Evaluating Asynchronous Parallel IO on HPC Systems

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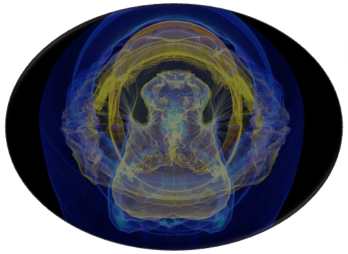
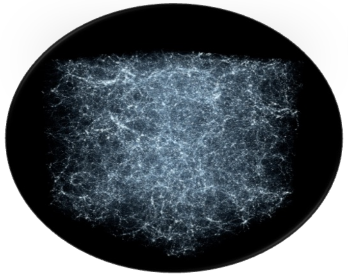
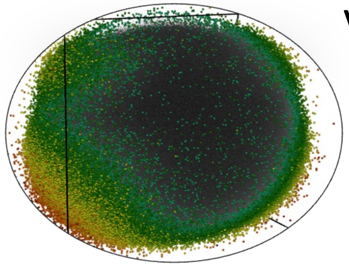
I/O – A critical tool for data storage and access



FLASH



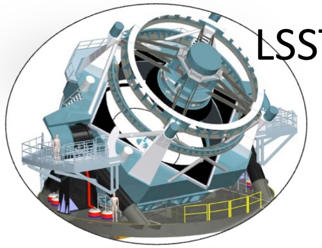
NyX



VPIC

- Simulations
  - Multi-physics (FLASH) – 10 PB
  - Cosmology (NyX) – 10 PB
  - Plasma physics (VPIC) – 1 PB
- Experimental and observational data (EOD)
  - LHC (100 PB),
  - LSST (60 PB),
  - Genomics (100 TB to 1 PB)

LHC

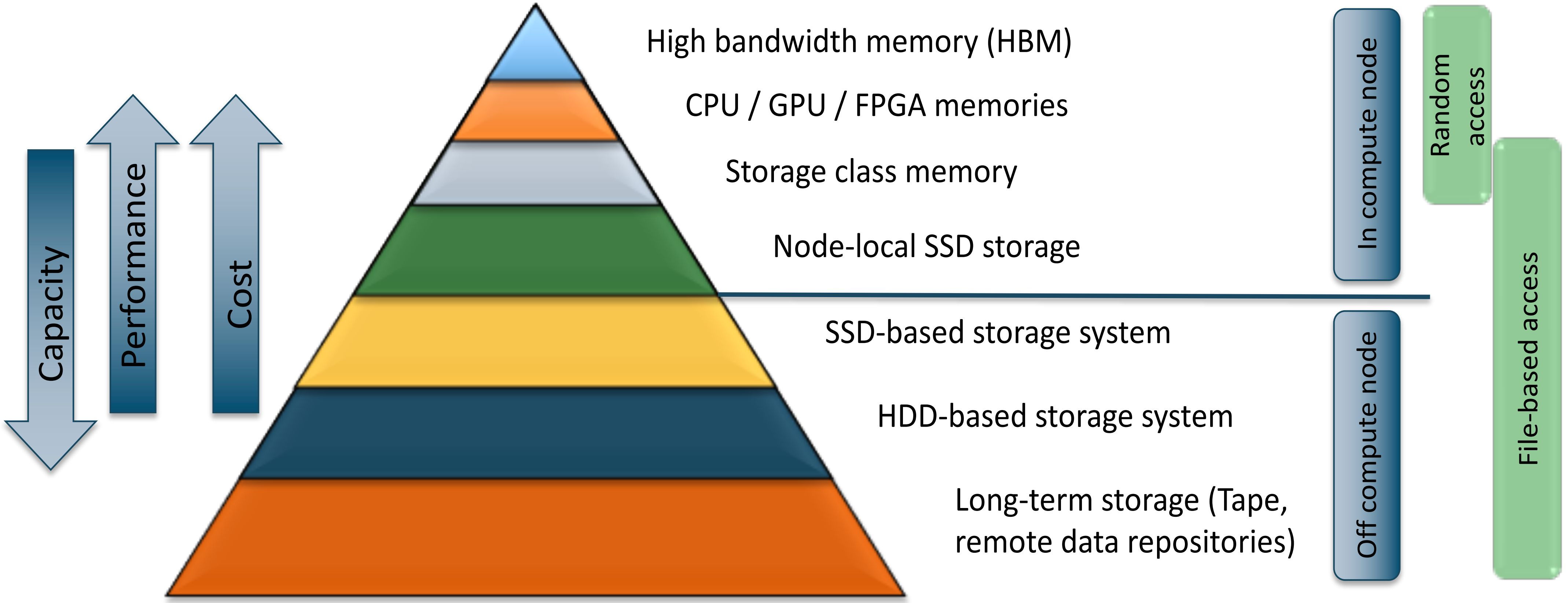


LSST

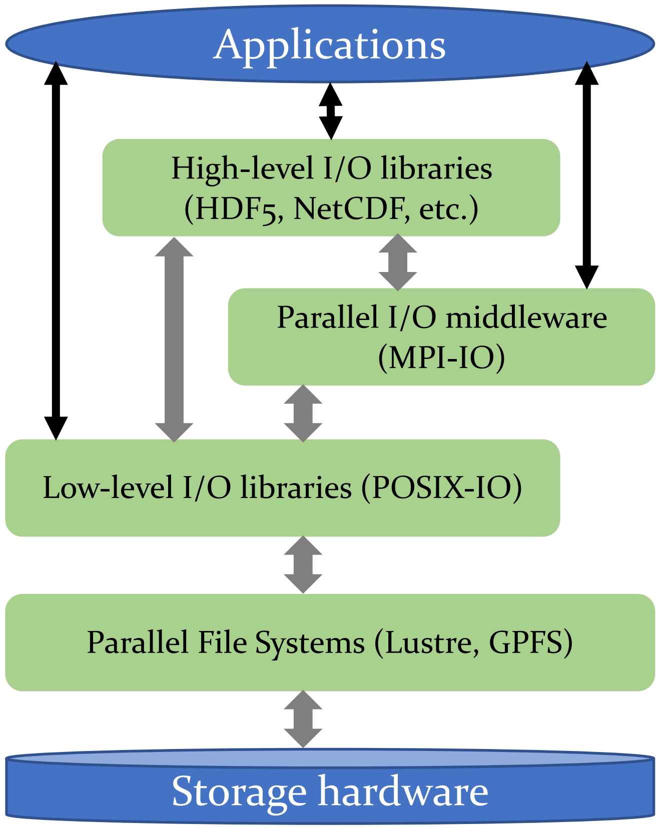
Genomics

Storage and I/O software and hardware are critical for storing and accessing these massive amounts of data.

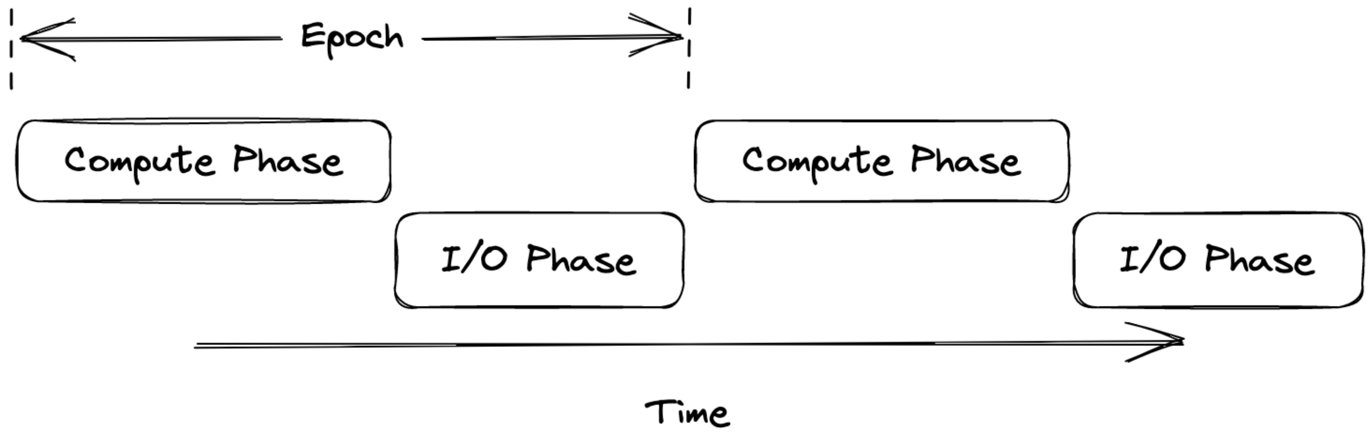
Architectural trends impacting I/O on HPC systems – deep memory and storage hierarchy



Parallel I/O – A stack of software libraries and hardware



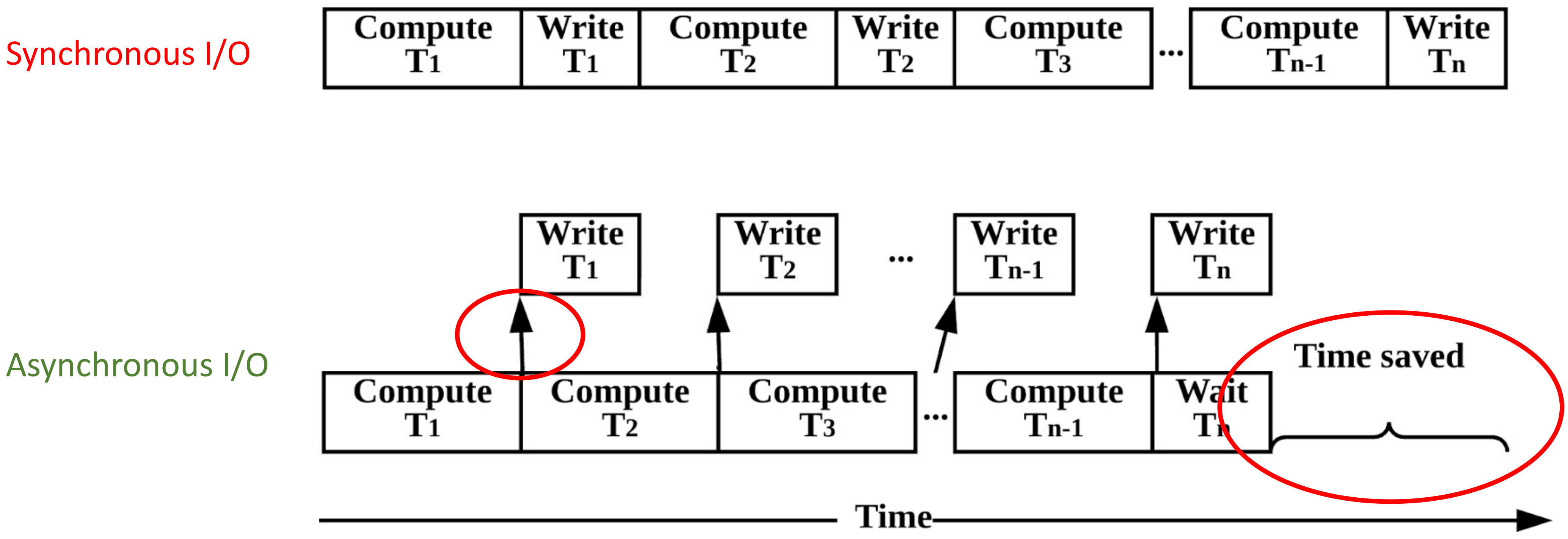
I/O phases could be slow and slowdown applications



- Many large-scale applications have distinct compute and I/O phases
- Simulations checkpoint state or save visualization data
  - *EQSIM* (earthquake simulator), *Nyx* and *Castro* (adaptive mesh refinement, cosmological hydrodynamics)
- Machine learning training iteratively reads data
  - *Cosmoflow (3D convolutional neural network)*

Asynchronous I/O to the rescue

- Hiding I/O latency by overlapping with computation → Common async I/O approach

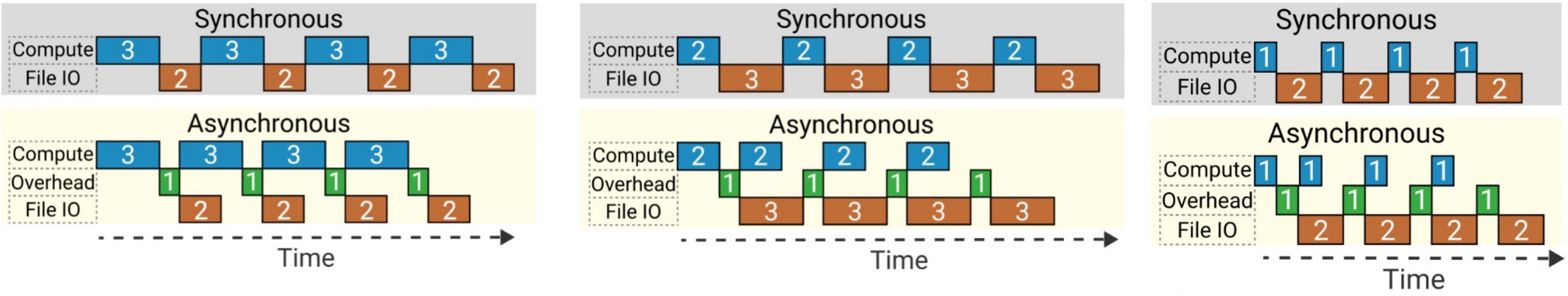


Asynchronous I/O – Implemented in several I/O libraries

- POSIX
- MPI-IO
- ADIOS
- Data Elevator and ARCHIE
- Proactive Data Containers (PDC)
- HDF5

A systematic study of benefits and limitations of asynchronous I/O is lacking

Asynchronous I/O Scenarios



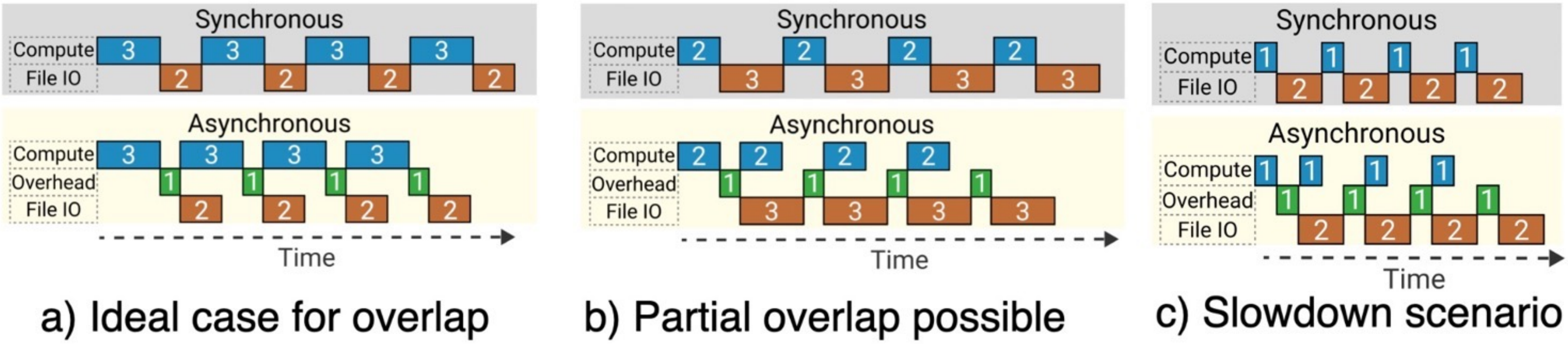
a) Compute Time > I/O Time

b) Compute Time < I/O Time

c) Compute Time <= Overhead

- Computation phase, Overhead for setting up async I/O, I/O latency
- Scenarios
  - Longer computation phases than I/O latency
  - Shorter computation phases than I/O latency

Latency with asynchronous I/O



$$t_{sync\_epoch} = t_{io} + t_{comp}$$

$$t_{async\_epoch} = max(t_{comp}, t_{io} - t_{comp}) + t_{transact\_overhead}$$

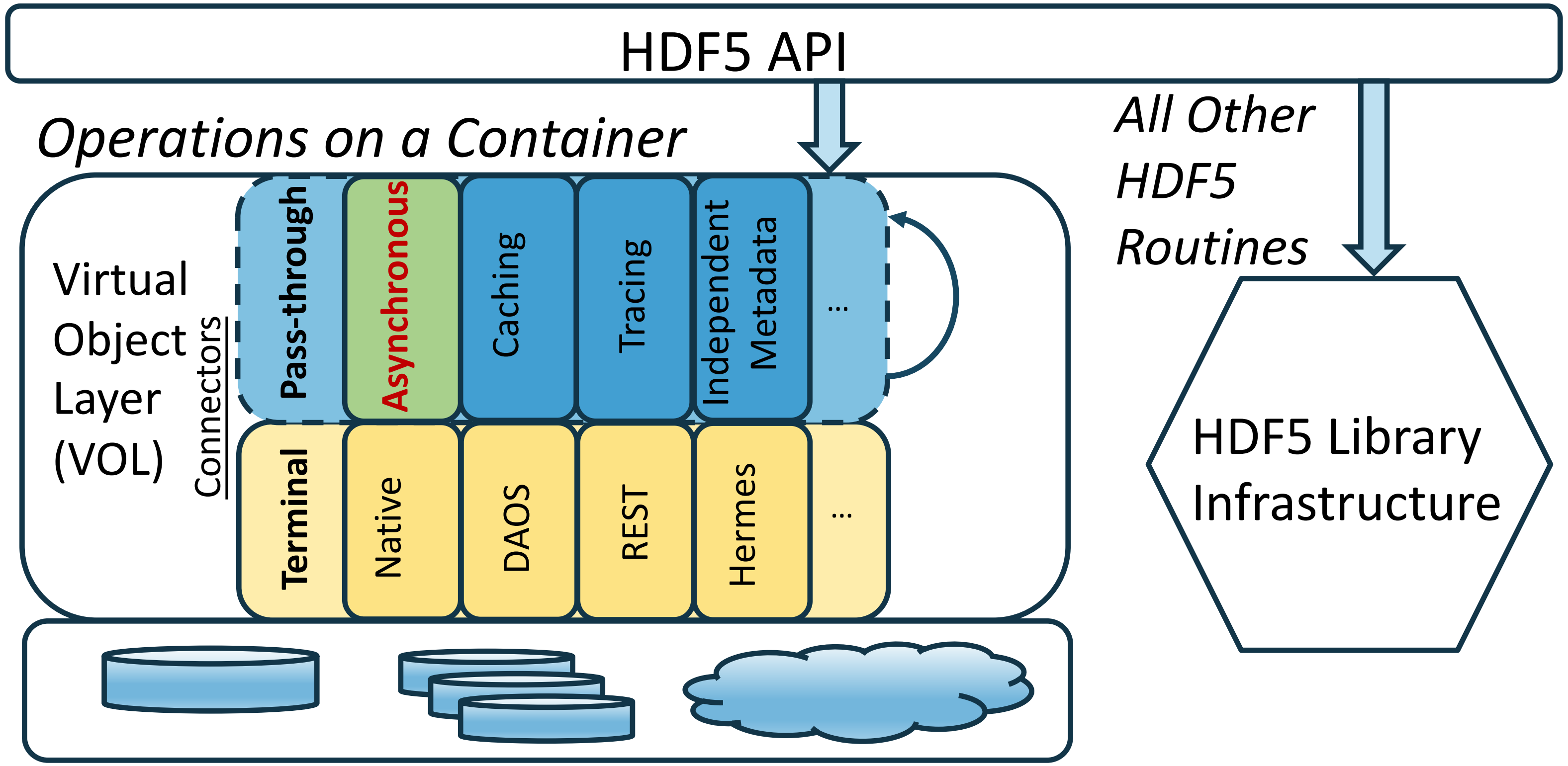
$$t_{io} = \frac{data\_size}{f_{io\_rate}}$$

Depends on an implementation of async I/O

- Background threads
- Extra buffering
- Communication for buffering
- Shared computation and communication resources
- Pressure on file system and I/O from other jobs

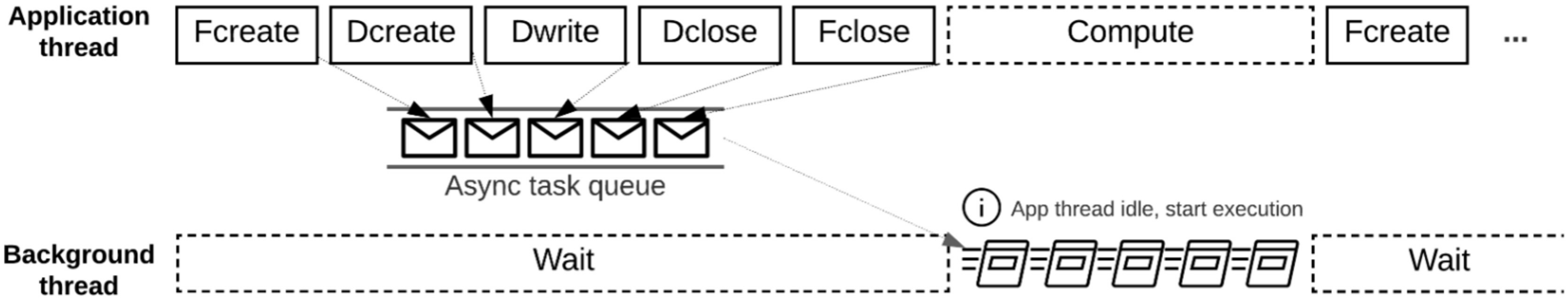
Asynchronous I/O in HDF5 – Intro to Virtual Object Layer (VOL)

- VOL allows “intercepting” HDF5 public API and implementing a different approach to storage and access



Asynchronous I/O in HDF5 – Using background threads

- A pass-through VOL connector for implementing asynchronous I/O
- Asynchronous task queue
- Transparent background thread execution



Explicit Control with Async and EventSet APIs

- Async version of HDF5 APIs
  - `H5Fcreate_async(fname, …, es_id);`
  - `H5Dwrite_async(dset, …, es_id);`
  - …

- Track and inspect multiple I/O operations with an ***EventSet ID***
  - `H5EScreate();`
  - `H5ESwait(es_id, timeout, &remaining, &op_failed);`
  - `H5ESget_err_info(es_id, ...);`
  - `H5ESclose(es_id);`

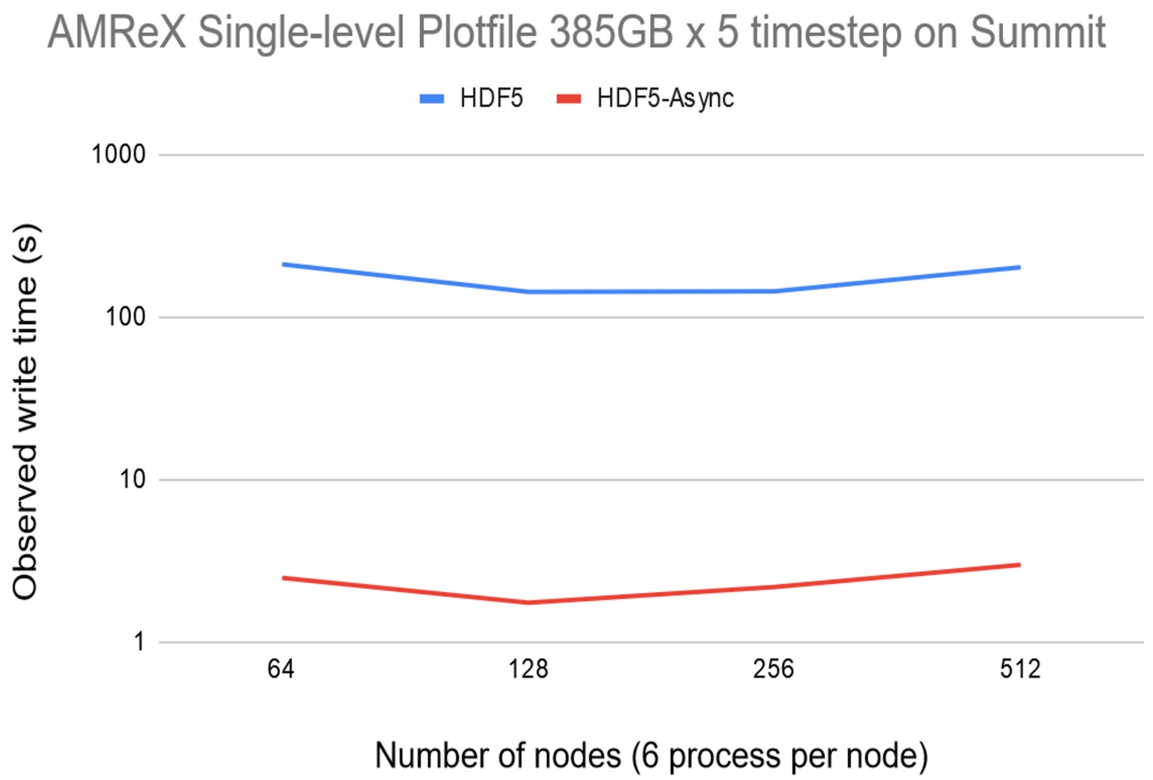
Converting Existing HDF5 Codes

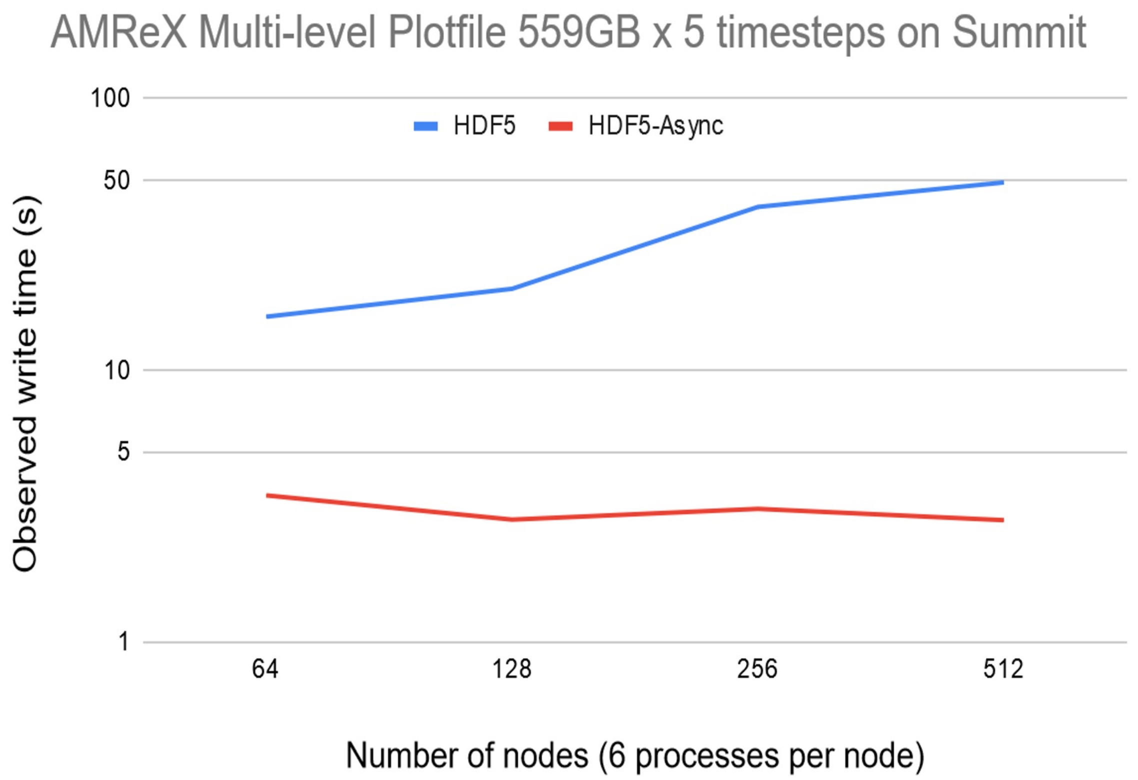
```
// Synchronous file create
fid = H5Fcreate(...);
// Synchronous group create
gid = H5Gcreate(fid, ...);
// Synchronous dataset create
did = H5Dcreate(gid, ..);
// Synchronous dataset write
status = H5Dwrite(did, ..);
// Synchronous dataset read
status = H5Dread(did, ..);
...
// Synchronous file close
H5Fclose(fid);
// Continue to computation

...

...
// Finalize
```

```
// Create an event set to track async operations
es_id = H5EScreate();
// Asynchronous file create
fid = H5Fcreate_async(.., es_id);
// Asynchronous group create
gid = H5Gcreate_async(fid, .., es_id);
// Asynchronous dataset create
did = H5Dcreate_async(gid, .., es_id);
// Asynchronous dataset write
status = H5Dwrite_async(did, .., es_id);
// Asynchronous dataset read
status = H5Dread_async(did, .., es_id);
...
// Asynchronous file close
status = H5Fclose_async(fid, .., es_id);
// Continue to computation, overlapping with asynchronous
    operations
...
// Finished computation, Wait for all previous operations in the
    event set to complete
H5ESwait(es_id, H5ES_WAIT_FOREVER, &n_running, &op_failed);
// Close the event set
H5ESclose(es_id);
...
// Finalize
```

Detailed description in https://github.com/hpc-io/vol-async

Async HDF5 VOL Connector – Benefits

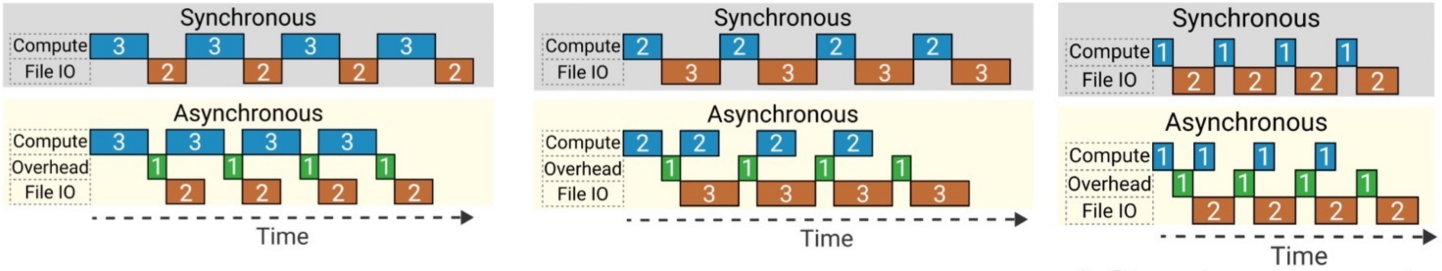




Houjun Tang, Quincey Koziol, John Ravi, and Suren Byna, "Transparent Asynchronous Parallel I/O using Background Threads", IEEE TPDS - Special Section on Innovative R&D toward the Exascale Era, 2021

Questions for a detailed evaluation

- For computation phases longer than I/O phases, async I/O is beneficial
- What about other conditions?
  - When does asynchronous I/O slow down applications?

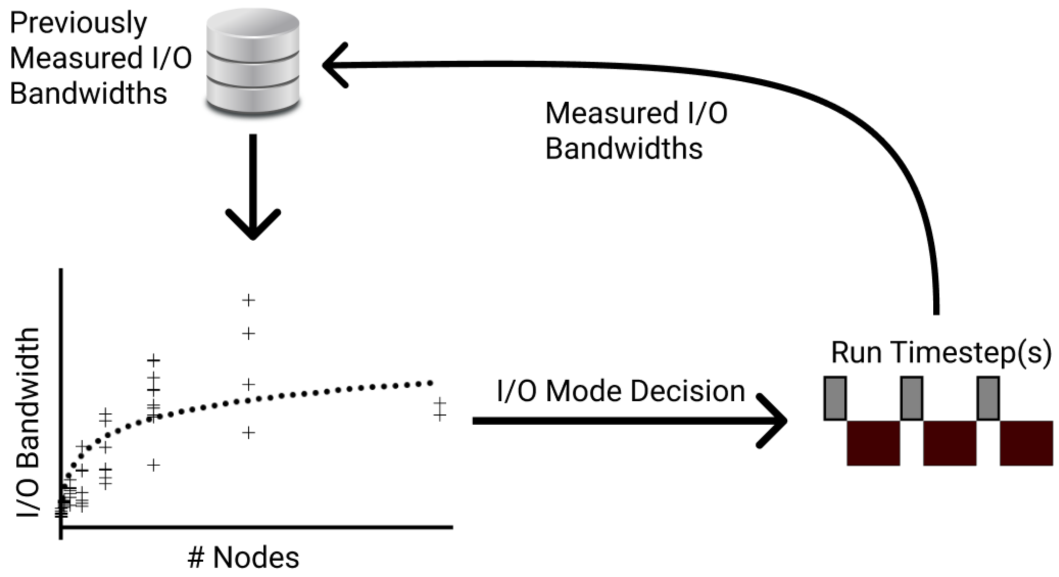


a) Ideal case for overlap b) Partial overlap possible c) Slowdown scenario

- Can we predict synchronous and asynchronous I/O time to decide on using them?

Experimental evaluation

- Systems
  - Summit at OLCF with ~4k nodes with GPFS Parallel File system
  - Cori at NERSC with ~12k nodes with Lustre Parallel File System
- Estimation of I/O cost
  - Empirical model using linear regression
  - Aggregate bandwidth scales with data size, # ranks for each I/O request



Benchmarks and Applications

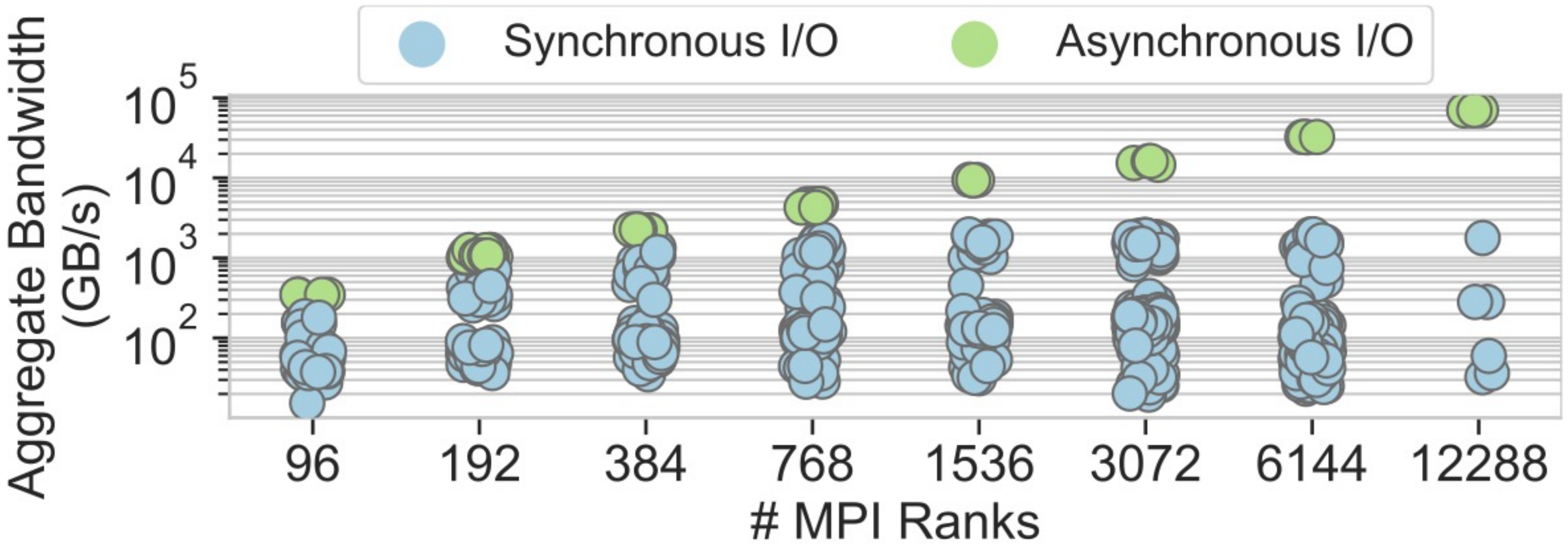
- VPIC-IO
  - A data write benchmark, extracted from a plasma physics simulation
- BD-CATS-IO
  - A read benchmark, extracted from a clustering analysis code
- Nyx
  - A massively parallel, adaptive mesh, cosmology simulation code
- Castro
  - A cosmology simulation solving compressible radiation & hydrodynamics equations
- EQSIM
  - A regional earthquake simulation code
- Cosmoflow
  - A deep learning code to process large 3D matter distributions using CNN

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

Configurations

I/O kernel / App	Data dimensions	Other notes
VPIC-IO	8 variables, 2^{10} particles	1D HDF5 dataset
BD-CATS-IO	Any number of given variables, 2^{10} particles	Same as VPIC-IO, read pattern
Nyx	Small: 256x256x256, every 20 time steps	20 MB data per time step
	Large: 2048x2048x2048 dimensions, every 50 time steps	10 GB data per time step
Castro	128x128x128 dimensions with 6 components in each multi-fab and 2 particles per cell	128 MB data per time step
EQSIM	Grid size of 50 with 30000x30000x17000 dimensions; checkpoint every 100 time steps	Computation phases are often very long compared to checkpointing phases
Cosmoflow	128^3 Voxels dataset, 4 epochs and with batch size of 8	Computation on GPUs, data for I/O is transferred to main memory before CPU performs I/O.

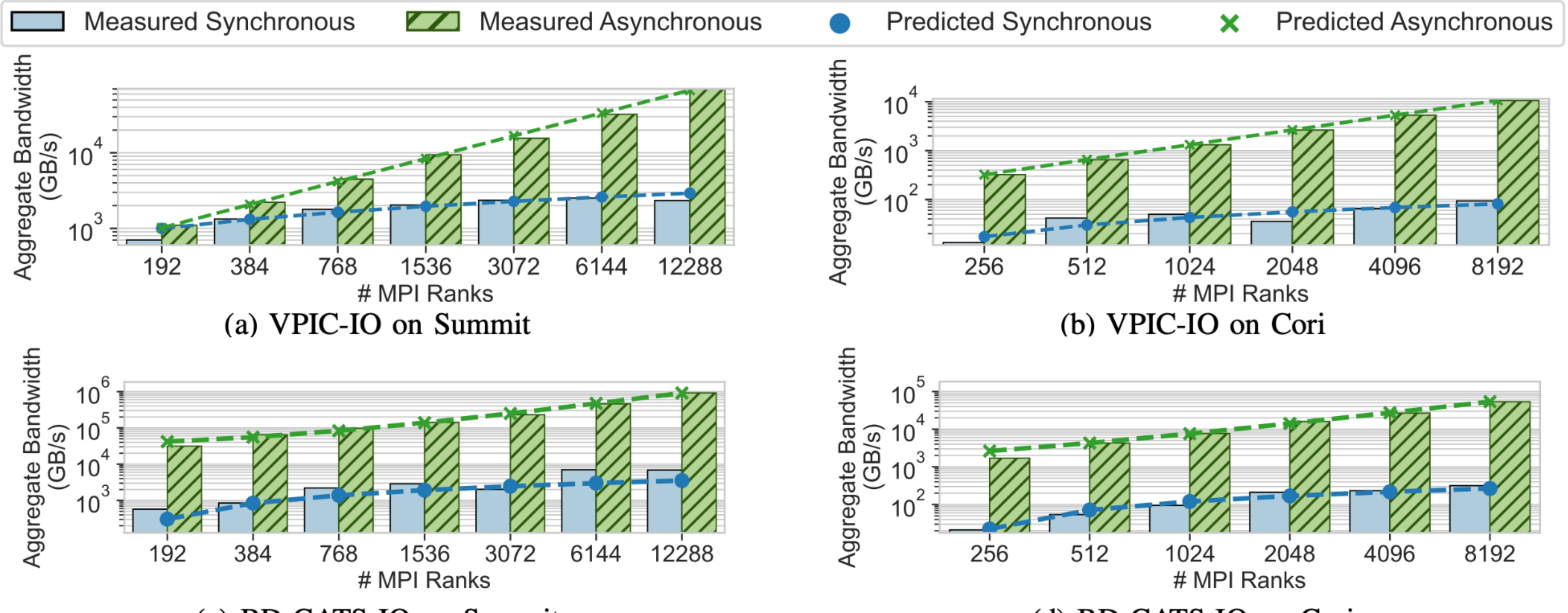
Estimation of I/O cost



VPIC-IO on Summit

- Each point represents a separate run at a different time
- Synchronous I/O varies in performance (about 2 orders of magnitude at high node count)
- History of best achieved bandwidth

Weak scaling tests on Summit and Cori

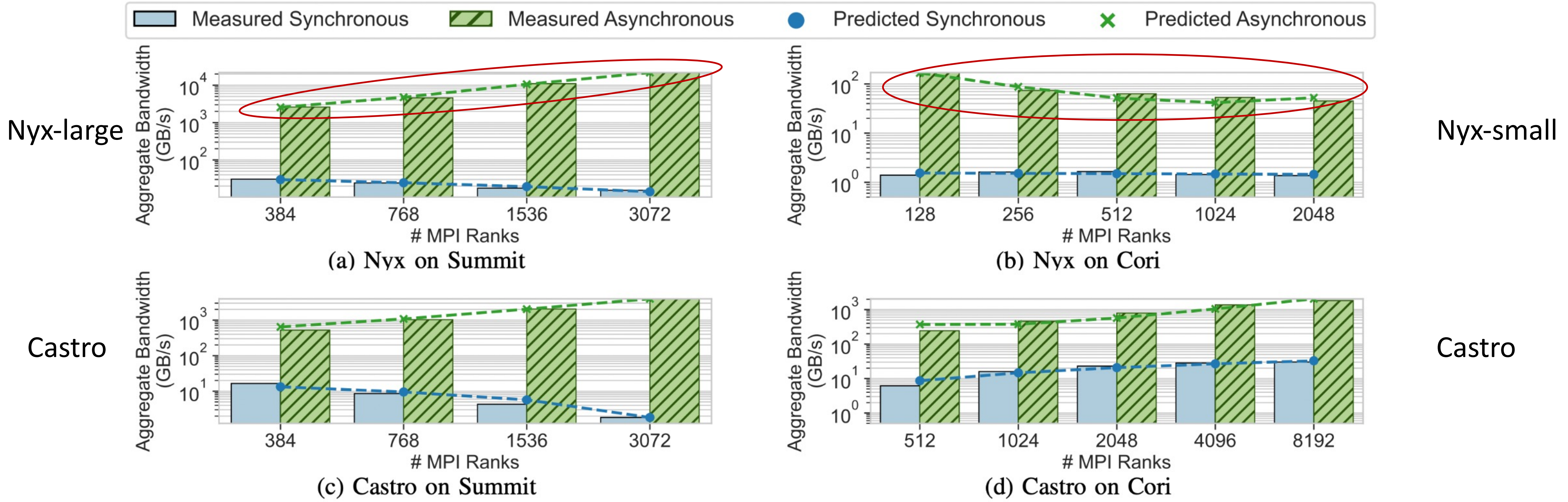


(a) VPIC-IO on Summit (b) VPIC-IO on Cori

(c) BD-CATS-IO on Summit (d) BD-CATS-IO on Cori

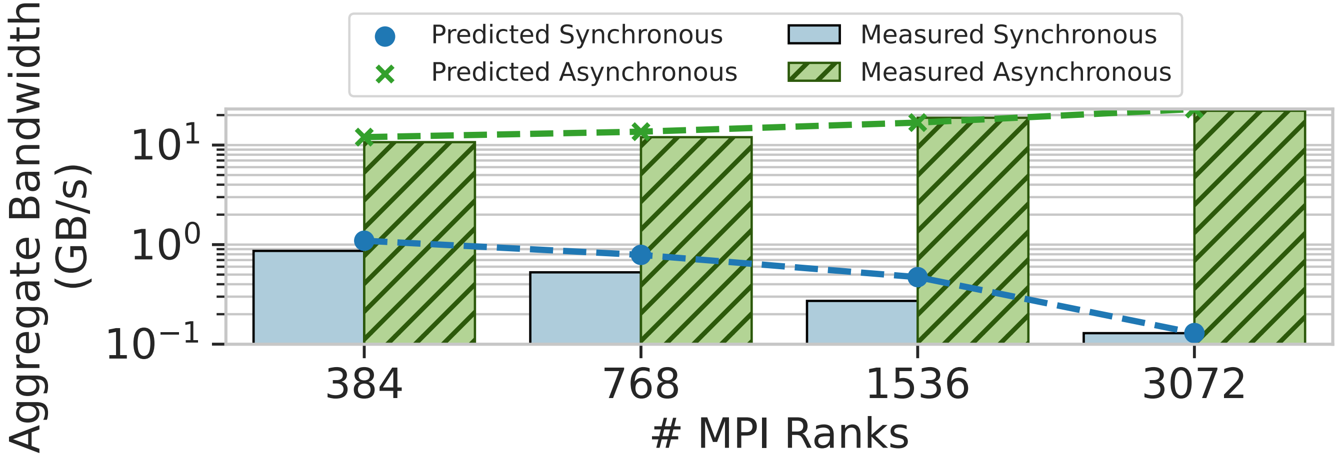
- *The aggregate bandwidth scales similarly on both systems for both synchronous and asynchronous epochs*
- *Analytical model fits well with the trend of synchronous write aggregate bandwidth which is based on a linear-log regression*

Strong scaling tests on Summit and Cori



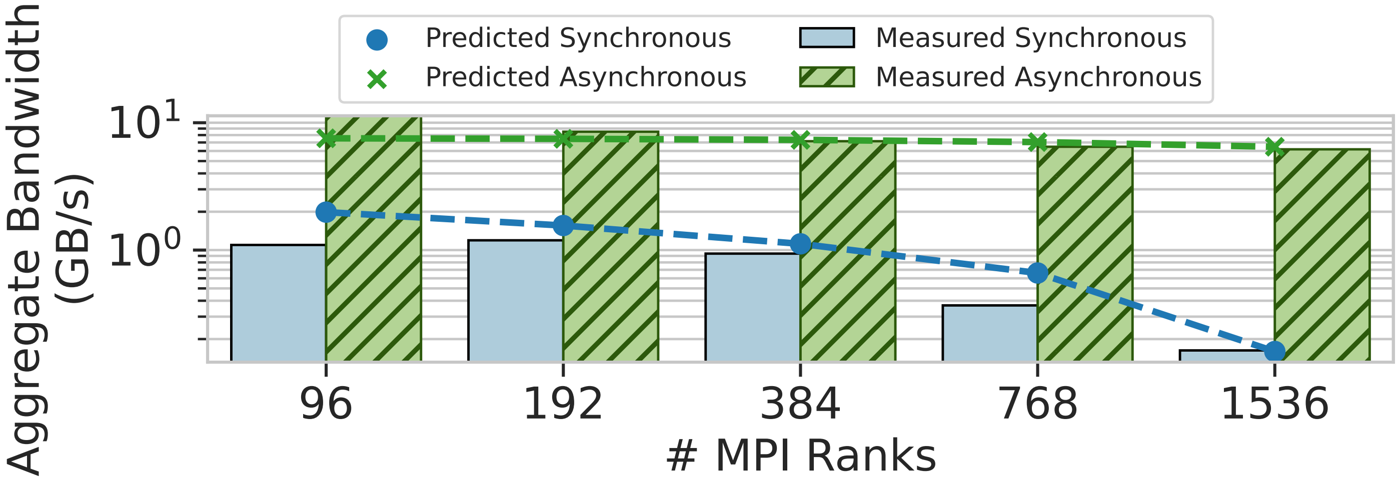
- *The async I/O overhead is low with smaller amount of data (with increasing number of ranks), increases async I/O rate on Summit*
- *On Cori, for smaller data size (Nyx-small configuration), increasing scale doesn't increase I/O rate much. Async I/O still much better than sync I/O*

EQSIM and Cosmoflow – Async I/O wins significantly

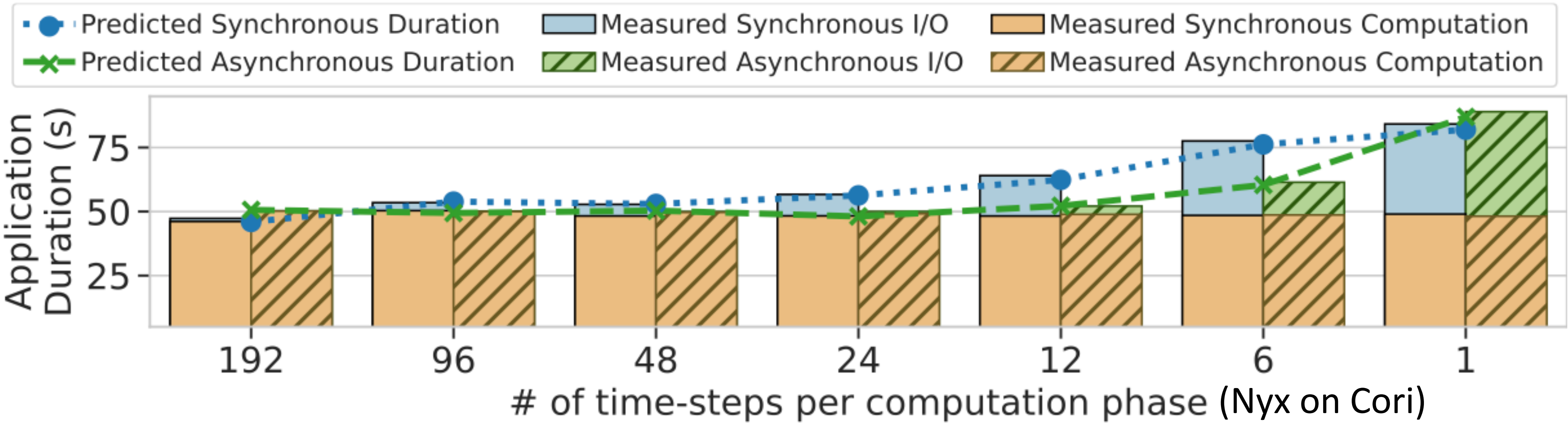


EQSIM on Summit – Synchronous I/O slows down with scale. Async I/O is effective.

Cosmoflow on Summit with GPUs – Synchronous I/O slows down after 128 nodes. Async I/O is effective (includes GPU to CPU memory copy overhead)



Frequent I/O phases with async I/O slows down applications



(Nyx on Cori)

- Checkpointing every timestep with asynchronous I/O enabled resulted in an overall slowdown
- Extra overhead introduced with asynchronous I/O could not be hidden
- Requires a dynamic decision at runtime to enable Asynchronous I/O

Conclusions

- Asynchronous I/O can hide I/O latency in cases where computation > async overhead + I/O time
- Analytical models for estimating I/O latency using linear regression to evaluate efficacy of async I/O
- Model-based automatic selection of async I/O → in progress
- Other Async I/O optimizations
  - Combine multiple small I/O requests → ESSA 2023 paper
  - Multi-dataset I/O in HDF5 to reduce the number of I/O requests

Contact: Suren Byna – https://sbyna.github.io

Async I/O with HDF5: https://github.com/hpc-io/vol-async

Back up slides

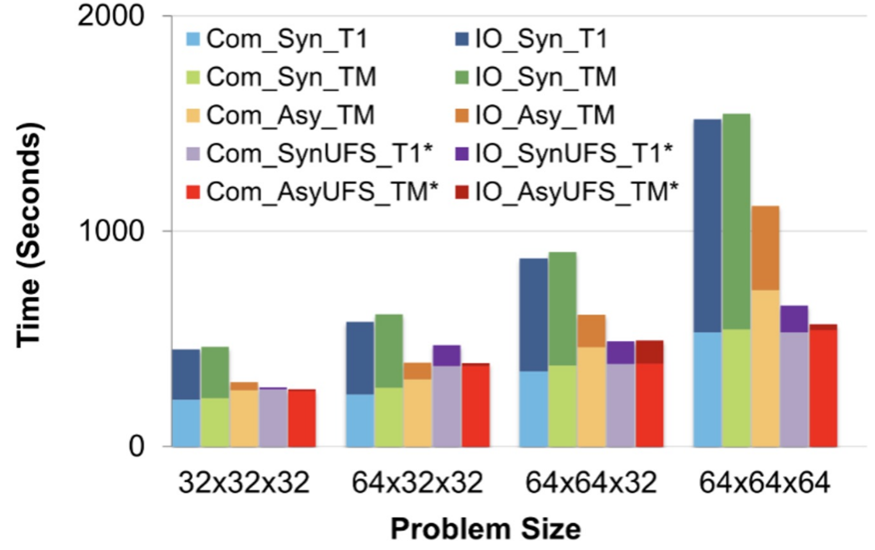
Results: Sod

Sod is a compressible flow explosion problem widely used for verification of shock-capturing simulation codes.

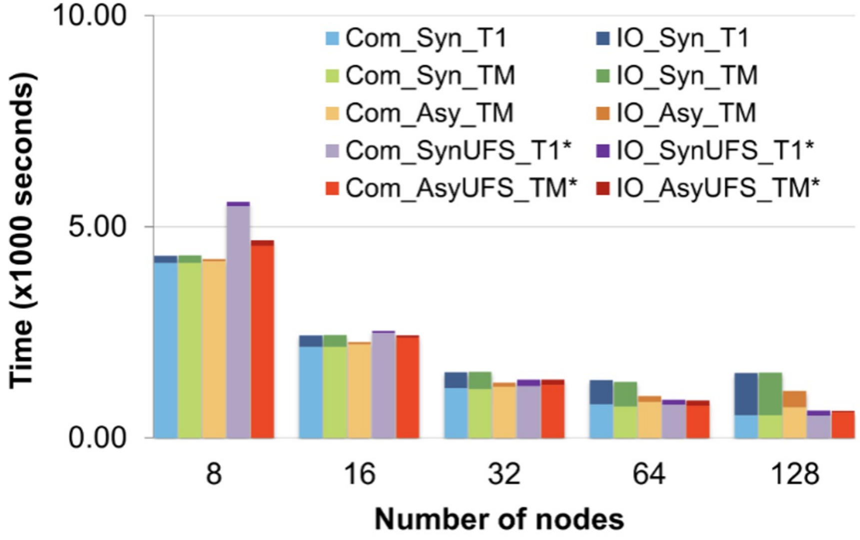
3D Sod problem with tracer particles.

Each runs for 109 steps, writes a checkpoint file every 33 steps, a plot file every 10 steps, and compared the total execution time with 5 different configurations that uses Synchronous and Asynchronous I/O, with and without MPI_THREAD_MULTIPLE, and using GPFS and UnifyFS.

- For cases with async, the majority of the write operations are overlapping with Flash-X's computation. Exceptions include the initial data writes and the last step as there is no computation to overlap with.



(a) Sod - weak scaling, 16 to 128 nodes



(b) Sod - strong scaling, problem size 64x64x64

Rajeev Jain, Houjun Tang, Akash Dhruv, Austin Harris, Suren Byna, Accelerating Flash-X Simulations with Asynchronous I/O, PDSW 2022

Results: Streaming Sine Wave

- The streaming sine wave test problem is a test problem for verifying the correctness of the streaming advection operator in thornado as well as the Flash-X interface to thornado.

- This problem uses GPU and CPU (threading).

- One GPU per MPI rank, and the data is copied from GPU to CPU memory automatically by FLASH-X before being written out

- At a higher number of nodes the interference between COM_ time and IO_ is higher as the I/O time as a whole increases: it is 27.1% for the 256-node synchronous case.

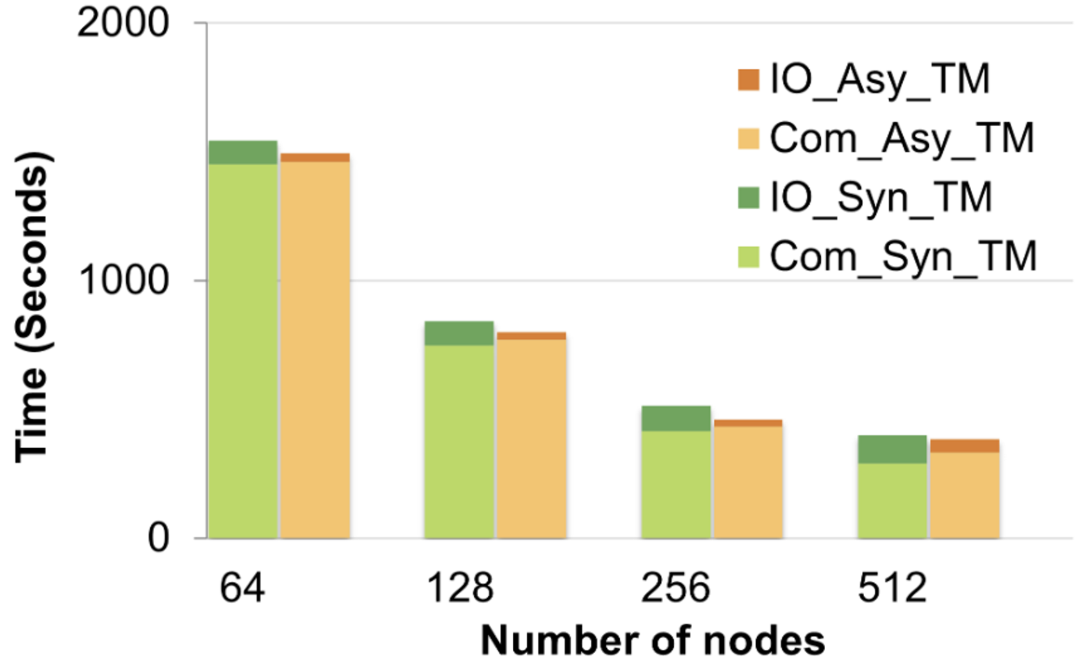


Fig. 7: Streaming sine wave - strong scaling

Results: Deforming Bubble Problem

- This is a benchmark problem for multiphase CFD applications in Flash-X. The deformation is computed by level-set advection and redistancing algorithm.
- For results shown in Fig. 6, the number of bubbles per MPI process is varied. Fig. 1 shows bubble undergo deformation under a velocity field.
- For the 64-node case the I/O time as a percentage of the total simulation time goes down from 22.3% to 4.7%.
- For the 256-node case, the I/O time is significantly higher for the synchronous case; this is due to the fact that a lot of communication is required to write the file to disk from 256 nodes (or 5,376 MPI ranks) and the GPFS file system on Summit does not scale well.
- The asynchronous I/O time for 256 nodes remains the same as for other cases, but the Com_ time has increased because a greater percentage of Com_ time overlaps with IO_ time.

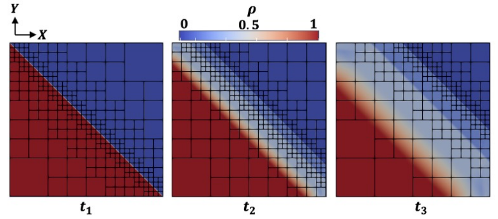


Fig. 1: Contours of energy (E) for time $t_3 > t_2 > t_1$, and an example of block structured AMR grids.

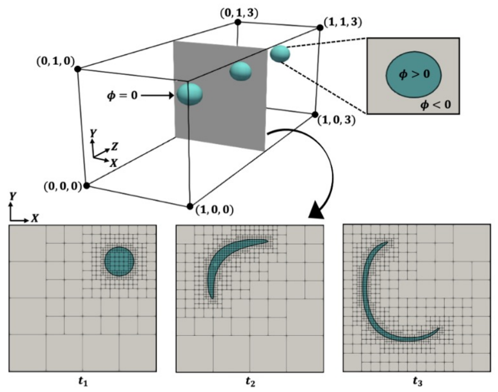


Fig. 2: Schematic of the deforming bubble problem: The bubbles are defined by using a signed distance function, ϕ, that undergoes deformation under a prescribed velocity field.

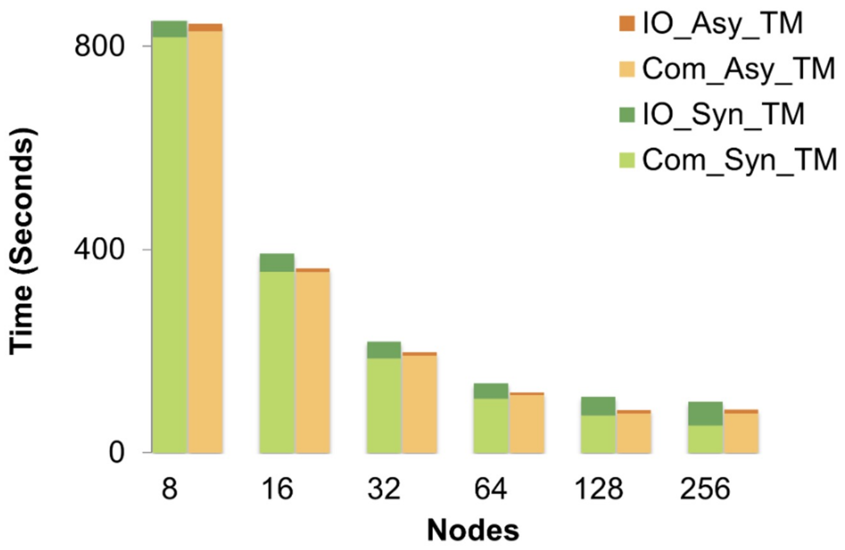


Fig. 6: Deforming bubble - strong scaling