Parallel I/O with HDF5 and Performance Tuning Techniques

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The HDF Group

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Outline

- Overview of parallel HDF5
- General best practices which effect parallel performance
- Best methods for HDF5 parallel I/O
- Using Parallel I/O instrumentation for tuning

Resources

The HDF Group

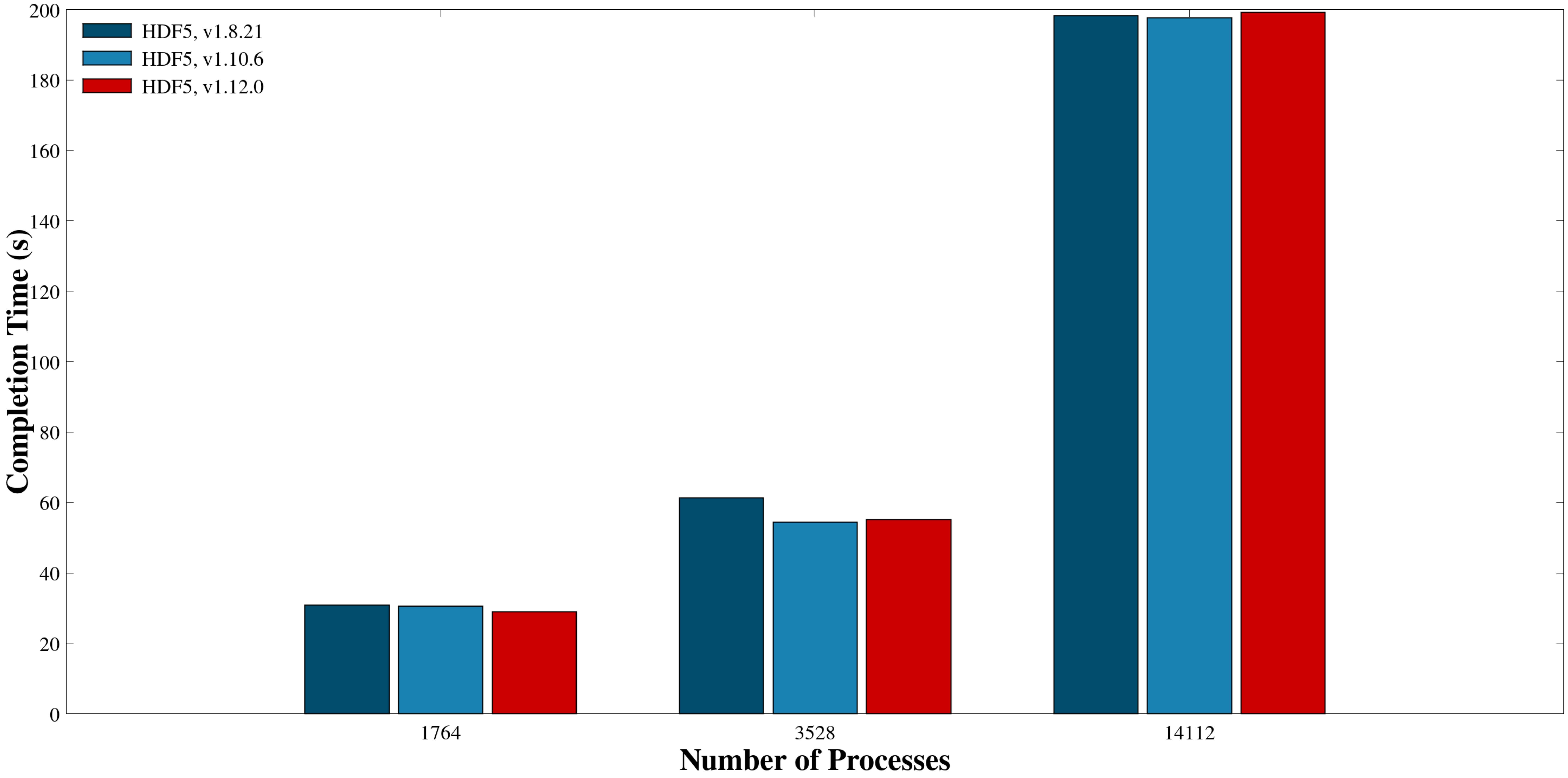
- HDF5 home page: http://hdfgroup.org/HDF5/
- HDF5 Jira: https://jira.hdfgroup.org
- Documentation: https://portal.hdfgroup.org/display/HDF5/HDF5

- HDF5 repo: https://bitbucket.hdfgroup.org/projects/HDFFV/repos/hdf5/
  - We are moving to Github! Stay tuned for announcement

- Latest releases: https://portal.hdfgroup.org/display/support/Downloads
  - HDF5 1.8.21
  - HDF5 1.10.6
  - HDF5 1.12.0

HDF5 Version for parallel HDF5

• CGNS scaling for different versions of HDF5 (Summit, ORNL).



Parallel HDF5 Overview

Parallel HDF5 Overview

- In this section we will remind you about basics of parallel HDF5
- If you are new to parallel HDF5, see:
  - Online tutorials https://portal.hdfgroup.org/display/HDF5/Introduction+to+Parallel+HDF5
  - In-person tutorials
    - Super Computing Conference (MPI IO)
    - ECP annual meetings
    - National Laboratories (Argonne Training Program on Extreme-Scale Computing (ATPESC))

Why Parallel HDF5?

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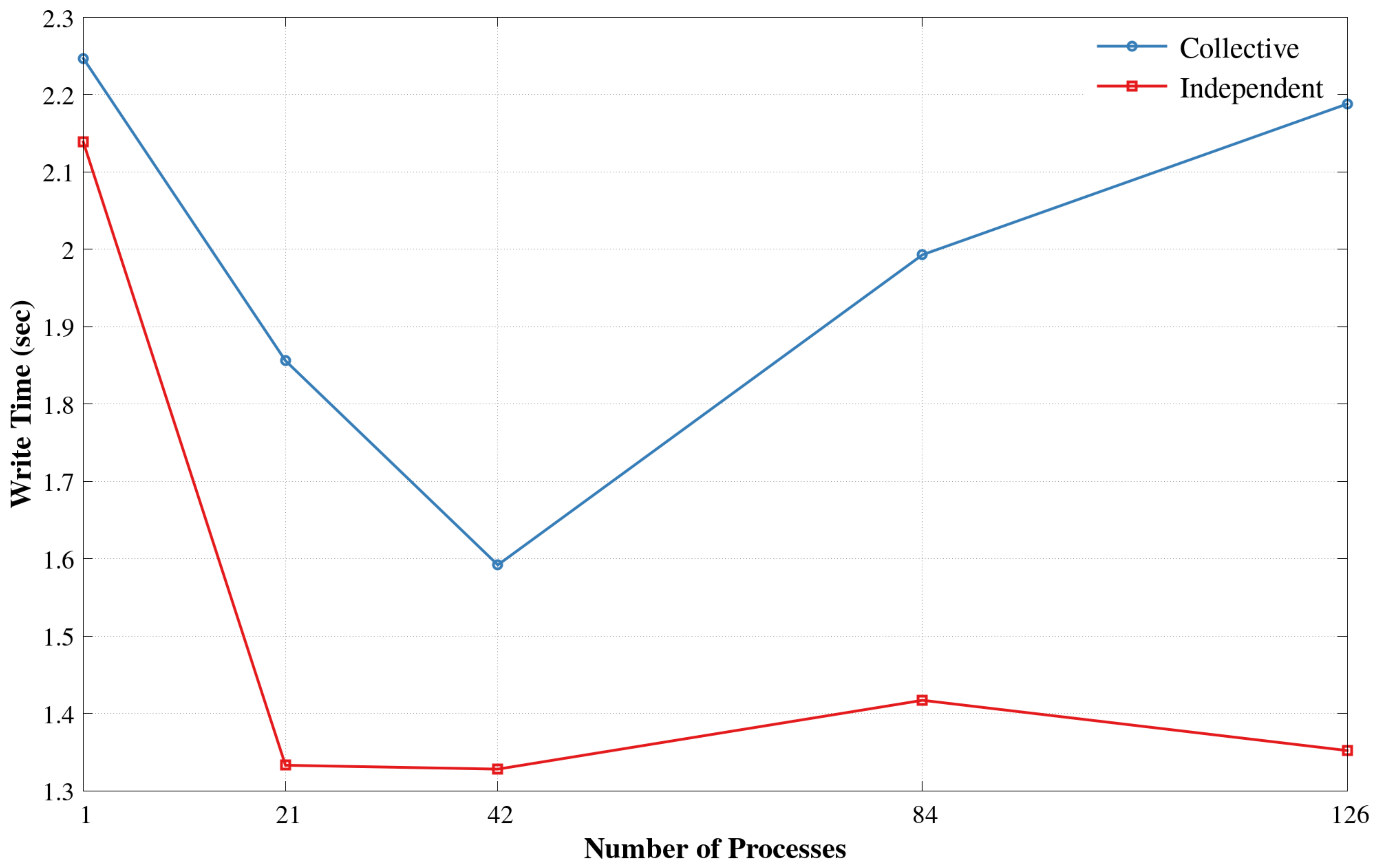
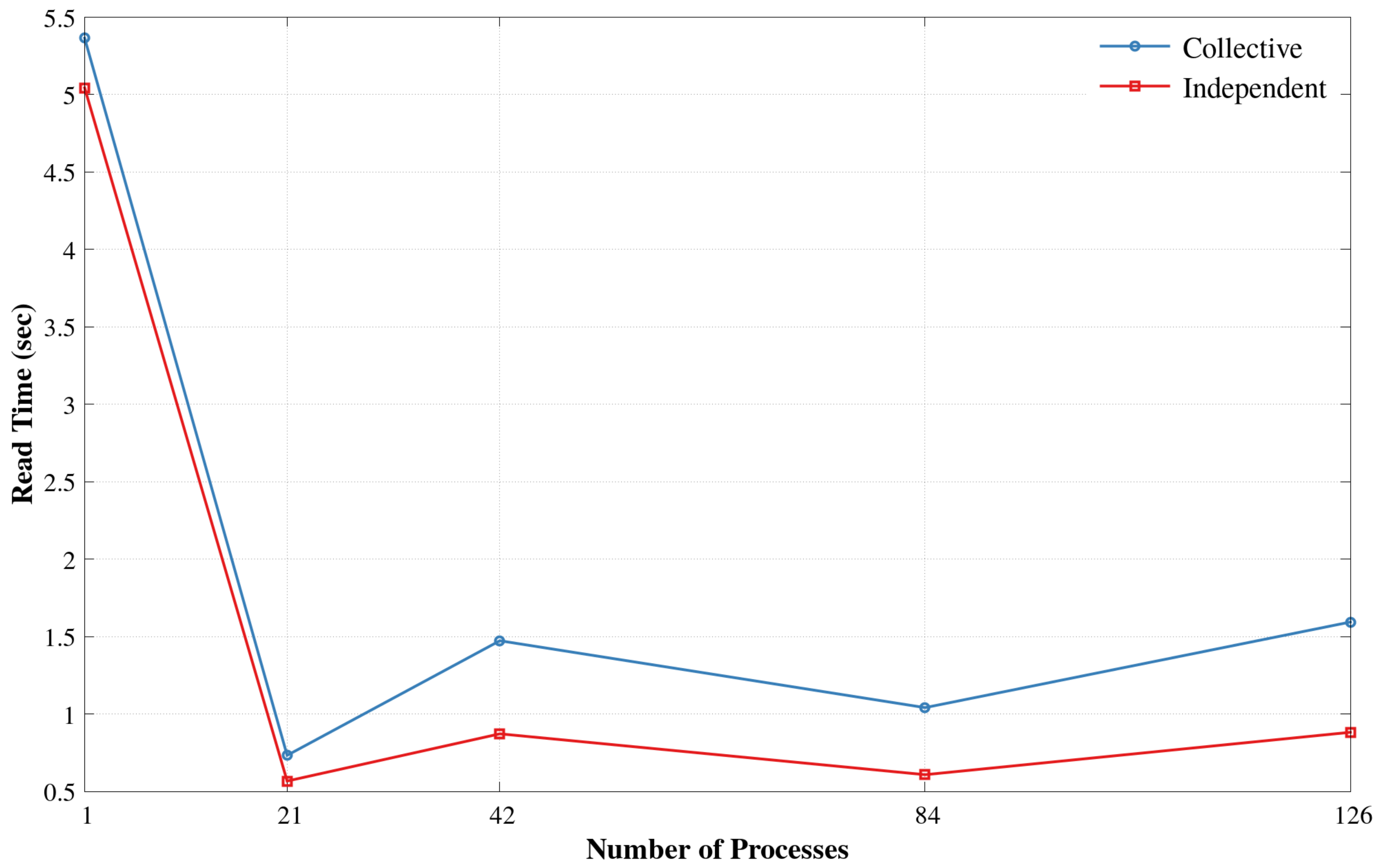
- Take advantage of high-performance parallel I/O while reducing complexity
  - Use a well-defined high-level I/O layer instead of POSIX or MPI-IO
  - Use only a single or a few shared files
    - “Friends don’t let friends use file-per-process!” 😕
- Maintained code base, performance and data portability
  - Rely on HDF5 to optimize for underlying storage system

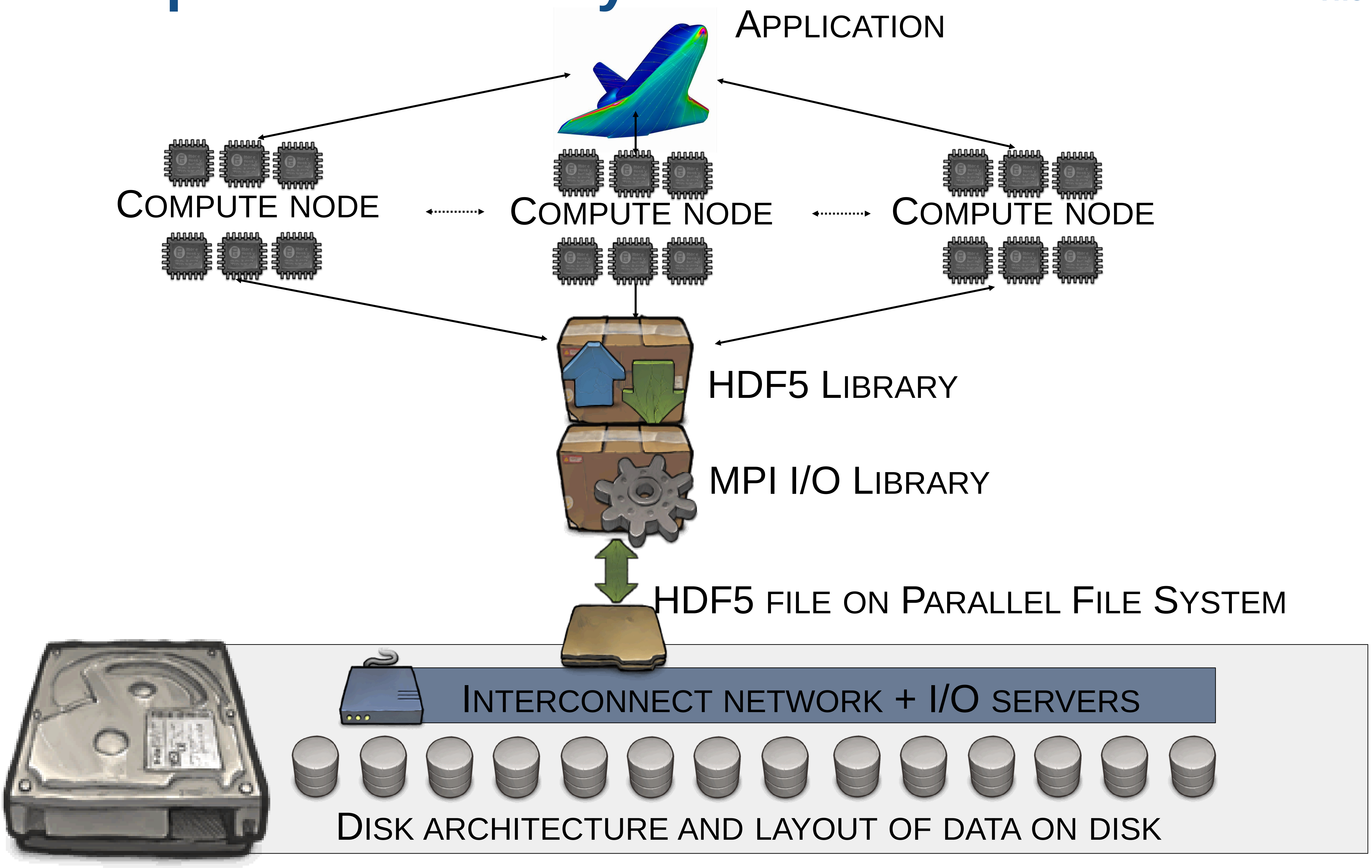
Benefit of Parallel I/O – Strong Scaling Example





CGNS – SUMMIT, ORNL

PHDF5 implementation layers



Parallel HDF5 (PHDF5) vs. Serial HDF5

- PHDF5 allows multiple MPI processes in an MPI application to perform I/O to a single HDF5 file
- Uses a standard parallel I/O interface (MPI-IO)
- Portable to different platforms
- PHDF5 files ARE HDF5 files conforming to the HDF5 file format specification
- The PHDF5 API consists of:
  - The standard HDF5 API
  - A few extra knobs and calls
  - A parallel “etiquette”

Parallel HDF5 Etiquette

- PHDF5 opens a shared file with an MPI communicator
  - Returns a file ID (as usual)
  - All future access to the file via that file ID
- Different files can be opened via different communicators
- All processes must participate in collective PHDF5 APIs
- All HDF5 APIs that modify the HDF5 namespace and structural metadata are collective!
  - File ops., group structure, dataset dimensions, object life-cycle, etc. https://support.hdfgroup.org/HDF5/doc/RM/CollectiveCalls.html
  - Raw data operations can either be collective or independent
    - For collective, all processes must participate, but they don't need to read/write data.

Example of a PHDF5 C Program

Starting with a simple serial HDF5 program:

```
file_id = H5Fcreate(FNAME, …, H5P_DEFAULT);
space_id = H5Screate_simple(…);
dset_id = H5Dcreate(file_id, DNAME, H5T_NATIVE_INT, space_id, …);


status = H5Dwrite(dset_id, H5T_NATIVE_INT, …, H5P_DEFAULT);
```

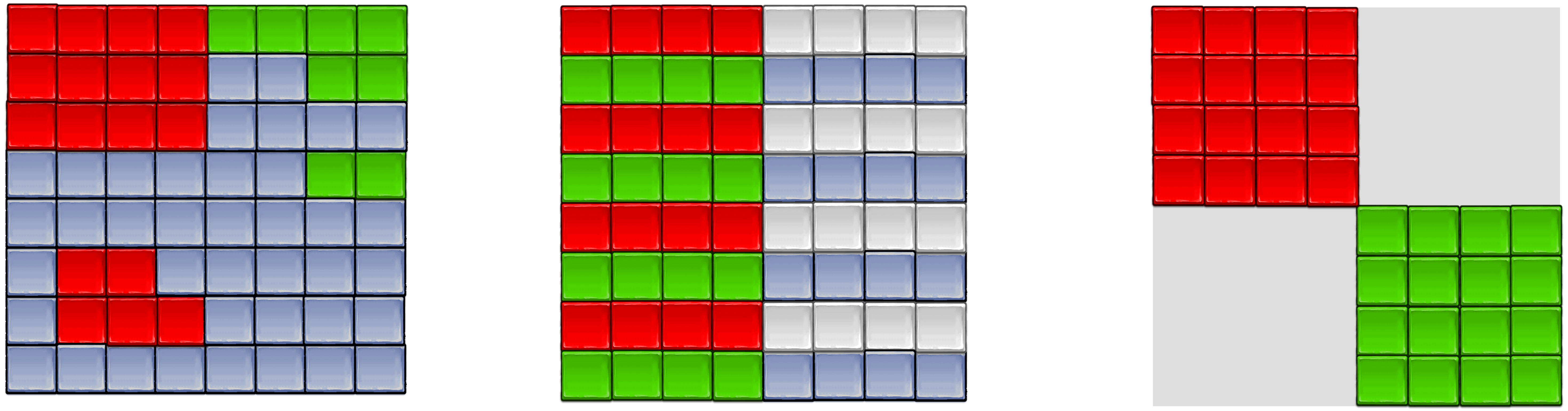
Example of a PHDF5 C Program

A parallel HDF5 program has a few extra calls:

```
MPI_Init(&argc, &argv);
…
fapl_id = H5Pcreate(H5P_FILE_ACCESS);
H5Pset_fapl_mpio(fapl_id, comm, info);
file_id = H5Fcreate(FNAME, …, fapl_id);
space_id = H5Screate_simple(…);
dset_id = H5Dcreate(file_id, DNAME, H5T_NATIVE_INT, space_id, …);
xf_id = H5Pcreate(H5P_DATASET_XFER);
H5Pset_dxpl_mpio(xf_id, H5FD_MPIO_COLLECTIVE);
status = H5Dwrite(dset_id, H5T_NATIVE_INT, …, xf_id);
…
MPI_Finalize();
```

General HDF5 Programming Parallel Model for raw data I/O

- Each process defines selections in memory and in file (aka HDF5 hyperslabs) using `H5Sselect_hyperslab`
- The hyperslab parameters define the portion of the dataset to write to
  - Contiguous hyperslab
  - Regularly spaced data (column or row)
  - Pattern
  - Blocks



- Each process executes a write/read call using selections, which can be either collective or independent

Collective vs. Independent Operations

- MPI Collective Operations:
  - All processes of the communicator must participate, in the right order. E.g.,

	Process1	Process2	
✓	call A(); call B();	call A(); call B();	…CORRECT
⊖	call A(); call B();	call B(); call A();	…WRONG

- Collective operations are not necessarily synchronous, nor must they require communication
  - It could be that only internal state for the communicator changes
- Collective I/O attempts to combine multiple smaller independent I/O ops into fewer larger ops; neither mode is preferable *a priori*

Object Creation (Collective vs. Single Process)

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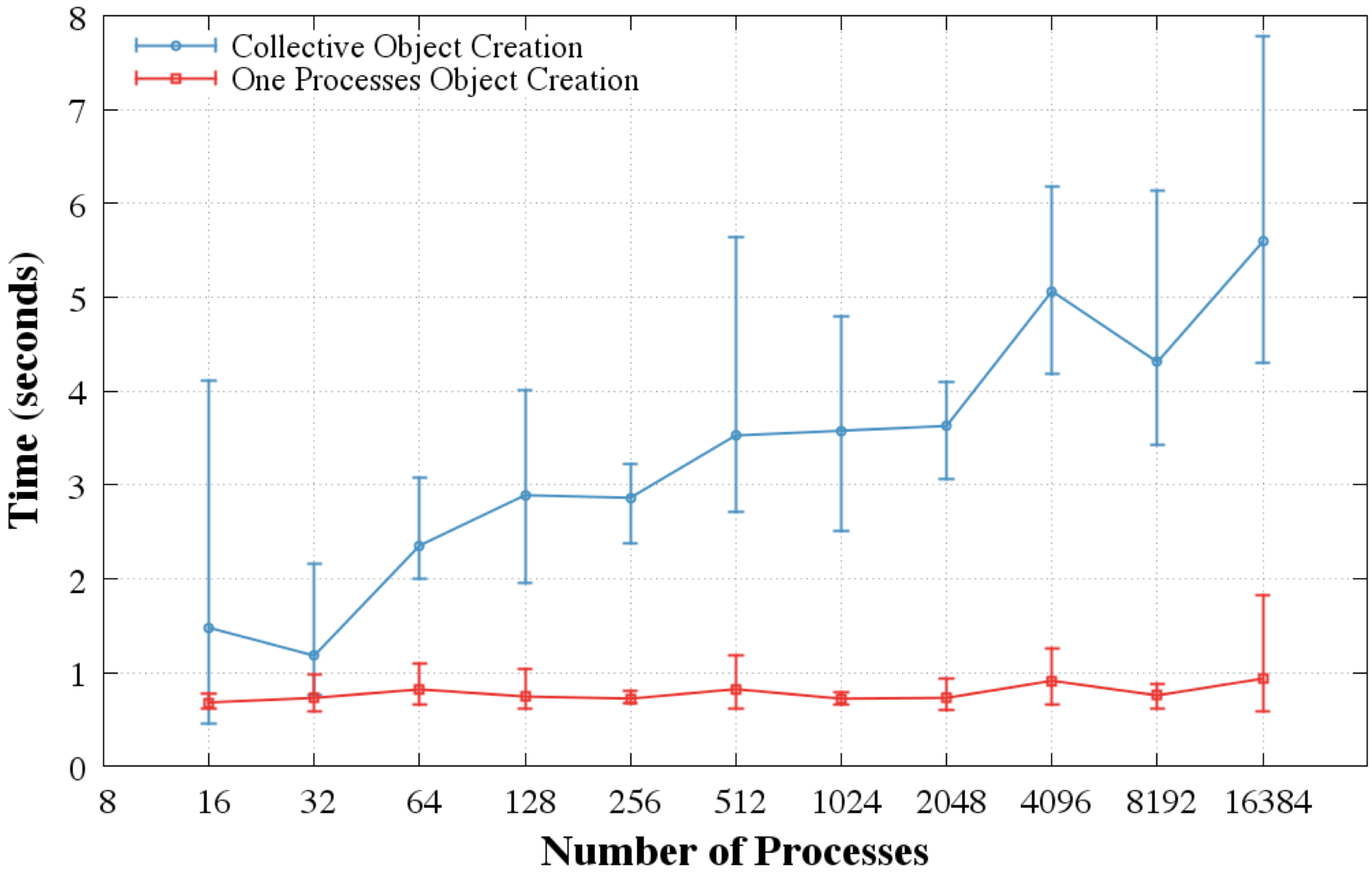

CAUTION: Object Creation (Collective vs. Single Process)

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- In sequential mode, HDF5 allocates chunks incrementally, i.e., when data is written to a chunk for the first time.
  - Chunk is also initialized with the default or user-provided fill value.

- In the parallel case, chunks are always allocated when the dataset is created (not incrementally).
  - The more ranks there are, the more chunks need to be allocated and initialized/written, which manifests itself as a slowdown

CAUTION: Object Creation (SEISM-IO, Blue Waters—NCSA)

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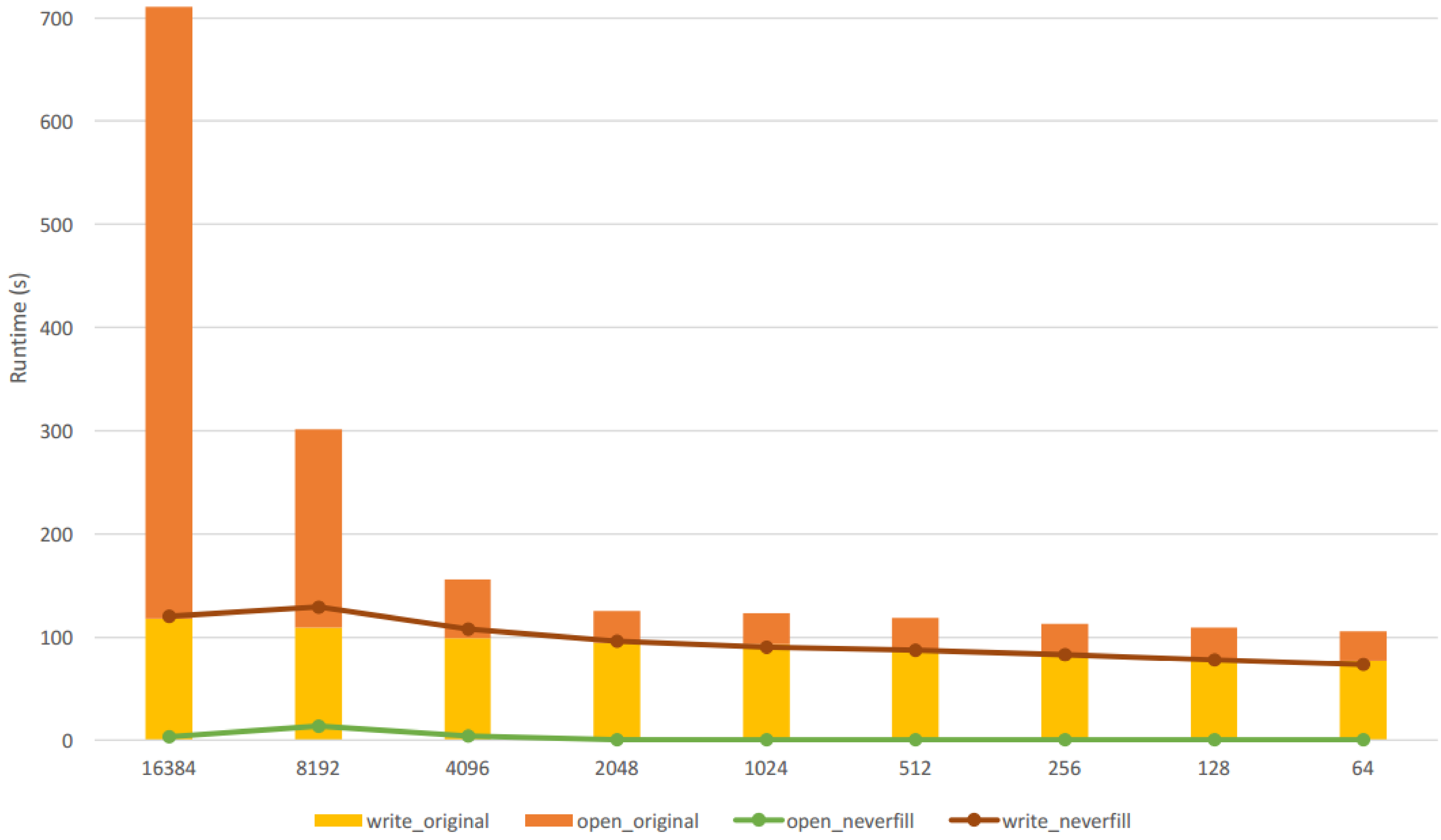
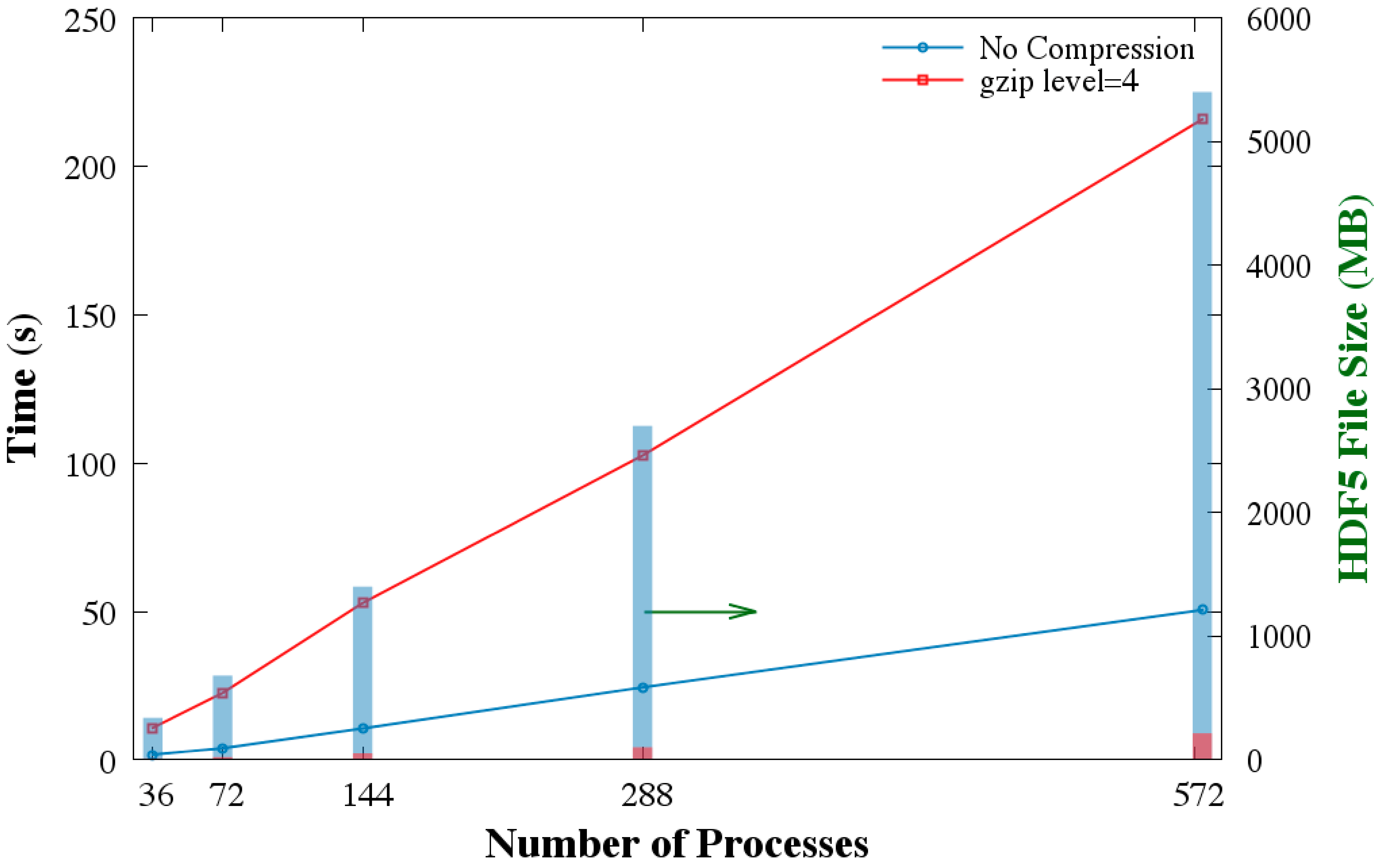
Set HDF5 to never fill chunks (H5Pset_fill_time with H5D_FILL_TIME_NEVER)



Parallel Compression (HDF5 1.10.2 and later)



General HDF5 Best Practices Effecting Parallel Performance

Memory considerations

- **Open Objects**
  - Open objects use up memory. The amount of memory used may be substantial when many objects are left open. Application should:
    - Delay opening of files and datasets as close to their actual use as is feasible.
    - Close files and datasets as soon as their use is completed.
    - If opening a dataspace in a loop, be sure to close the dataspace with each iteration, as this can cause a large temporary "memory leak".
- There are APIs to determine if objects are left open. H5Fget_obj_count will get the number of open objects in the file, and H5Fget_obj_ids will return a list of the open object identifiers.

HDF5 Dataset I/O

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- Issue large I/O requests
  - At least as large as file system block size
- Avoid **datatype conversion**
  - Use the same data type in the file as in memory
- Avoid **dataspace conversion**
  - One dimensional buffer in memory to two-dimensional array in the file

Can break collective operations; check what mode was used H5Pget_mpio_actual_io_mode, and why H5Pget_mpio_no_collective_cause

HDF5 Dataset – Storage Type

- Use **contiguous storage** if no data will be added and compression is not used
  - Data will no be cached by HDF5
- Use **compact** storage when working with small data (<64K)
  - Data becomes part of HDF5 internal metadata and is cached (metadata cache)
- Avoid data duplication to reduce file sizes
  - Use links to point to datasets stored in the same or external HDF5 file
  - Use VDS to point to data stored in other HDF5 datasets

HDF5 Dataset – Chunked Storage

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- Chunking is required when using extendibility and/or compression and other filters
- **I/O** is always performed **on a whole chunk**
- Understand how **chunking cache** works https://portal.hdfgroup.org/display/HDF5/Chunking+in+HDF5 and consider
  - Do you access the same chunk often?
  - What is the best chunk size (especially when using compression)?

HDF5 Parallel Performance

Performance Tuning is a Multi-layer Problem

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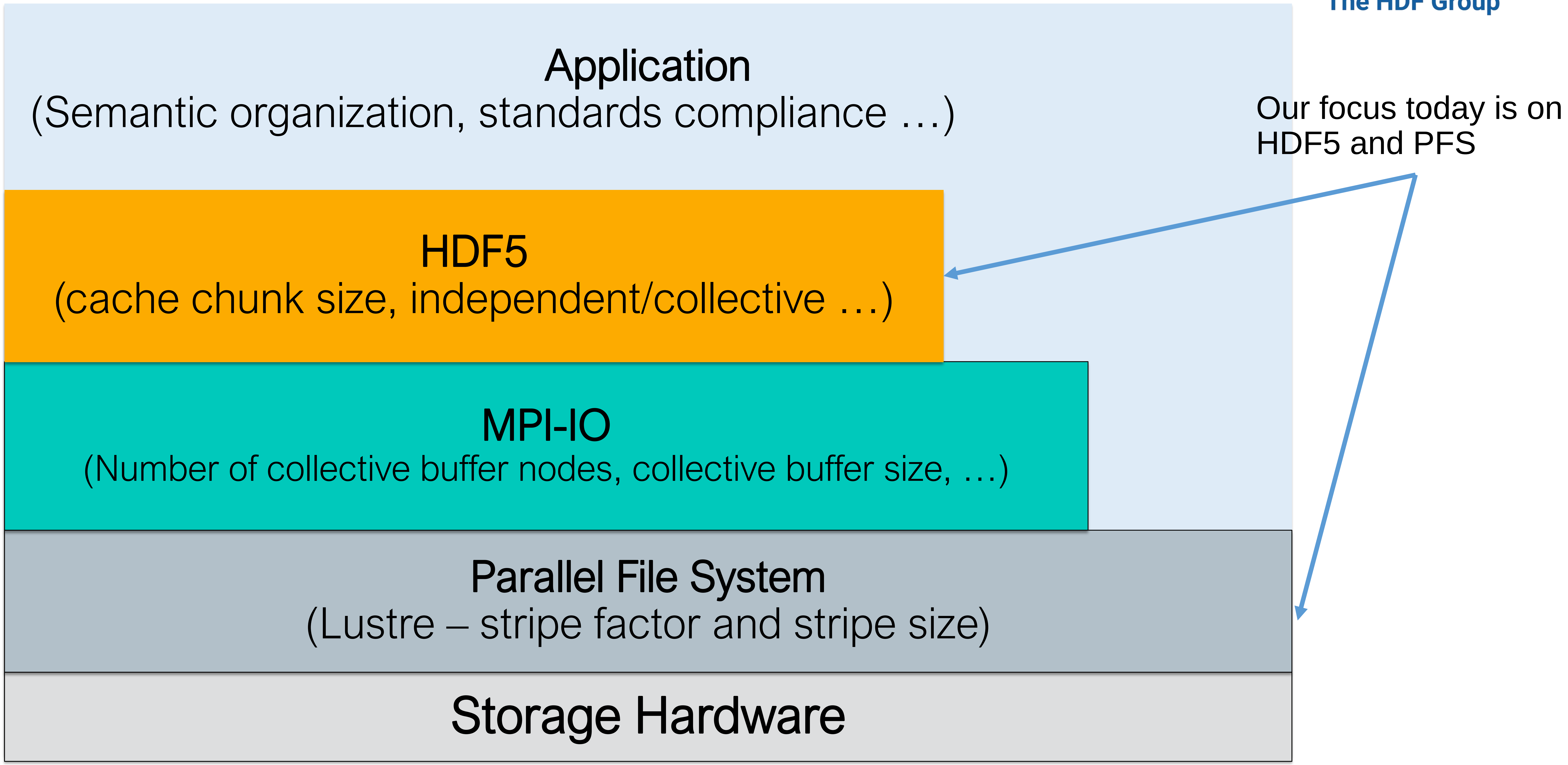

Parallel File Systems – Lustre, GPFS, etc.

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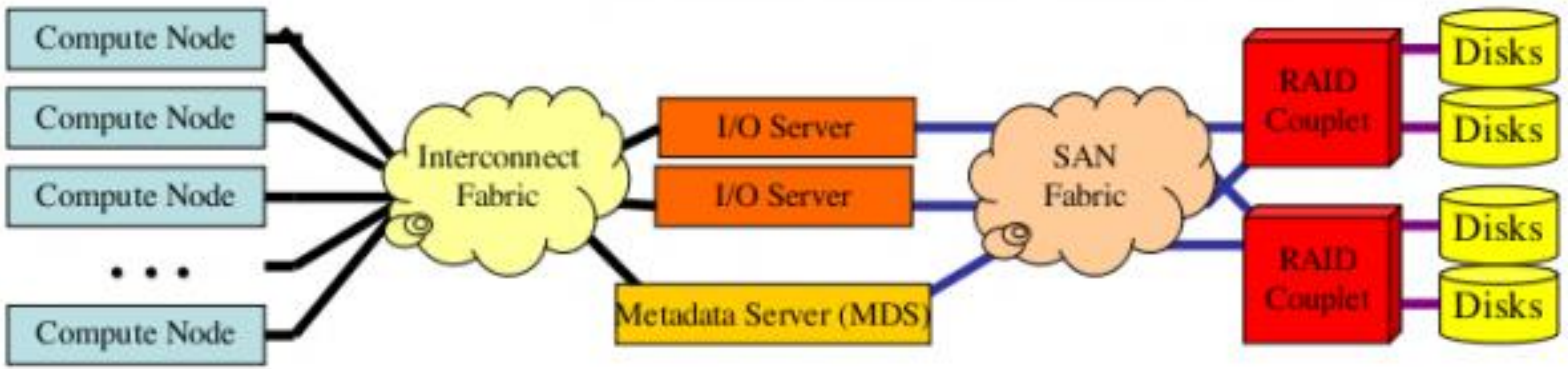
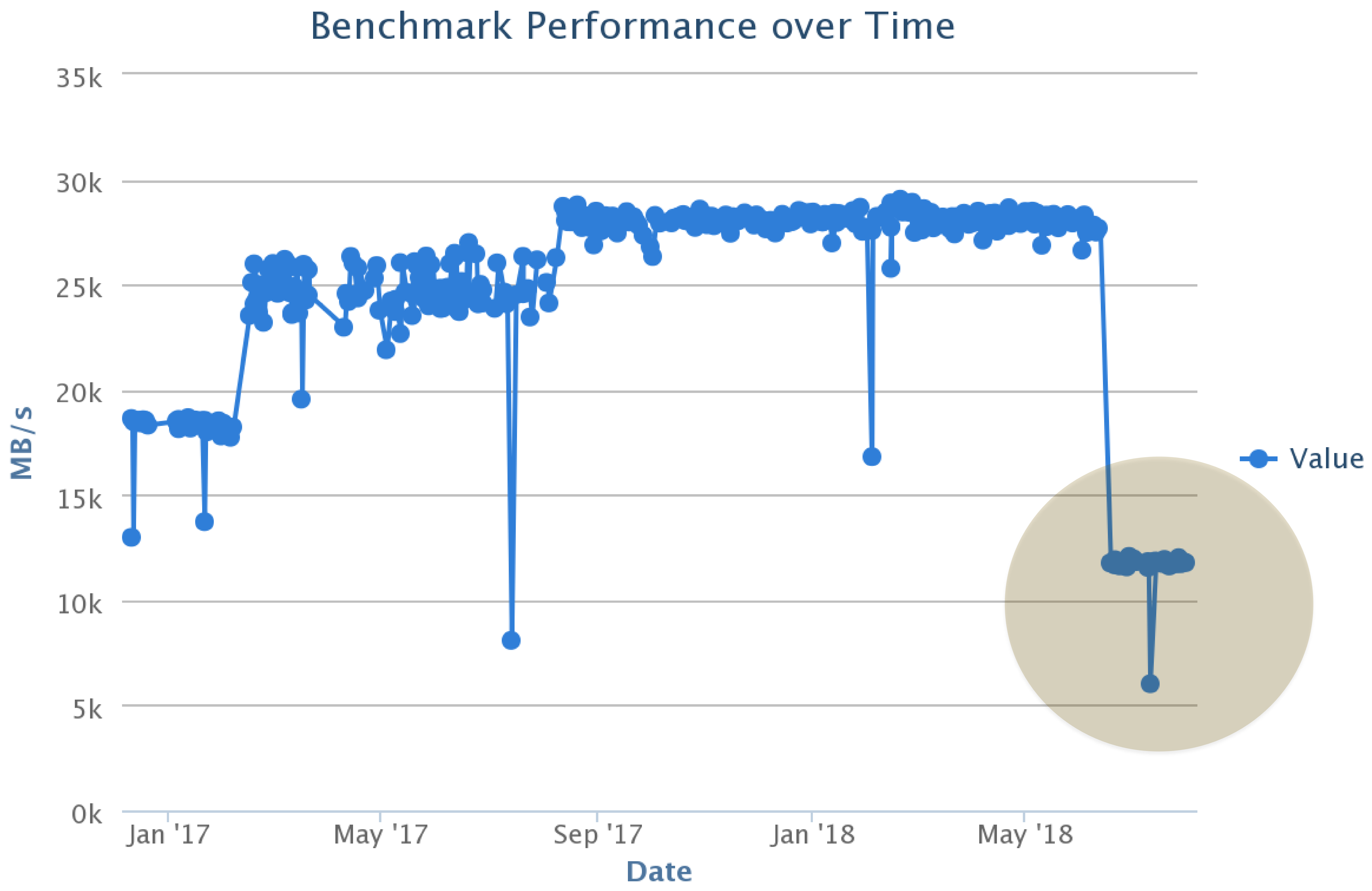


- Scalable, POSIX-compliant file systems designed for large, distributed-memory systems
- Uses a client-server model with separate servers for file metadata and file content

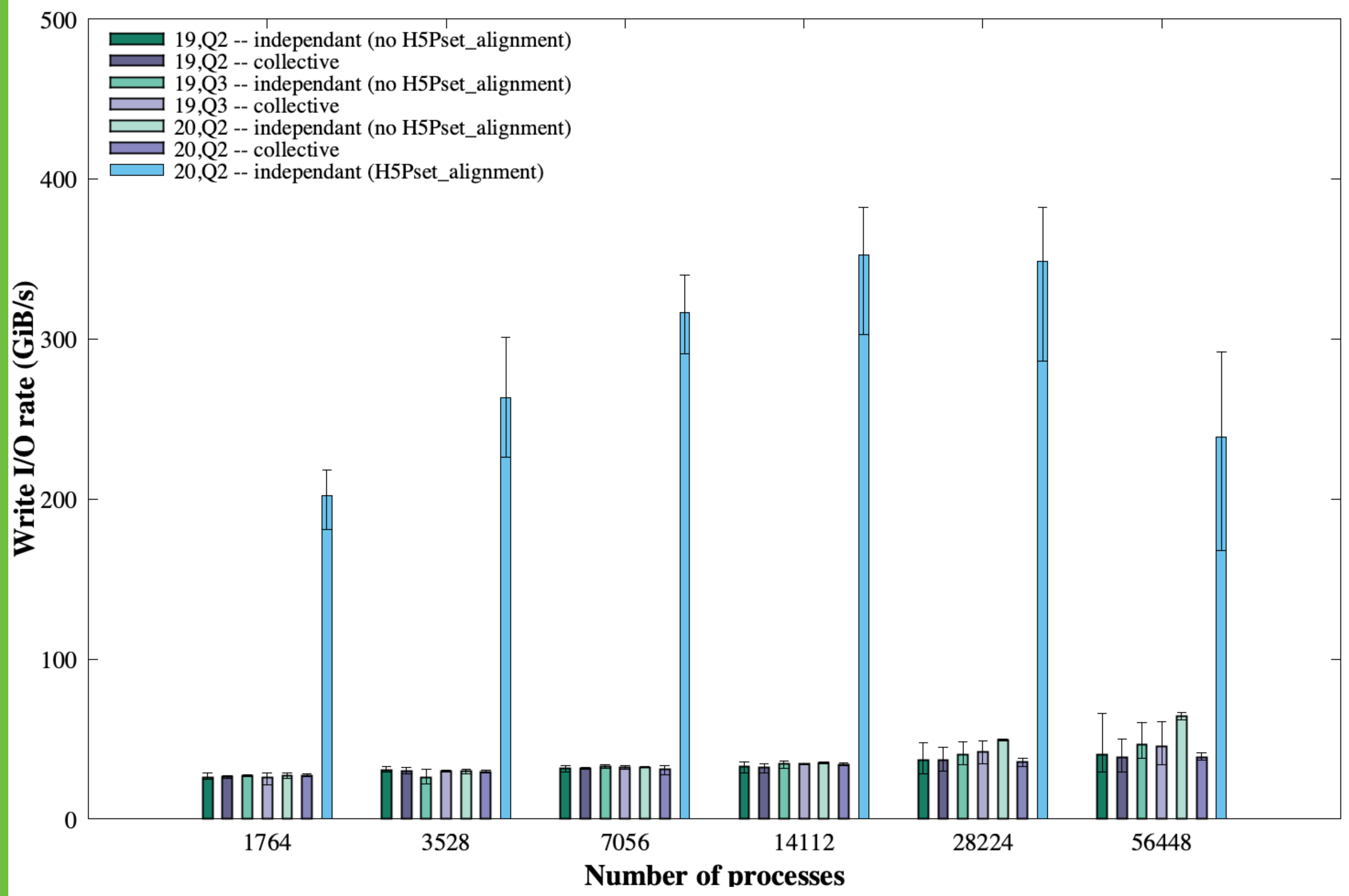
Effects of Software/Hardware Changes

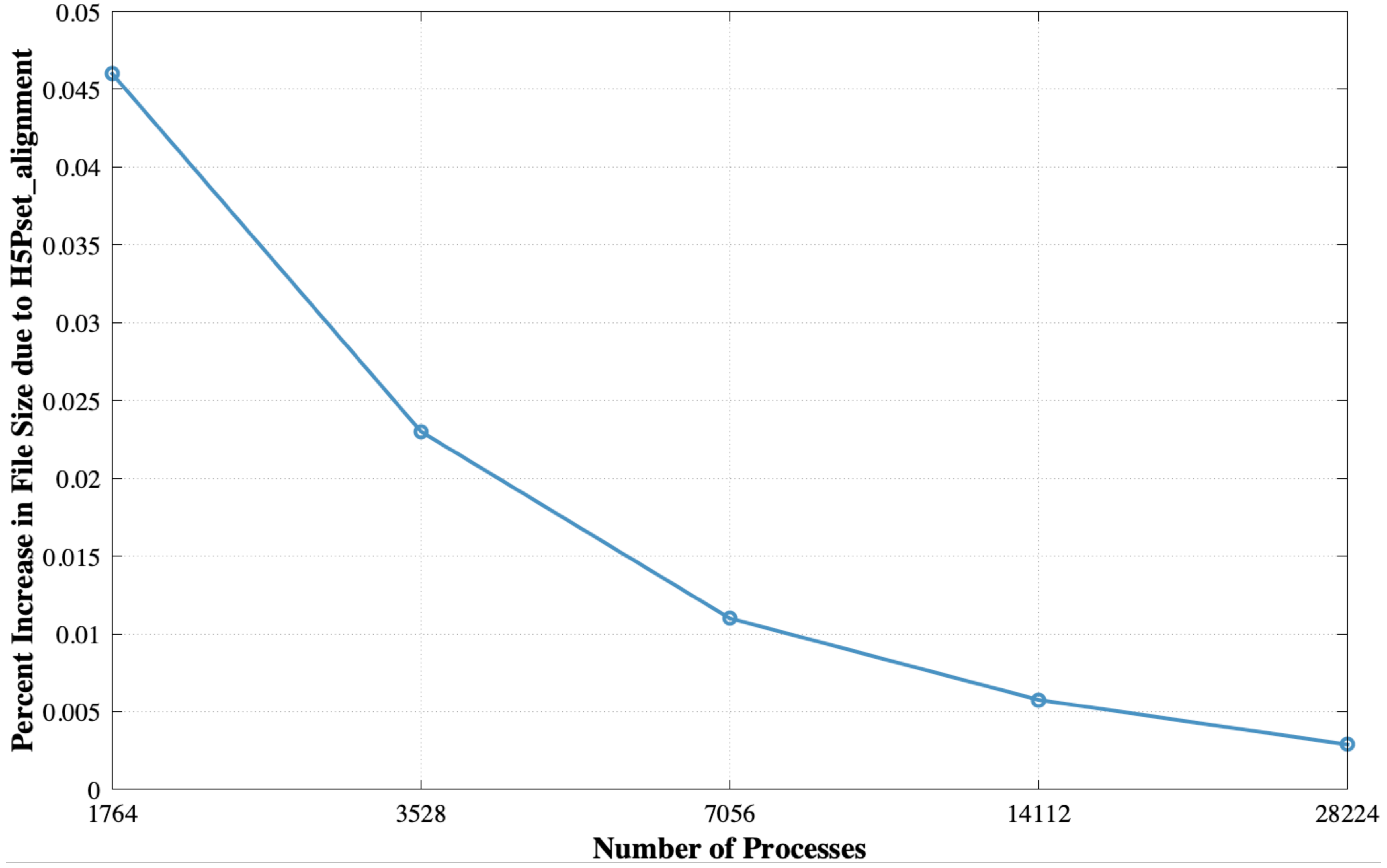
- Poor/Improved performance can be a result of FS changes
- Single shared file using MPI-IO performance degradation [Byna, NERSC].



Effects of influencing object’s in the file layout

- H5Pset_alignment – controls alignment of file objects on addresses.





VPIC, Summit, ORNL

How to pass hints to MPI from HDF5

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- To set hints for MPI using HDF5, see: H5Pset_fapl_mpio
- Use the 'info' parameter to pass these kinds of low-level MPI-IO tuning tweaks.
- C Example – Controls the number of aggregators on GPFS:

```
MPI_Info info;
MPI_Info_create(&info); /* MPI hints: the key and value are strings */
MPI_Info_set(info, "bg_nodes_pset", "1");
H5Pset_fapl_mpio(plist_id, MPI_COMM_WORLD, info);
/* Pass plist_id to H5Fopen or H5Fcreate */
file_id = H5Fcreate(H5FILE_NAME, H5F_ACC_TRUNC, H5P_DEFAULT, plist_id);
```

Use Case CGNS

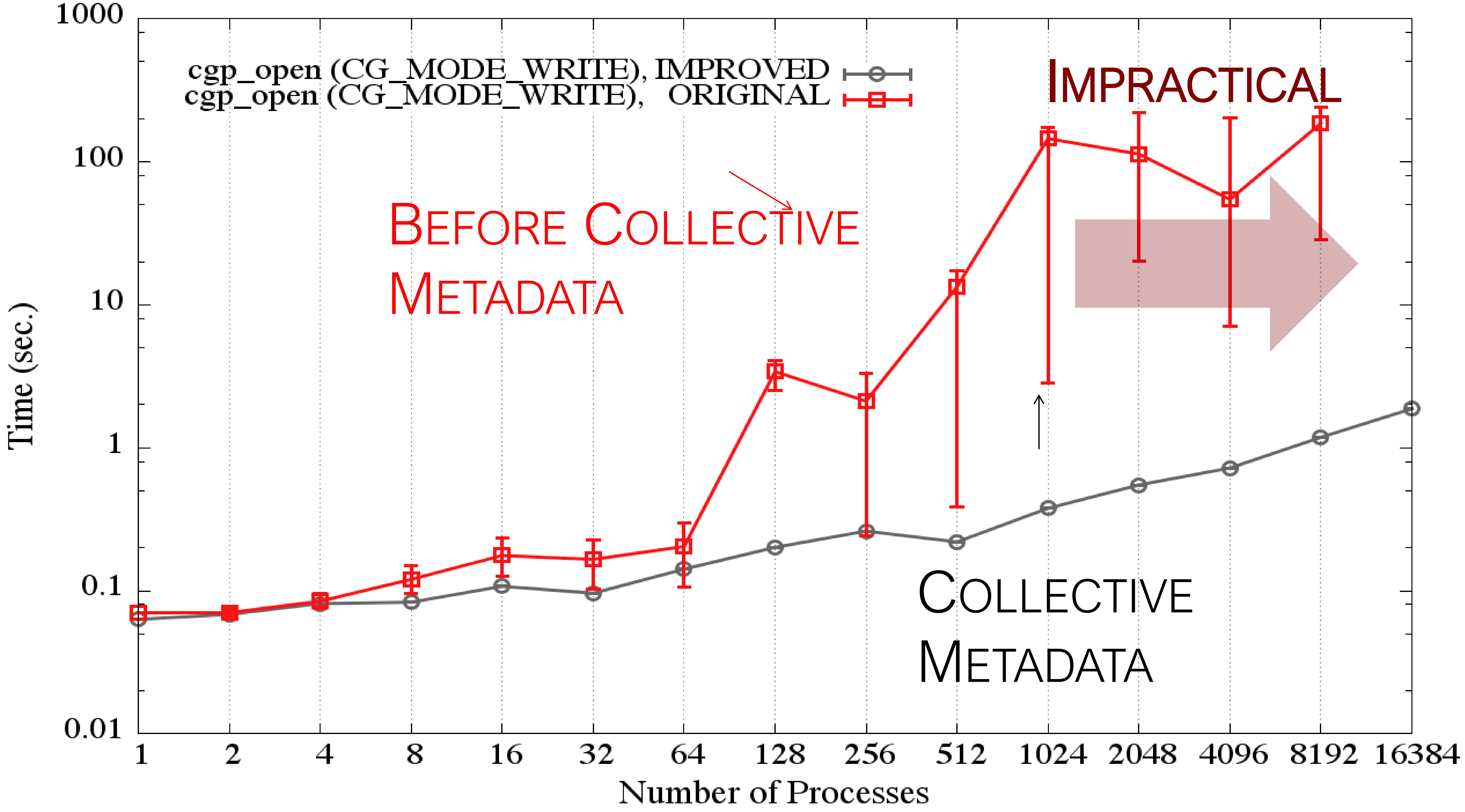
Performance tuning

- CGNS = Computational Fluid Dynamics (CFD) General Notation System
- An effort to standardize CFD input and output data including:
  - Grid (both structured and unstructured), flow solution
  - Connectivity, boundary conditions, auxiliary information.
- Two parts:
  - A standard format for recording the data
  - Software that reads, writes, and modifies data in that format.
- An American Institute of Aeronautics and Astronautics Recommended Practice

Performance issue: Slow opening of an HDF5 File …

- Opening an existing file
  - CGNS reads the entire HDF5 file structure, loading a lot of (HDF5) metadata
  - Reads occur independently on ALL ranks competing for the same metadata

”Read Storm”



Metadata Read Storm Problem (I)

- All metadata "write" operations are required to be collective:

```
if(0 == rank)
    H5Dcreate("dataset1");
else if(1 == rank)
    H5Dcreate("dataset2");
```

```
/* All ranks have to call */
H5Dcreate("dataset1");
H5Dcreate("dataset2");
```

- Metadata read operations are not required to be collective:

```
if(0 == rank)
    H5Dopen("dataset1");
else if(1 == rank)
    H5Dopen("dataset2");
```

```
/* All ranks have to call */
H5Dopen("dataset1");
H5Dopen("dataset2");
```

HDF5 Metadata Read Storm Problem (II)

The HDF Group

- HDF5 metadata read operations are treated by the library as independent read operations.
- Consider a very large MPI job size where all processes want to open a dataset that already exists in the file.
- All processes
  - Call `H5Dopen(“/G1/G2/D1”);`
  - Read the same metadata to get to the dataset and the metadata of the dataset itself
    - IF metadata not in cache, THEN read it from disk.
  - Might issue read requests to the file system for the same small metadata.

Read Storm

Avoiding a Read Storm

- Hint that metadata access is done collectively
  - `H5Pset_coll_metadata_write, H5Pset_all_coll_metadata_ops`
- A property on an access property list
- If set on the file access property list, then all metadata read operations will be required to be collective
- Can be set on individual object property list
- If set, MPI rank 0 will issue the read for a metadata entry to the file system and broadcast to all other ranks

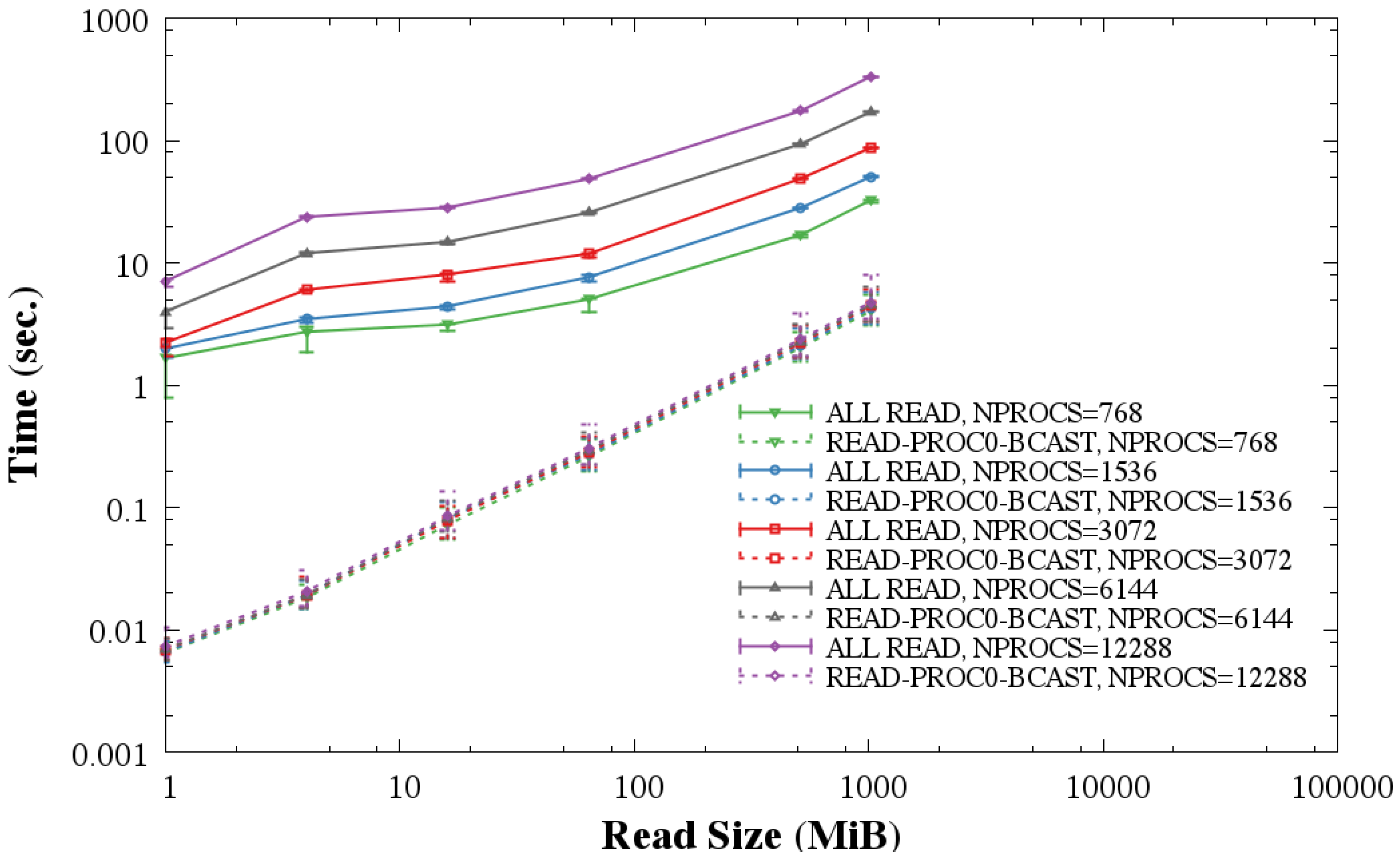
Improve the performance of reading/writing H5S_all selected datasets

(1) New in HDF5 1.10.5

- If:
  - All the processes are reading/writing the same data
  - And the dataset is less than 2GB
- Then
  - The lowest process id in the communicator will read and broadcast the data or will write the data.

(2) Use of compact storage, or

- For compact storage, this same algorithm gets used.



SCALING OPTIMIZATIONS

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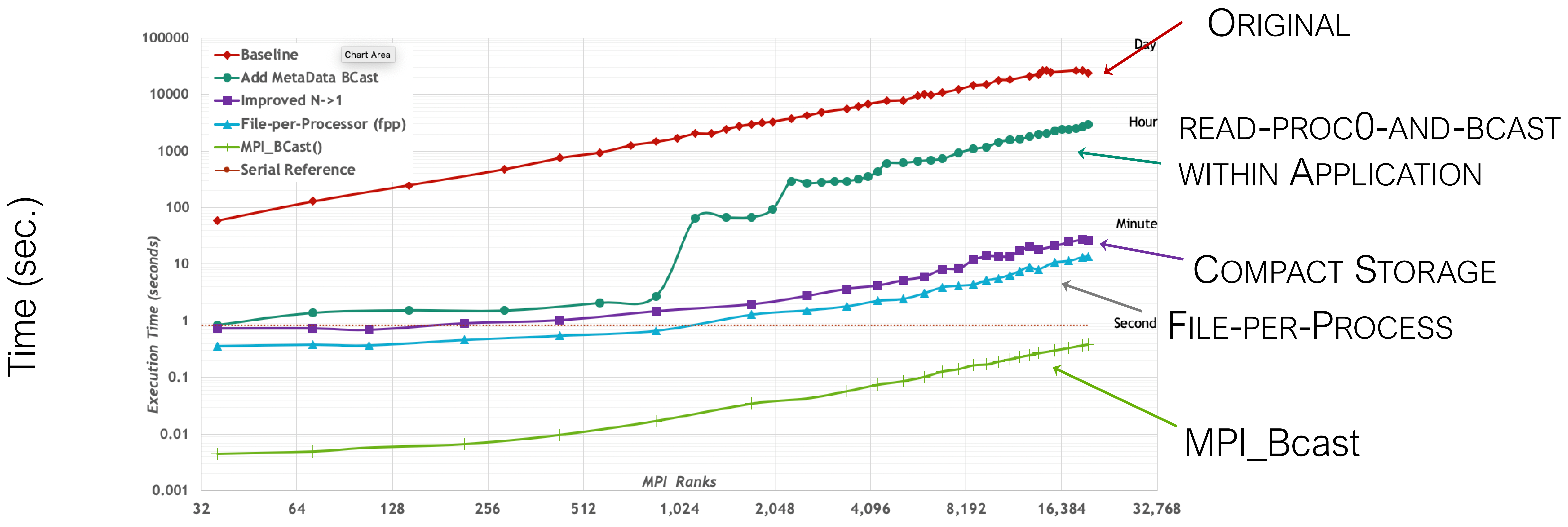


Greg Sjaardema, Sandia National Labs

CGNS cfd data standard

Diagnostics and Instrumentation Tools

I/O monitoring and profiling tools

The HDF Group

- Two kinds of tools:
  - I/O benchmarks for measuring a system's I/O capabilities
  - I/O profilers for characterizing applications' I/O behavior
  - Profilers have to compromise between
    - A lot of detail ➔ large trace files and overhead
    - Aggregation ➔ loss of detail, but low overhead
- Examples of I/O benchmarks:
  - h5perf (in the HDF5 source code distro and binaries)
  - IOR https://github.com/hpc/ior
- Examples of profilers
  - Darshan https://www.mcs.anl.gov/research/projects/darshan/
  - Recorder https://github.com/uiuc-hpc/Recorder
  - TAU built with HDF5
    https://github.com/UO-OACISS/tau2/wiki/Configuring-TAU- to-measure-IO-libraries

“Poor Man’s Debugging”

The HDF Group

- Build a version of PHDF5 with

```
./configure --enable-build-mode=debug --enable-parallel …
```

```
setenv H5FD_mpio_Debug “rw”
```

- This allows the tracing of MPIO I/O calls in the HDF5 library such as `MPI_File_read_xx` and `MPI_File_write_xx`

- You’ll get something like this…

"Poor Man's Debugging"(cont'd)
Example - Chunked by Column

```
% setenv H5FD_mpio_Debug 'rw'
% mpirun -np 4 ./a.out 1000
```

Indep., Chunked by column.

```
in H5FD_mpio_write  mpi_off=0       size_i=96
in H5FD_mpio_write  mpi_off=0       size_i=96
in H5FD_mpio_write  mpi_off=0       size_i=96
in H5FD_mpio_write  mpi_off=0       size_i=96
in H5FD_mpio_write  mpi_off=3688    size_i=8000
in H5FD_mpio_write  mpi_off=11688   size_i=8000
in H5FD_mpio_write  mpi_off=27688   size_i=8000
in H5FD_mpio_write  mpi_off=19688    size_i=8000
in H5FD_mpio_write  mpi_off=96      size_i=40
in H5FD_mpio_write  mpi_off=136     size_i=544
in H5FD_mpio_write  mpi_off=680     size_i=120
in H5FD_mpio_write  mpi_off=800     size_i=272
…
```

HDF5 metadata

Dataset elements

HDF5 metadata

“Poor Man’s Debugging” (cont’d) Debugging Collective Operations

`setenv` **H5_COLL_API_SANITY_CHECK 1**

- HDF5 library will perform an MPI_Barrier() call inside each metadata operation that modifies the HDF5 namespace.
- Helps to find which rank is hanging in the MPI barrier

Use Case

Tuning PSDNS with Darshan

Darshan (ECP DataLib team)

The HDF Group

- Design goals:
  - Transparent integration with user environment
  - Negligible impact on application performance
- Provides aggregate figures for:
  - Operation counts (POSIX, MPI-IO, HDF5, PnetCDF)
  - Datatypes and hint usage
  - Access patterns: alignments, sequentially, access size
  - Cumulative I/O time, intervals of I/O activity
- An excellent starting point

New feature in Darshan 3.2.0+

Darshan Use-Case (Blue Waters, NCSA)

The HDF Group

- PSDNS code solves the incompressible Navier-Stokes equations in a periodic domain using pseudo-spectral methods.
- Uses custom sub-filing by collapsing the 3D in-memory layout into a 2D arrangement of HDF5 files
- Uses virtual dataset which combines the datasets distributed over several HDF5 files into a single logical dataset

Slow read times.

Ran experiments on 32,768 processes with **Darshan** 3.1.3 to create an I/O profile.

Darshan Use-Case (Blue Waters, NCSA)

…
total_POSIX_SIZE_READ_0_100: 196608
total_POSIX_SIZE_READ_100_1K: 393216
total_POSIX_SIZE_READ_1K_10K: 617472
total_POSIX_SIZE_READ_10K_100K: 32768
total_POSIX_SIZE_READ_100K_1M: 2097152
total_POSIX_SIZE_READ_1M_4M: 0
total_POSIX_SIZE_READ_4M_10M: 0
total_POSIX_SIZE_READ_10M_100M: 0
total_POSIX_SIZE_READ_100M_1G: 0
total_POSIX_SIZE_READ_1G_PLUS: 0
…

Large numbers of reads of only small amounts of data.

Multiple MPI ranks independently read data from a small restart file which contains a virtual dataset.

Darshan Use-Case (Blue Waters, NCSA)

The HDF Group

- "Broadcast" the restart file:

1. Rank 0: read the restart file as a byte stream into a memory buffer.
2. Rank 0: broadcasts the buffer.
3. All MPI ranks open the buffer as an HDF5 *file image,* and proceed as if they were performing reads against an HDF5 file stored in a file system.

Eliminates the "read storm",

….

total_POSIX_SIZE_READ_0_100: 6
total_POSIX_SIZE_READ_100_1K: 0
total_POSIX_SIZE_READ_1K_10K: 0
total_POSIX_SIZE_READ_10K_100K: 2
total_POSIX_SIZE_READ_100K_1M: 0
total_POSIX_SIZE_READ_1M_4M: 0
total_POSIX_SIZE_READ_4M_10M: 0
total_POSIX_SIZE_READ_10M_100M: 0
total_POSIX_SIZE_READ_100M_1G: 32768
total_POSIX_SIZE_READ_1G_PLUS: 0

…

Use Case

Tuning HACC (Hardware/Hybrid Accelerated Cosmology Code) with Recorder

Recorder

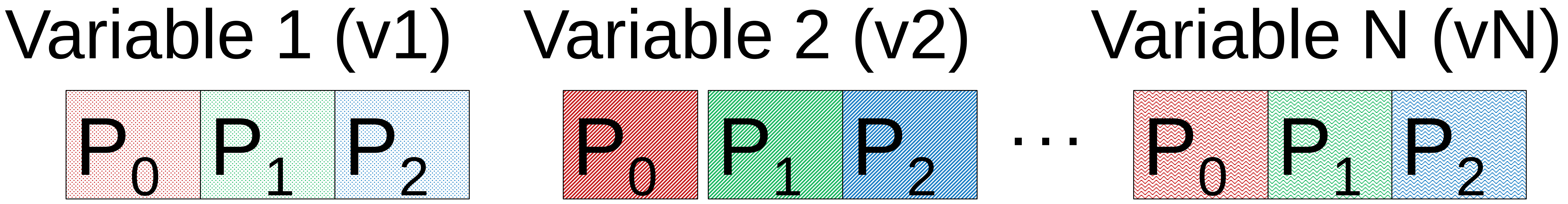
- Multi-level I/O tracing library that captures function calls from HDF5, MPI and POSIX.
- It keeps every function and its parameters. Useful to exam access patterns.
- Built-in visualizations for access patterns, function counters, I/O sizes, etc.
- Also reports I/O conflicts such as write-after-write, write-after-read, etc. Useful for consistency semantics check (File systems with weaker consistency semantics).

Wang, Chen, Jinghan Sun, Marc Snir, Kathryn Mohror, and Elsa Gonsiorowski. "Recorder 2.0: Efficient Parallel I/O Tracing and Analysis." In IEEE International Workshop on High-Performance Storage (HPS), 2020.

https://github.com/uiuc-hpc/Recorder

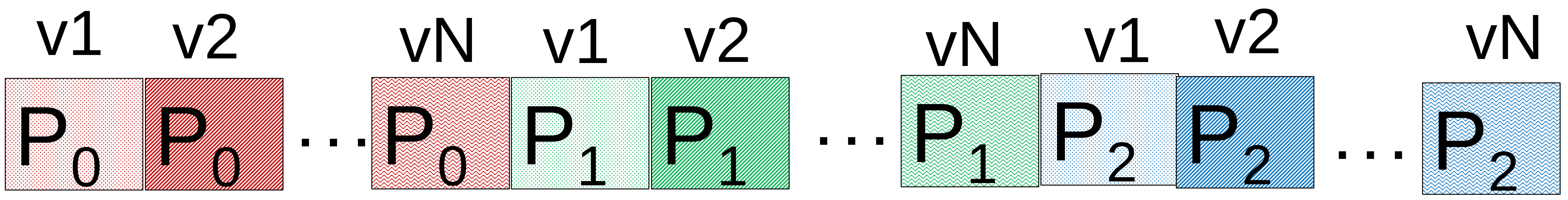
Write Pattern Effects – Data location in the file

Pattern 1 – HDF5 pattern



Variables are **contiguously** stored in the file

Pattern 2 – MPI-IO pattern (or HDF5 compound datatype)



Variables are **interleaved** in the file

HACC-IO: MPI vs HDF5, why HDF5 is slow?

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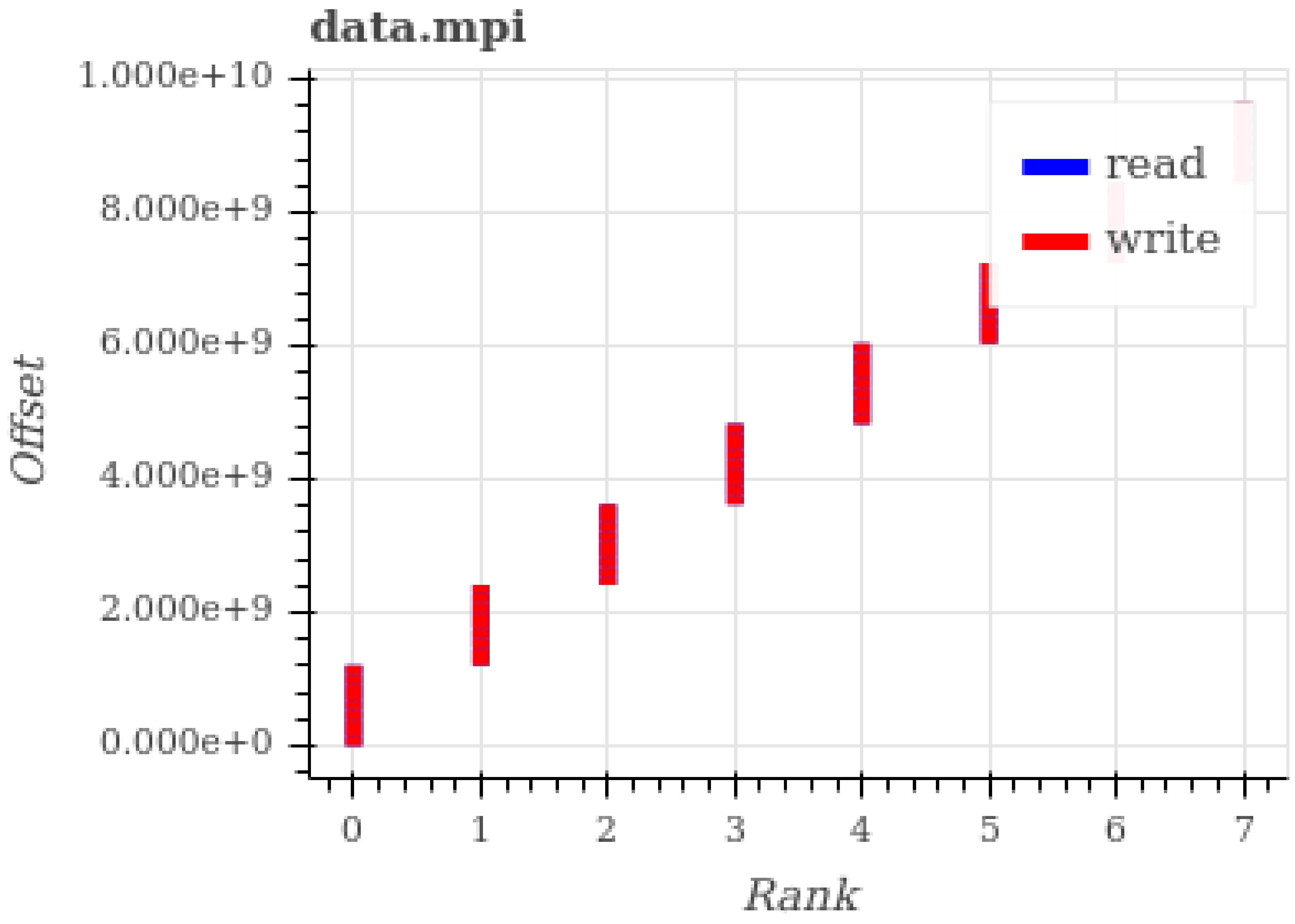
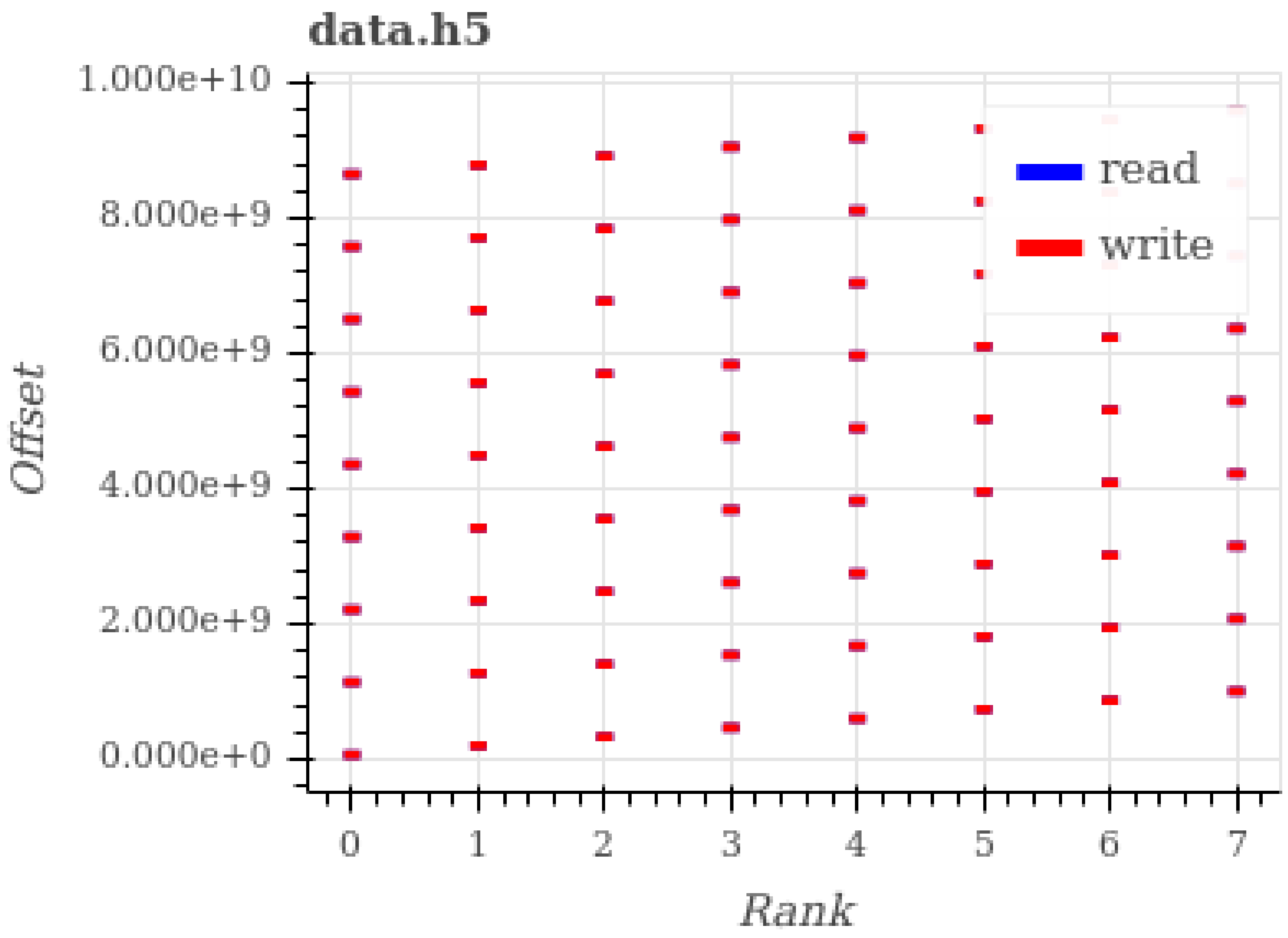
Example of access patterns with 8 ranks writing 9GB.



MPI-IO Access Pattern



HDF5 with individual dataset

HACC-IO: HDF5 access patterns

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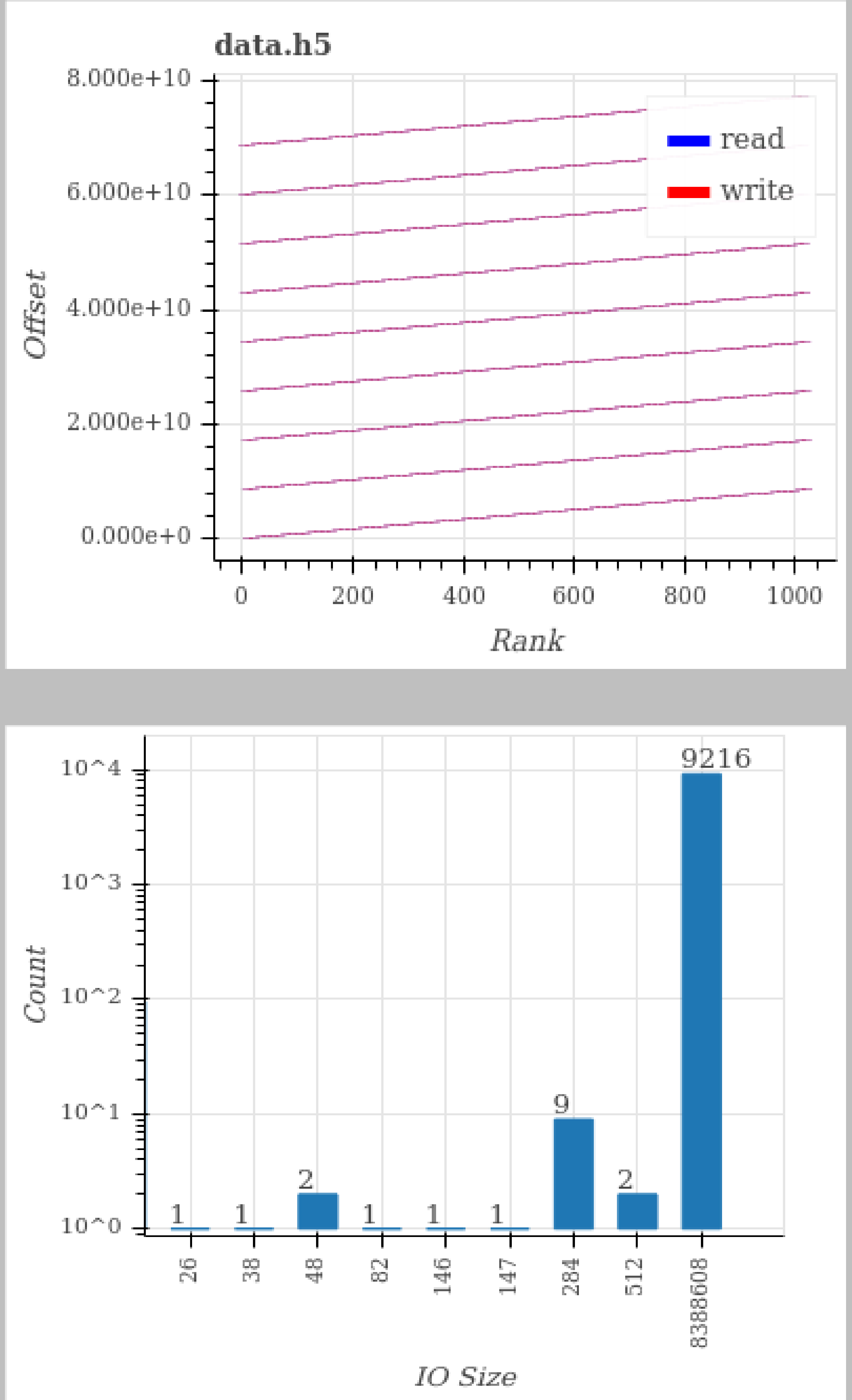
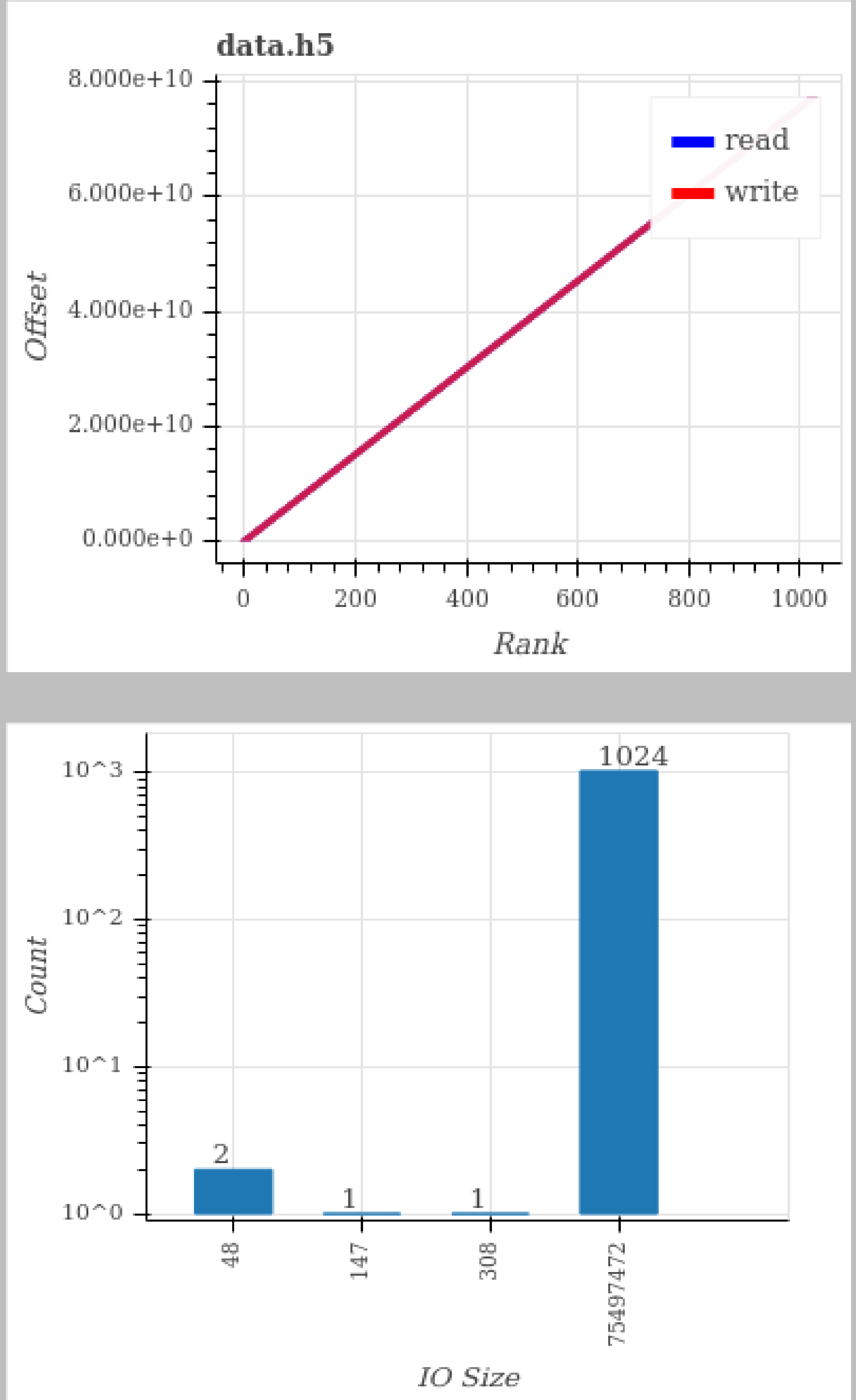
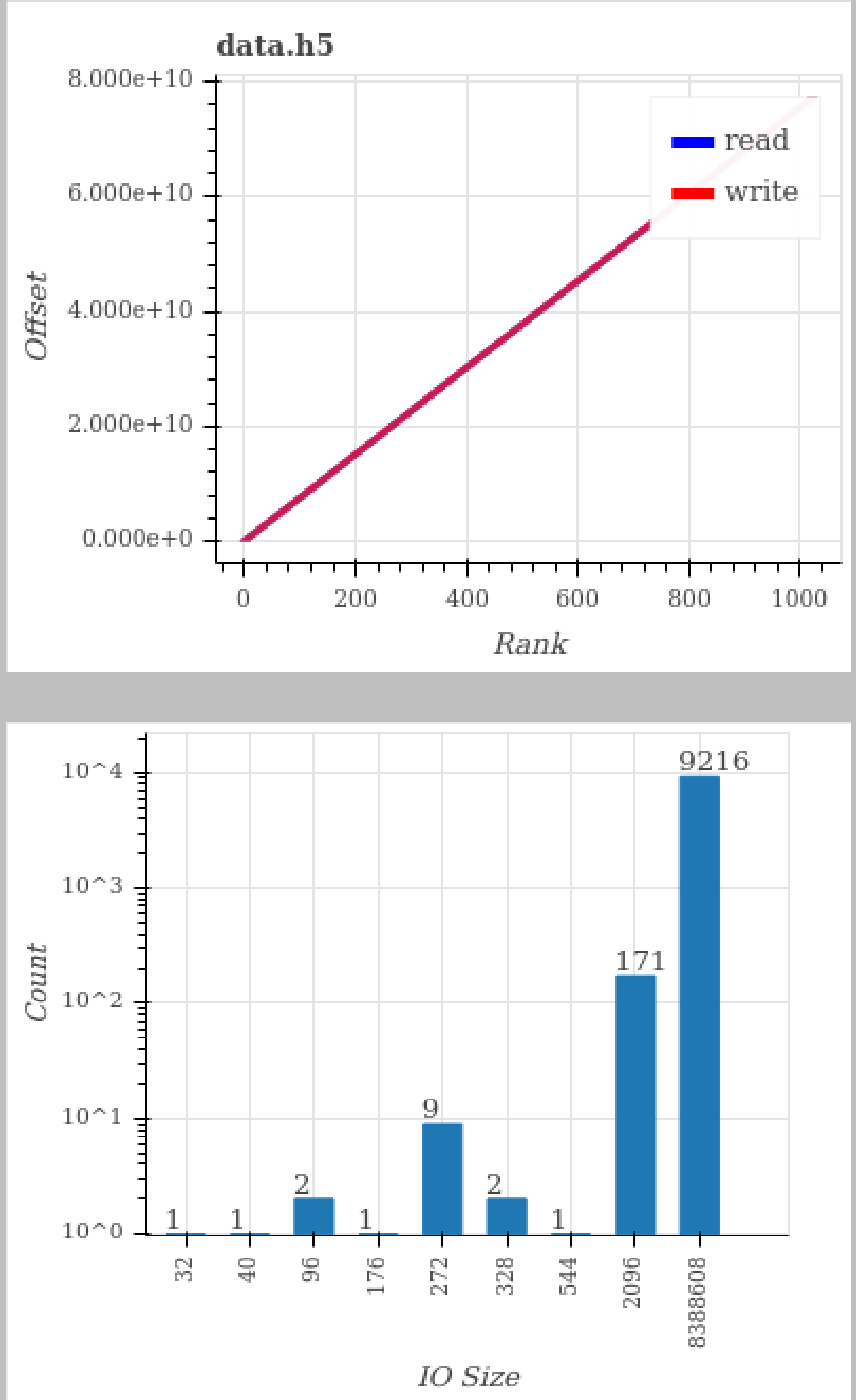


HDF5 with individual dataset



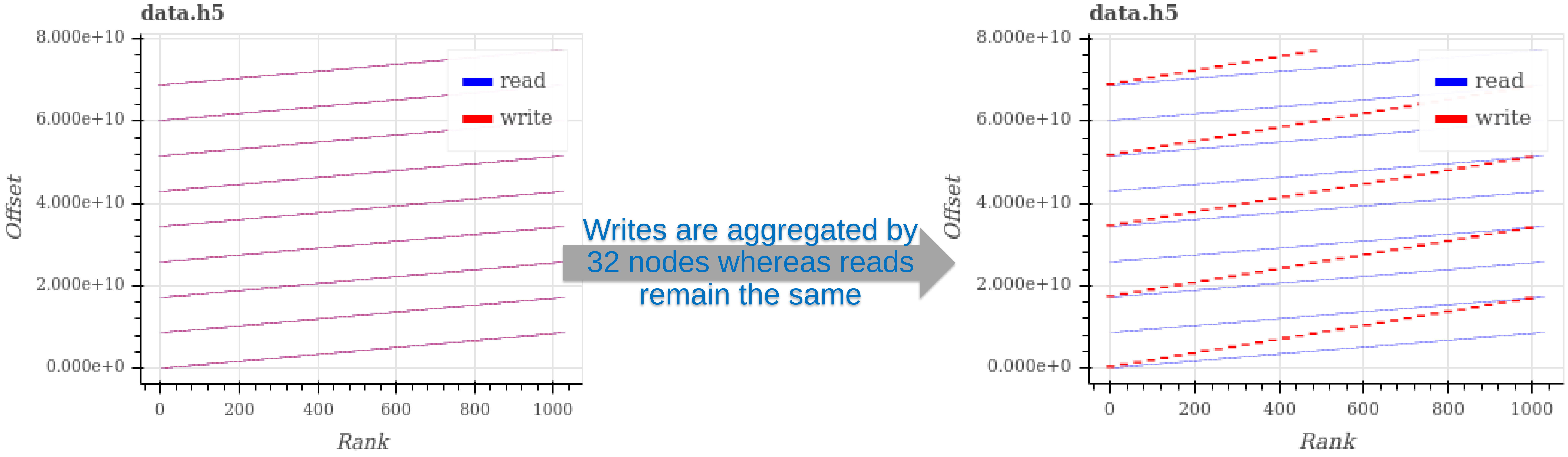
HDF5 with compound datatype



HDF5 with allocate multi

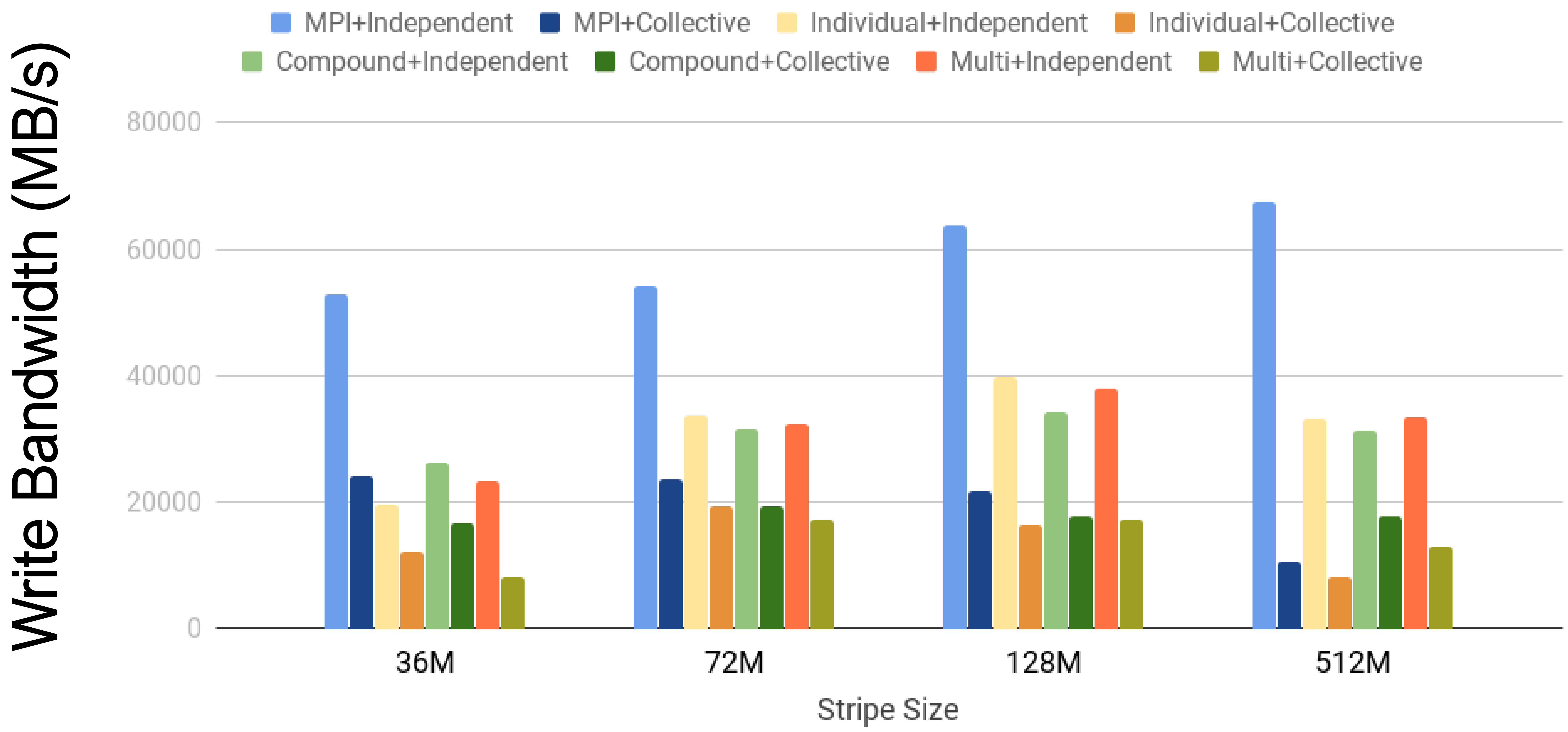
HACC-IO: access patterns of HDF5 with collective I/O

- Will Collective I/O make the access pattern (on the left) of individual dataset better?
  - Problem size: 8GB per variable, 72GB in total
  - Lustre config: Stripe count 32, Stripe Size 512M
  - Each rank writes 9 variables
  - The size of each write is 8GB/1024 Processes = 8MB
- ROMIO:
  - romio_cb_read/write = automatic
  - **"When set to automatic, ROMIO will use heuristics to determine when to enable the optimization."**



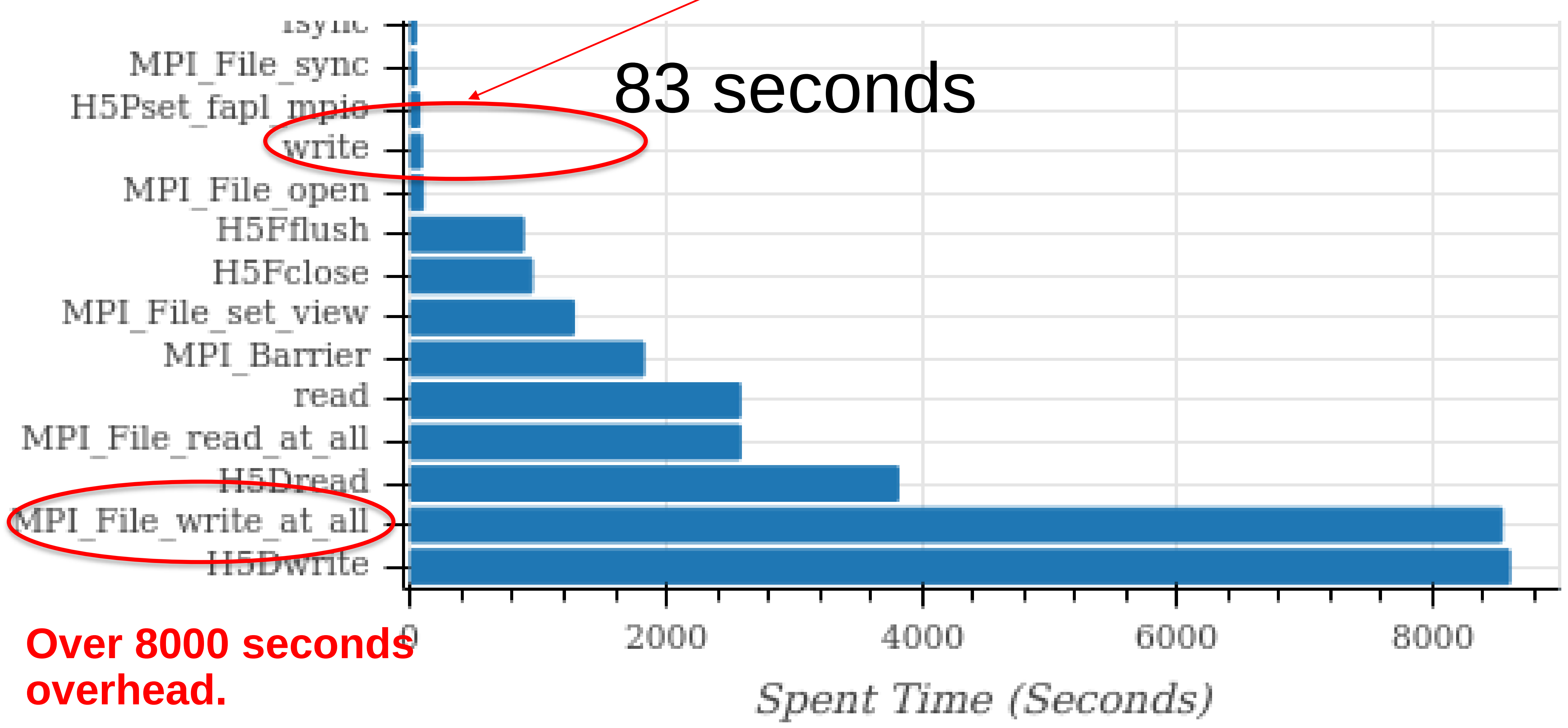
Interleaved is not always better, and neither is collective IO

- Write bandwidth with different stripe size.
- Individual dataset is better when using large stripe sizes.



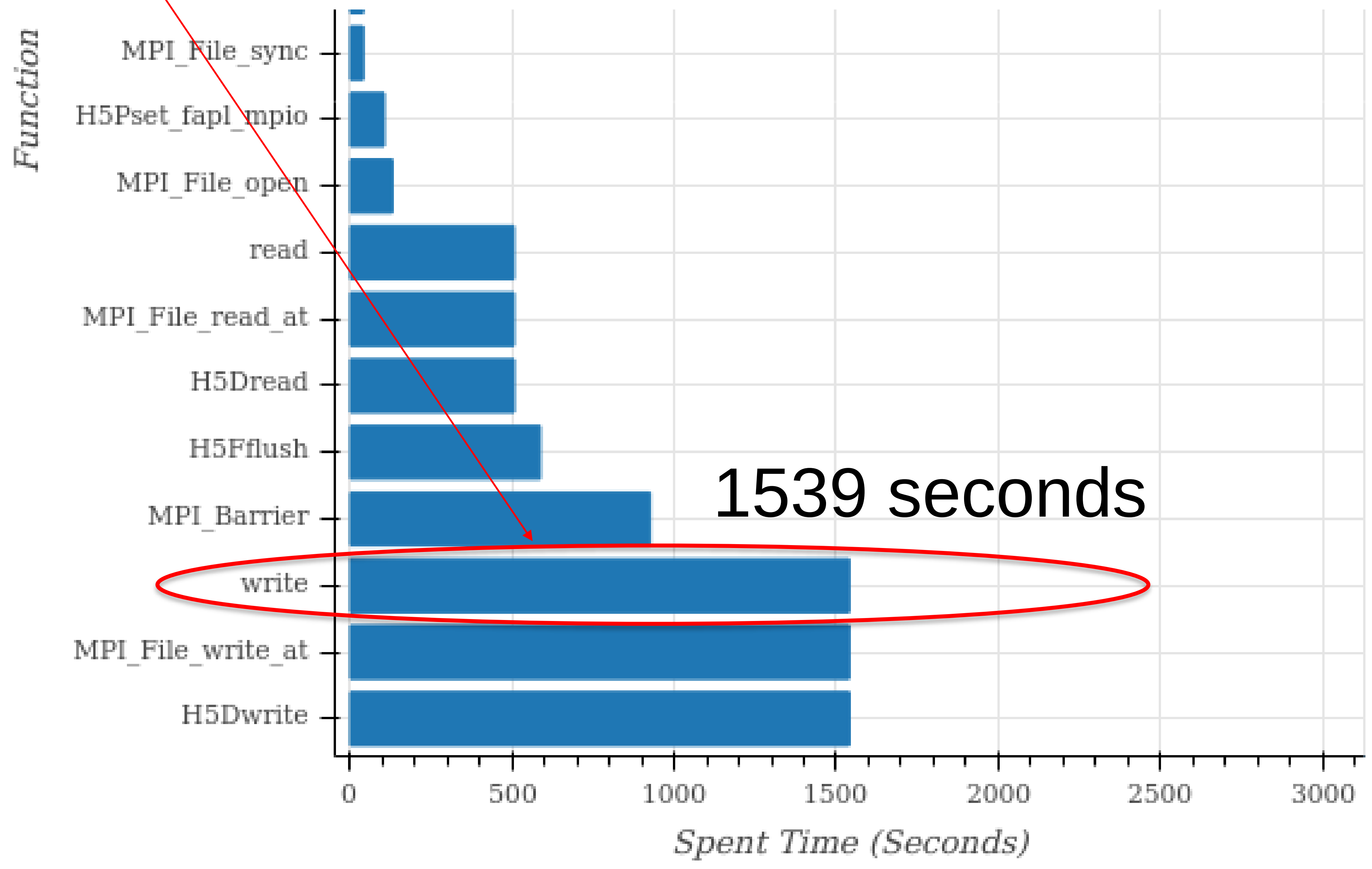
Interleaved is not always better, and neither is collective IO

- When the request size is big, the collective communication overhead increases and the benefits from collective I/O becomes limited.
- Request size is 8MB in our case.
- Collective writes are indeed much faster: 83 seconds vs 1539 seconds in independent mode.
- However, the cost for communication is too high



Over 8000 seconds overhead.

Collective

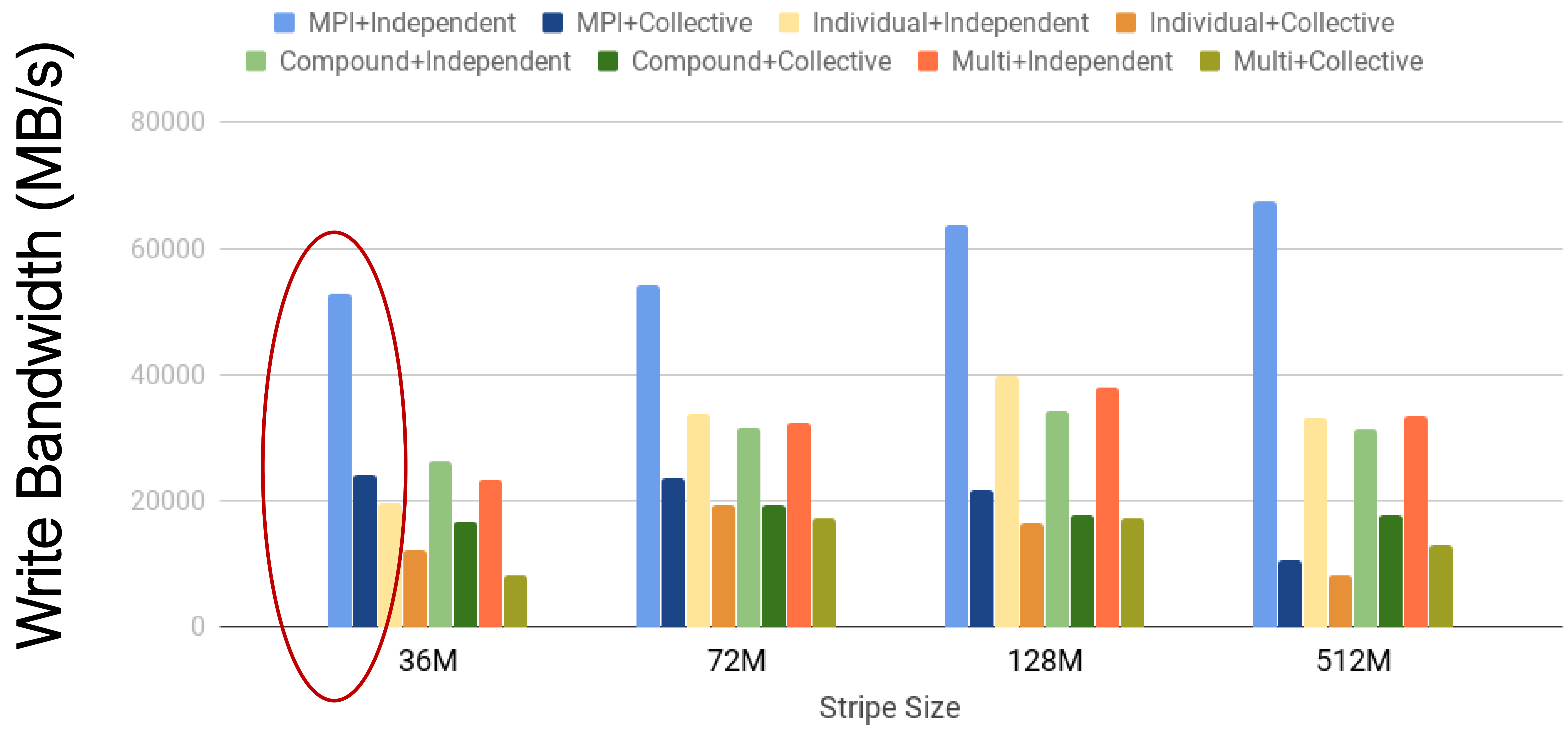


Independent

Accumulated time spent on each function

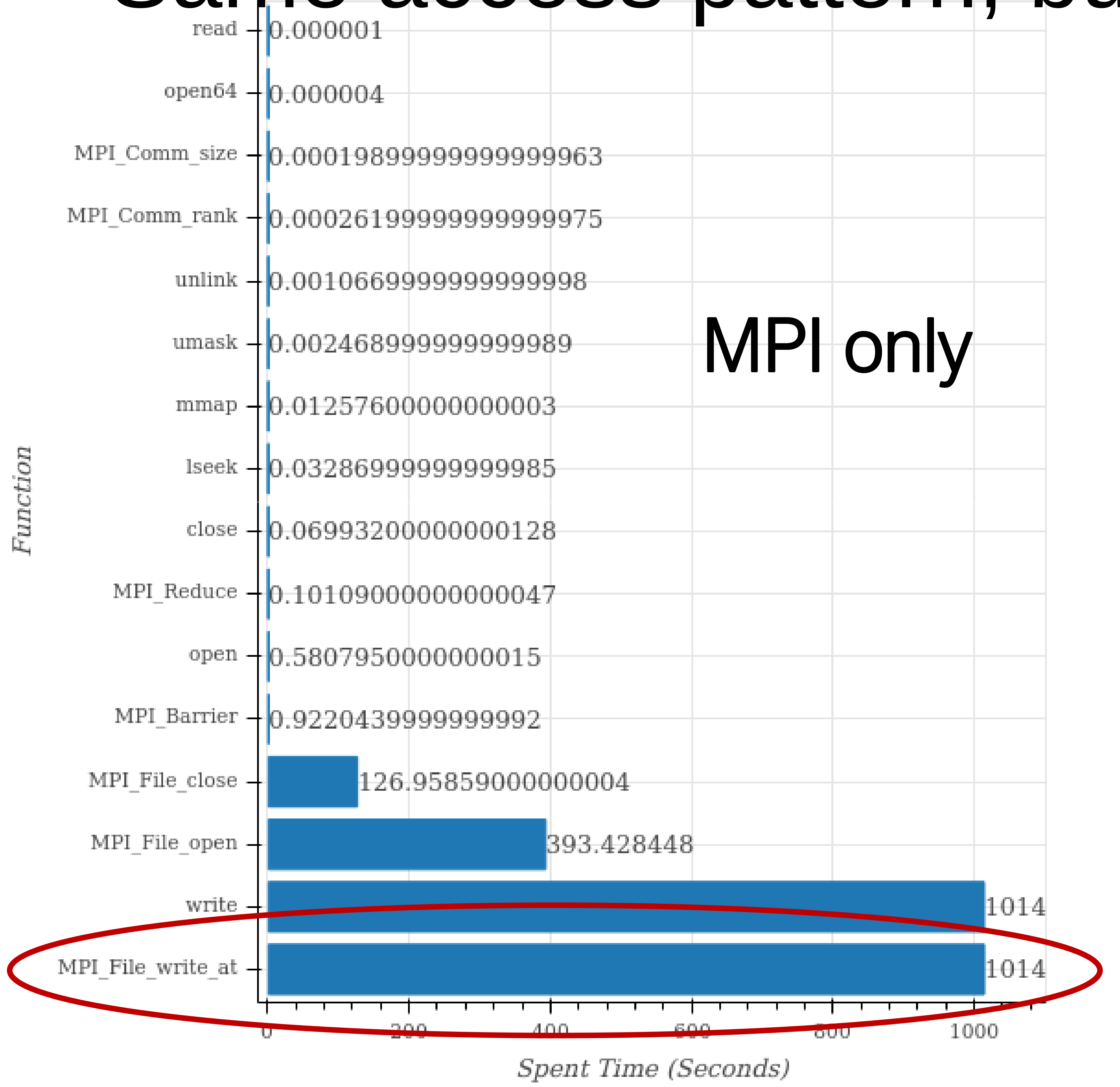
Interleaved is not always better, and neither is collective IO

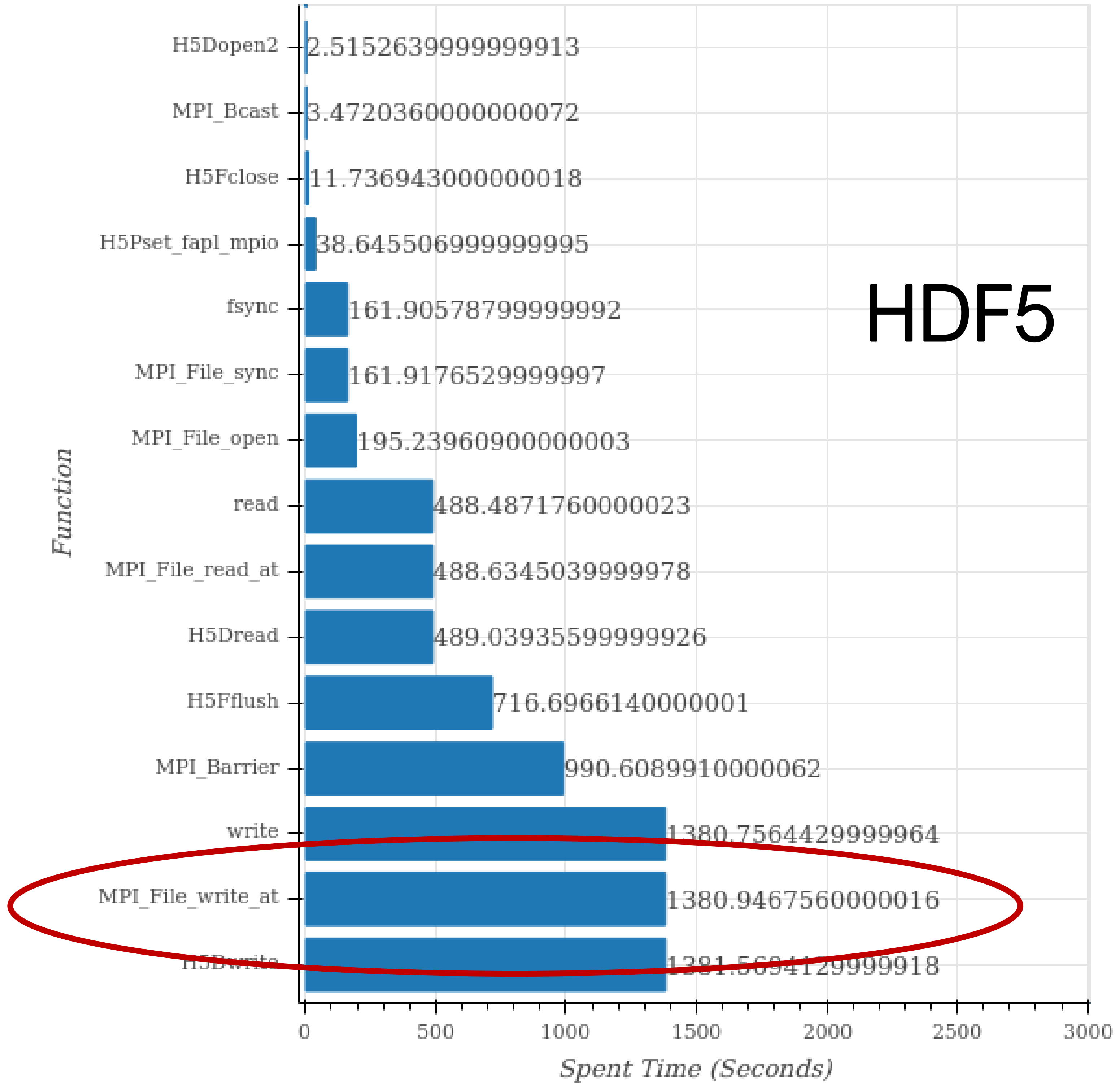
- Write bandwidth with different stripe size.
- Individual dataset is better when using large stripe sizes.



HACC-IO: MPI vs HDF5

- Same access pattern, but why MPI is faster?





MPI_File_write_at is slower in HDF5?

```
7093442 7093810 0 H5Dopen2 ['dset_id,', 'id', '0']
7093820 7093856 0 H5Sselect_hyperslab ['file_space_id', '0', '0x7fffffffb280', '(nil)', '0x7fffffffb288', '(nil)']
7093859 7093860 0 H5Sselect_hyperslab ['mem_space_id', '0', '0x7fffffffb290', '(nil)', '0x7fffffffb298', '(nil)']
7093864 7147935 0 H5Dwrite ['dset_id', 'H5T_NATIVE_DOUBLE,', 'mem_space_id', 'file_space_id', '0', '0x2aaacae4b010']
7094119 7147912 0 MPI_File_write_at ['0x8a6c58', '2048', '0x2aaacae4b010', '8388608', 'MPI_BYTE', '0x7ffffff93c0']
7094136 7094142 0 lseek ['8', '2048', '0']
7094144 7147900 0 write ['8', '0x2aaacae4b010', '8388608']
7147940 7148015 0 H5Dclose ['dset_id']
```

- HDF5 writes 2048 bytes metadata at the beginning of the file.
- This causes the alignment issue for the data writes.

Need help 

- HDF Knowledge base
  https://portal.hdfgroup.org/display/knowledge/Parallel+HDF5
- HDF-FORUM https://forum.hdfgroup.org/
- HDF Helpdesk help@hdfgroup.org

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THANK YOU!

Questions & Comments?