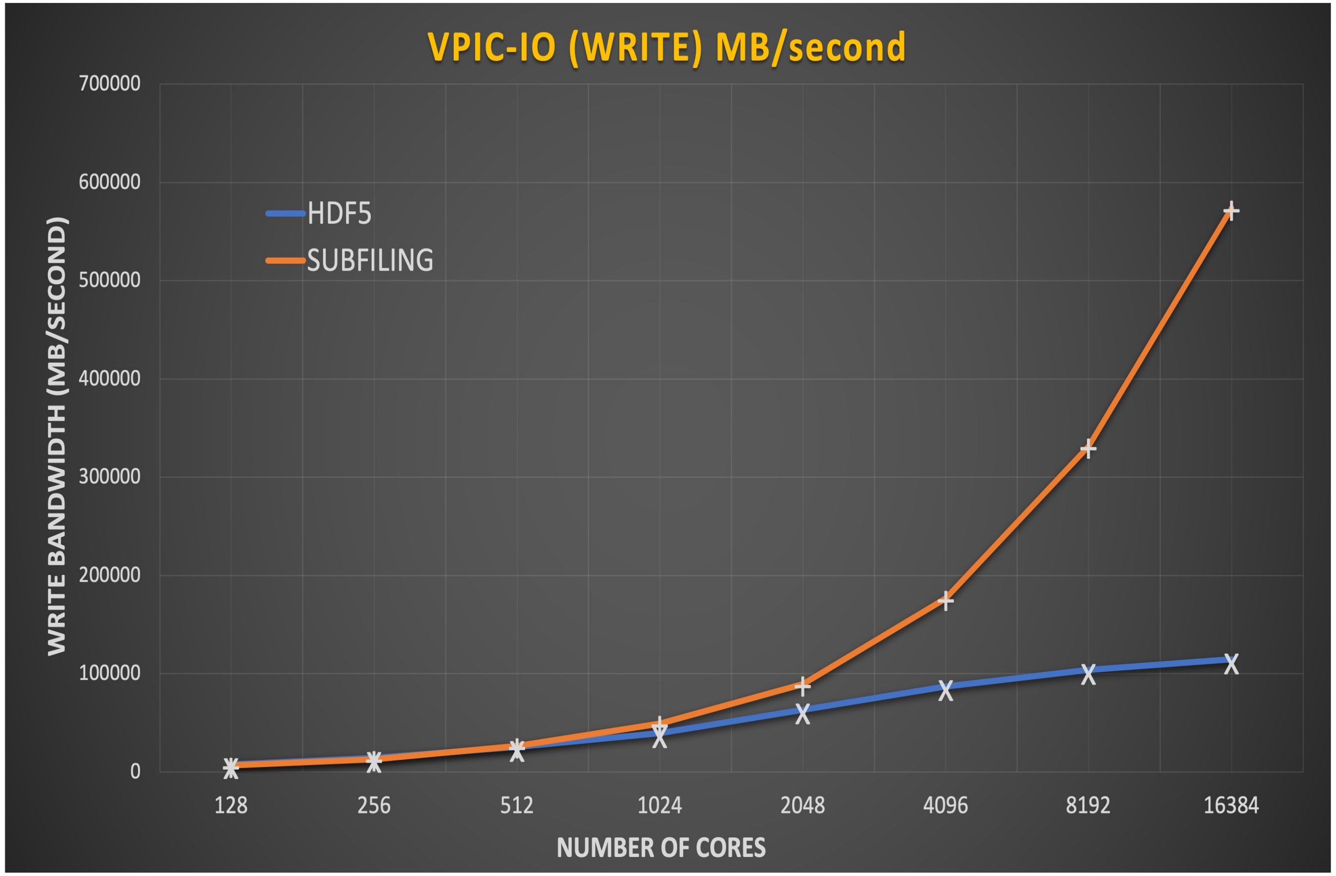


- Benefits
  - Better use of parallel I/O subsystem
  - Reduces the complexity of *fpp*
  - Reduced locking and contention issues to improve performance at larger processor counts over *sff*

Subfiling - Initial results

(h5bench – write benchmark)

- Parallel runs on *SUMMIT* showing results from 256 to 16384 cores.
- The number of *Subfiles* utilized range from **6** (for a 256 MPI rank application run) to **391** (for the 16K MPI rank application); based on 42 cores per node.



Feature: Querying datasets

Main developer: THG devs

Objective

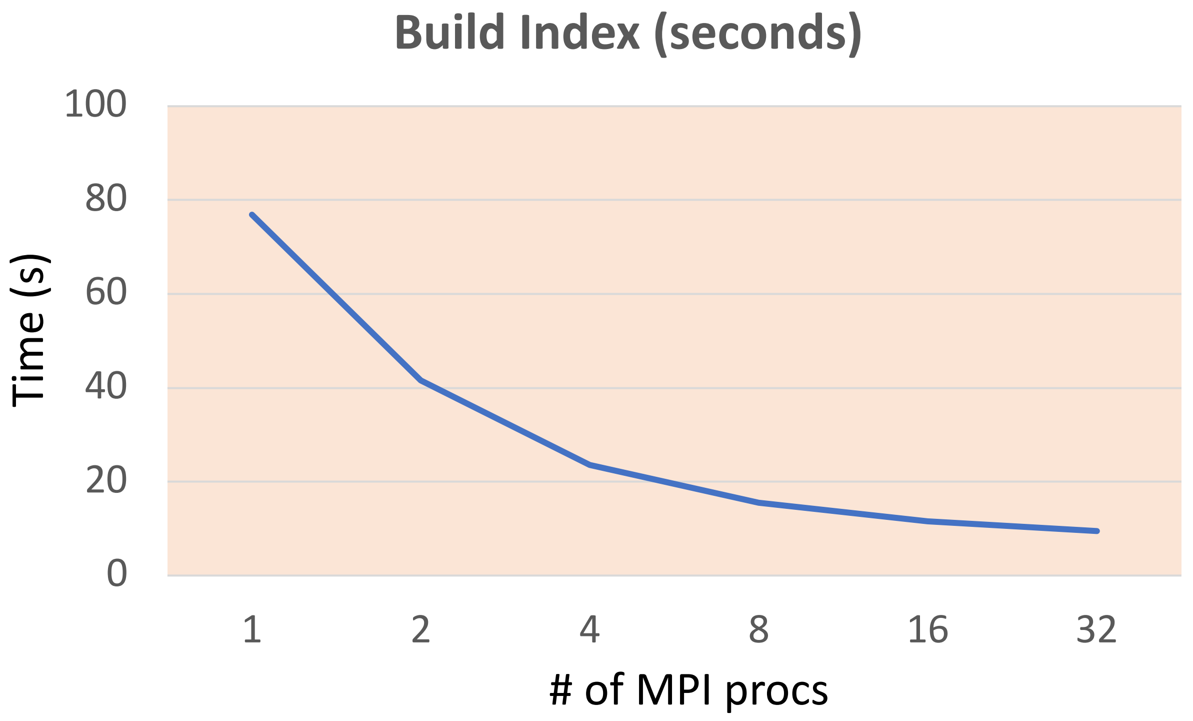
- Create complex queries on both metadata and data elements within a HDF5 container
- Retrieve the results of applying those query operations.

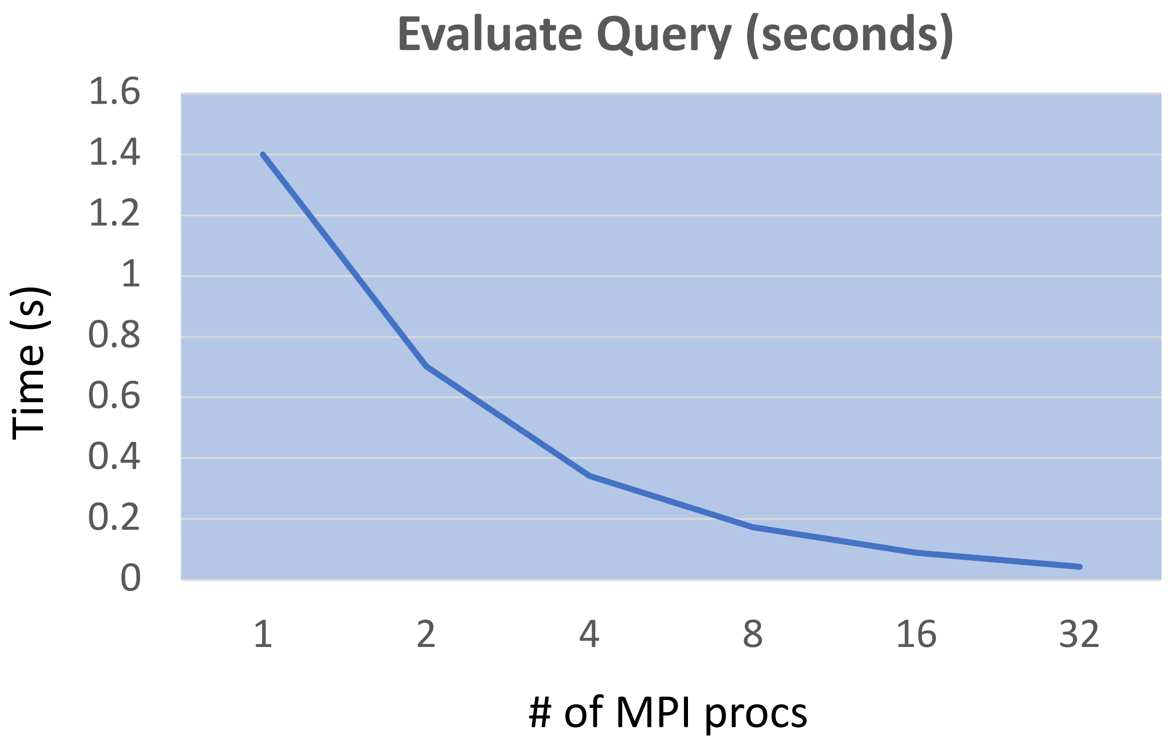
Solution

- HDF5 *query* API routines enable the construction of query requests for execution on HDF5 containers
  - H5Qcreate
  - H5Qcombine
  - H5Qapply
  - H5Qclose
- HDF5 *index* API routines allow the creation of indexes on the contents of HDF5 objects, to improve query performance

HDF5 github repo containing the *querying and indexing* source code:
https://github.com/HDFGroup/hdf5/tree/feature/indexing

Querying and Indexing





Parallel scaling of index generation and query resolution is evidenced even for small-scale experiments.

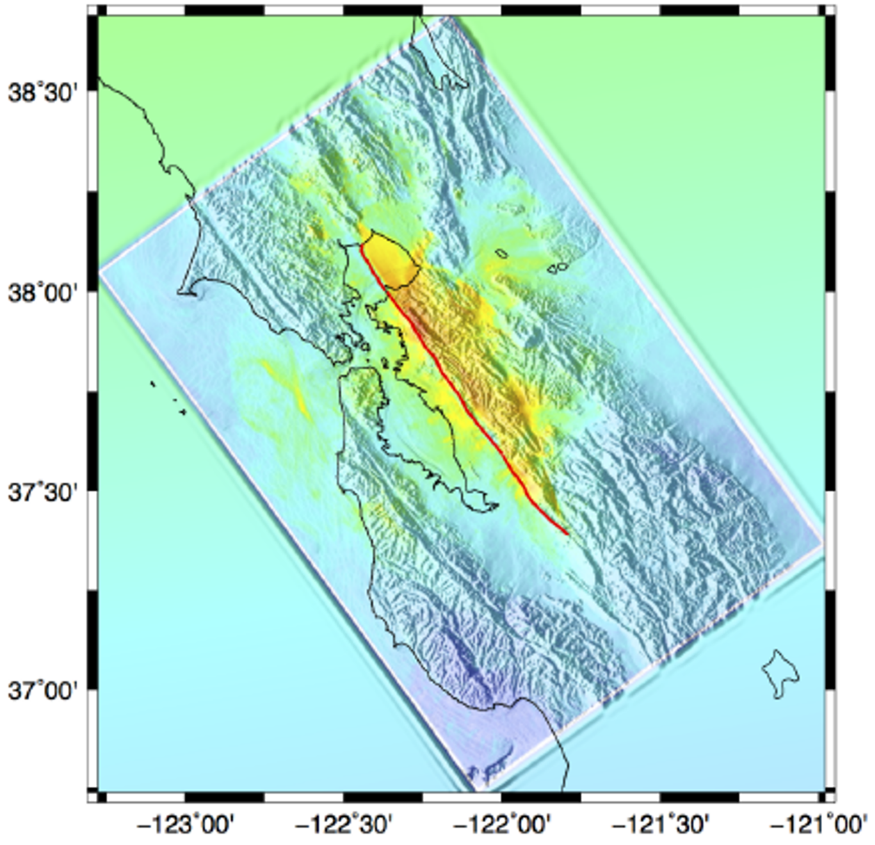
ECP HDF5 Applications

EQSIM

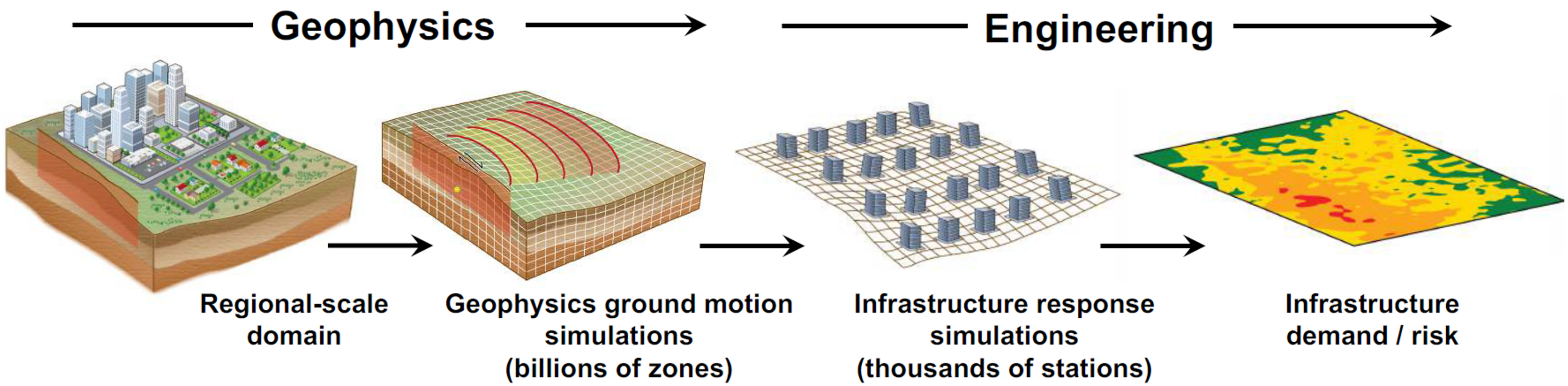
- High-Performance, Multidisciplinary Simulation for Regional-Scale Earthquake Hazard and Risk Assessments

- Provide the first **strong coupling** and **linkage** between simulations of earthquake ***hazards*** (ground motions) and ***risk*** (structural system demands).

- **SW4**, main code to simulate seismic wave propagation.



EQSIM Workflow



Geophysics

Engineering

Regional-scale domain

Geophysics ground motion simulations (billions of zones)

Infrastructure response simulations (thousands of stations)

Infrastructure demand / risk

- Seismologists sets up an earthquake event for simulation.

Various input data

- SW4 generates and outputs ground motions for specified locations.

1D, 2D, 3D, 4D output data

- Analysis codes (OpenSees, ESSI) produces building response.

Visualization and analysis data

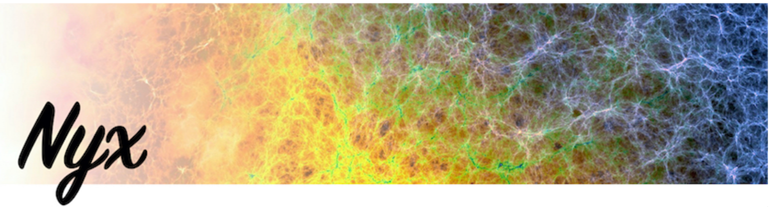
SW4 I/O with HDF5 integration

- **Input**
  - Material model and topography: **sfile**: ½ size, 3x faster, new curvilinear grid.
  - Forcing function: **SRF-HDF5**: 1/3 size, 5x faster.
  - Station location: **inputHDF5**: single file.

- **Output**
  - Time-series
    - Station output: **SAC-HDF5**: 1/5 USGS, same as SAC, ***single*** file
    - Subsurface output: **SSI**, with ZFP compression (**155GB** / **38TB**), 3x faster
  - Image: **imgHDF5**, same as native, easy to access
  - Checkpoint: **chkHDF5** with ZFP compression - 4x to 6x less data (optimization WIP)

AMReX Applications

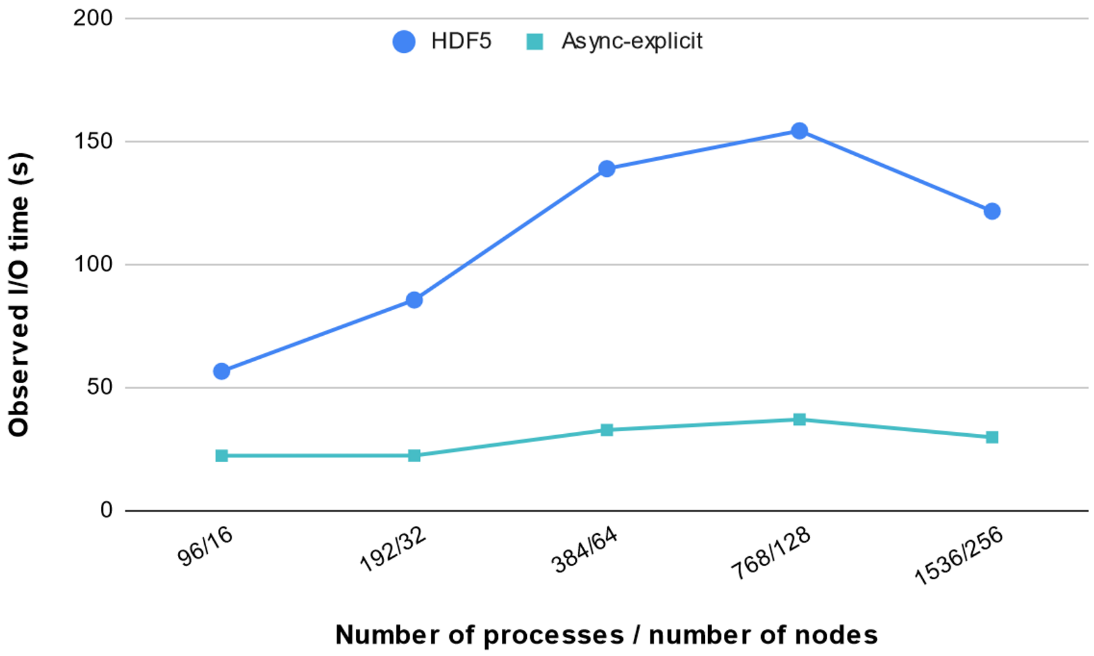
- AMReX is a software framework for massively parallel, block-structured adaptive mesh refinement (AMR) applications.
- HDF5 output format is supported for writing plotfiles and particle data, asynchronous I/O can also be enabled.



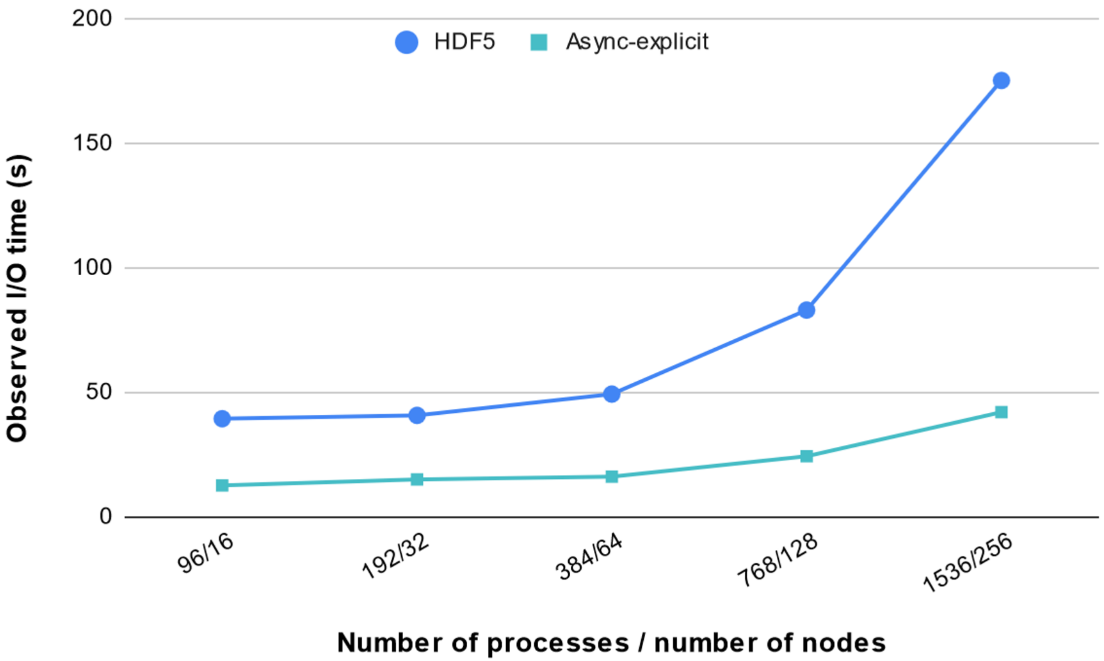
Nyx is an adaptive mesh, massively-parallel, cosmological simulation code.

Castro is an adaptive-mesh compressible radiation / MHD / hydrodynamics code for astrophysical flows.

Results on Summit



Single-level (Nyx) Workload

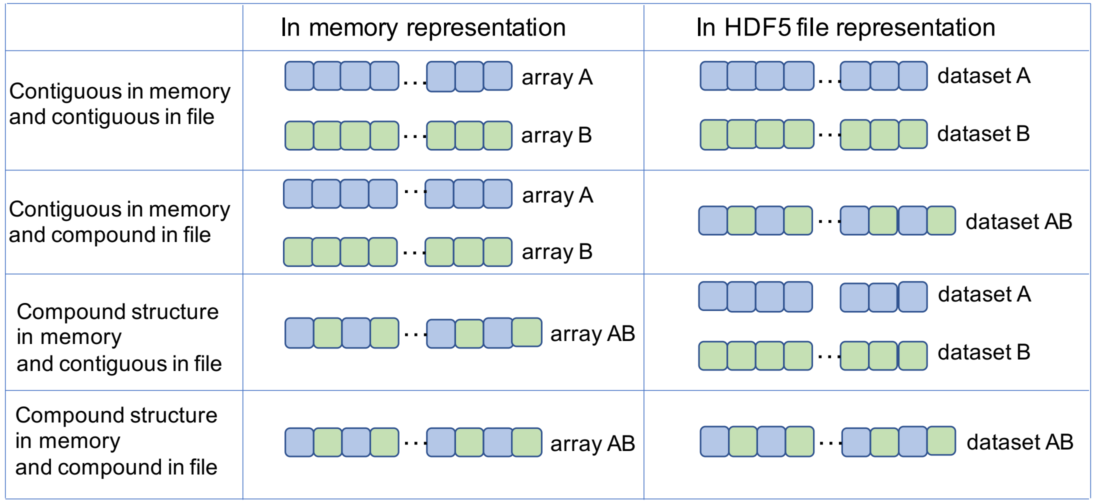


Multiple-level (Castro) Workload

h5bench - A suite of HDF5 benchmarks

https://github.com/hpc-io/h5bench

- Captures various I/O patterns
    - Locality in memory and in files
        - Contiguous, strided, compound data types
    - Array dimensionality - 1D, 2D, and 3D
- I/O modes
    - Synchronous
    - Asynchronous - Implicit and explicit
- Processor type - CPUs and GPUs
- MPI-IO modes
    - Collective buffering on or off
- File system configuration
    - Alignment and striping



	In memory representation	In HDF5 file representation
Contiguous in memory and contiguous in file	array A array B	dataset A dataset B
Contiguous in memory and compound in file	array A array B	dataset AB
Compound structure in memory and contiguous in file	array AB	dataset A dataset B
Compound structure in memory and compound in file	array AB	dataset AB

Conclusions

- Testing of stacking of asynchronous I/O and cache VOL is in progress
- Try h5bench for verifying HDF5 performance at scale
  - Feedback and adding more I/O patterns are welcome
- Subfiling development is in progress
- Contact us if you have any querying use cases
- Contact us with any HDF5 performance or functionality problems
  - The HDF Group: Helpdesk at help@hdfgroup.org
  - HDF5 resources: https://www.hdfgroup.org/
  - ECP ExaIO: SByna@lbl.gov

Useful links and info

- HDF5 tutorials
  - https://github.com/HDFGroup/Tutorial
  - Parallel HDF5 hands-on tutorial examples
    - https://github.com/HDFGroup/Tutorial/tree/main/Parallel-hands-on-tutorial
- HUG 2021 (HDF5 User Group) meeting
  - https://www.hdfgroup.org/hug/hug21
  - Contact: hug@hdfgroup.org
- *HPC Data Management Systems Postdoctoral Scholar position available at LBNL*
  - https://tinyurl.com/2021-sdm-postdoc