Parallel I/O with HDF5

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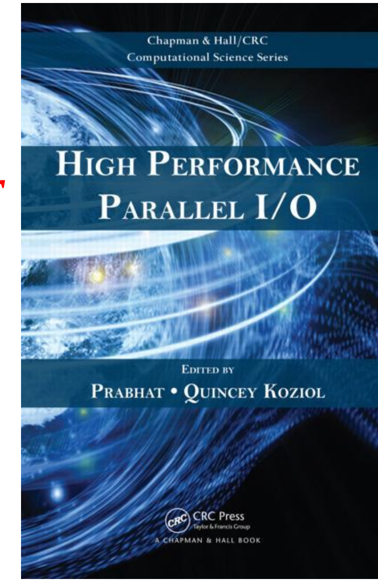
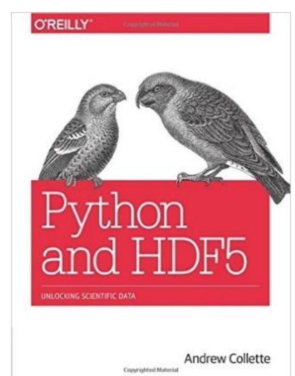
Outline

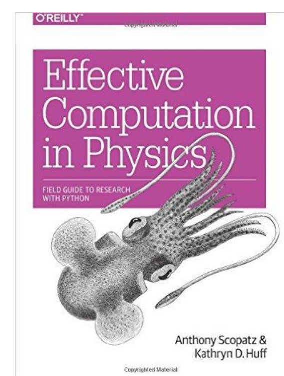
- Problems and Goals
- Methodology
- Tools
  - Parallel HDF5
  - Diagnostics & Instrumentation
- Two Examples
  - VPIC
  - CGNS
- HDF5 from Python

The answers to most of your I/O-related questions Can be found here ➔



We've ~~plundered~~ re-used the best parts in this presentation 🡐





PROBLEMS AND GOALS

Problems

"A supercomputer is a device for turning compute-bound problems into I/O-bound problems." (Ken Batcher)

- My application spends too much time in I/O.
- It doesn't scale because of I/O.
- I'm told my system is capable of X, but I'm getting less than 1% of X.
- …

Common Causes of I/O Problems

1. Undersized I/O system for the compute partition
2. Misconfigured system (for the application)
3. Interference with other running applications
4. The way your application reads and writes data leads to poor I/O performance

While 1 - 3 are possibilities, 4 is the most likely scenario. (… and it's not always your fault!)

Towards Achievable Goals

- Rule out / quantify 1 - 3 through benchmarking and repeated application runs
- Characterize application I/O through profiling
- Create a performance improvement plan
  - “Spectrum of control”
    - My I/O layer] ← … → [Closed-source 3rd-party lib.
  - Know your system’s capabilities and your resources (budget, skills, …)
  - Be prepared to settle for a lot less (sometimes).

Most of this is common sense, but deserves to be repeated.

METHODOLOGY

Prepare a Baseline

- Full application vs. I/O kernel
- Performance model
  - Back-of-the-envelope calculations
- Benchmarks
- Application runs with representative workloads
- Metrics (examples)
  - I/O size in megabytes read and written
  - I/O rate in MB/s
  - Percentage of application time spent in I/O
  - Distribution of write and read sizes

Define the Search Space

- Goal is to establish the “fundamentals” (or rule out certain causes)
- Define lines (loops!) of investigation
- Walk the loop(s) and document setup and results
  - Low hanging fruit first (if there are any)
- Fewer variables are better than too many
  - NEVER change more than one variable at a time
- Depends on level of control and budget

Know When to Stop

You might have:

- Reached your goal (unlikely)
- Exhausted your budget (frequently)
- Gotten on a path of diminishing returns (most likely)
- New problem in a different part of the application (always)

TOOLS

Tools

- Parallel HDF5
- Diagnostics and Instrumentation
- Basic facts about your machine's I/O stack

Tools

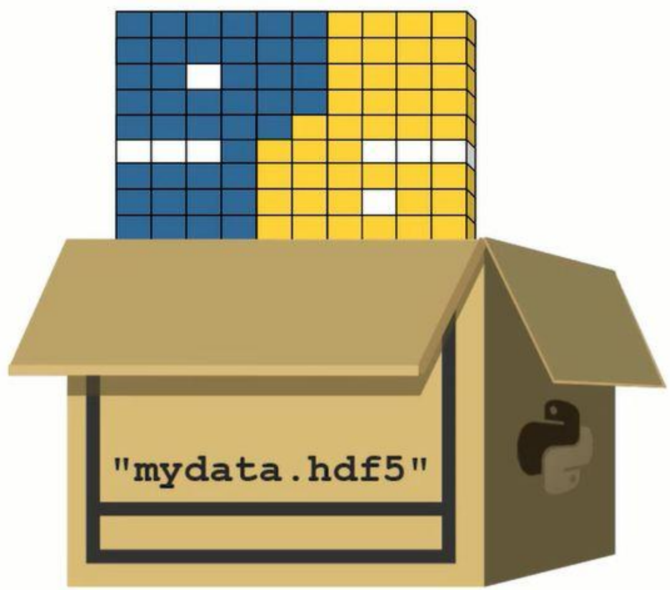
PARALLEL HDF5

HDF5 in 2 Slides and 2 Movies

1. **Who's** behind all this?
   The HDF Group, 1800 S. Oak St., Champaign, IL...
2. **What** is HDF5? What is it not?
   A Smart data container, not a Big Data buzz word
3. **Where** is it being used?
   Academia, enterprise, government, research, ...
4. **When** should I consider using it? When not?
   Always! Erm, actually not... => Ask the experts!
5. **Why** does my neighbor make jokes about HDF5?
   Give us her address and we'll take care of it...
6. **How** can I get up to speed – fast? *=> This talk + refs.*

Showtime – Part 1

Introduction to HDF5 with Python



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HDF5 Data Model

- Groups – provide structure among objects
- Datasets – where the primary data goes
  - Data arrays
  - Rich set of datatype options
  - Flexible, efficient storage and I/O
- Attributes, for metadata

Everything else is built essentially from these parts.

Showtime – Part 2

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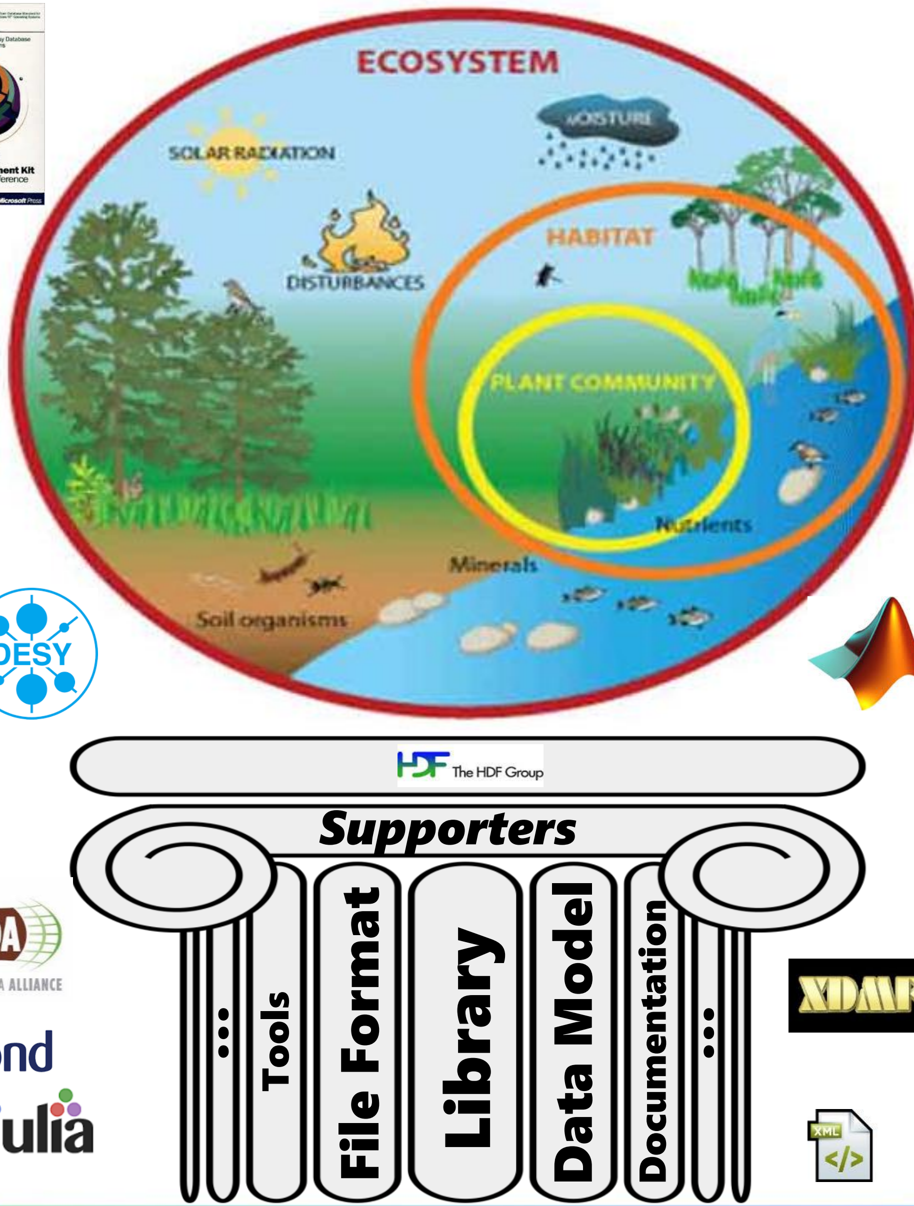
Core Topics Introduction
Data Model and Basic Usage

HDF5 Ecosystem



Terminology

- DATA ➔ problem-size data, e.g., large arrays
- METADATA – is an overloaded term
- In this presentation:
    - Metadata "=" HDF5 metadata
  - For each piece of application metadata, there are many associated pieces of HDF5 metadata
  - There are also other sources of HDF5 metadata

Why Parallel HDF5?

- Take advantage of high-performance parallel I/O while reducing complexity
  - Add a well-defined layer to the I/O stack
  - Keep the dream of a single or a few shared files alive
  - “Friends don’t let friends use one file per process!”
- Make performance portable

What We'll Cover Here

- Parallel vs. serial HDF5
- Implementation layers
- HDF5 files (= composites of data & metadata) in a parallel file system
- PHDF5 I/O modes: collective vs. independent
- Data and metadata I/O

What We Won’t Cover

- Consistency semantics
- Metadata server
- Virtual Object Layer (VOL)
- Automatic tuning
- Single Writer Multiple-Reader (SWMR)
- Virtual Datasets (VDS)
- BigIO
- …
- Come see us during the break or after the presentation!

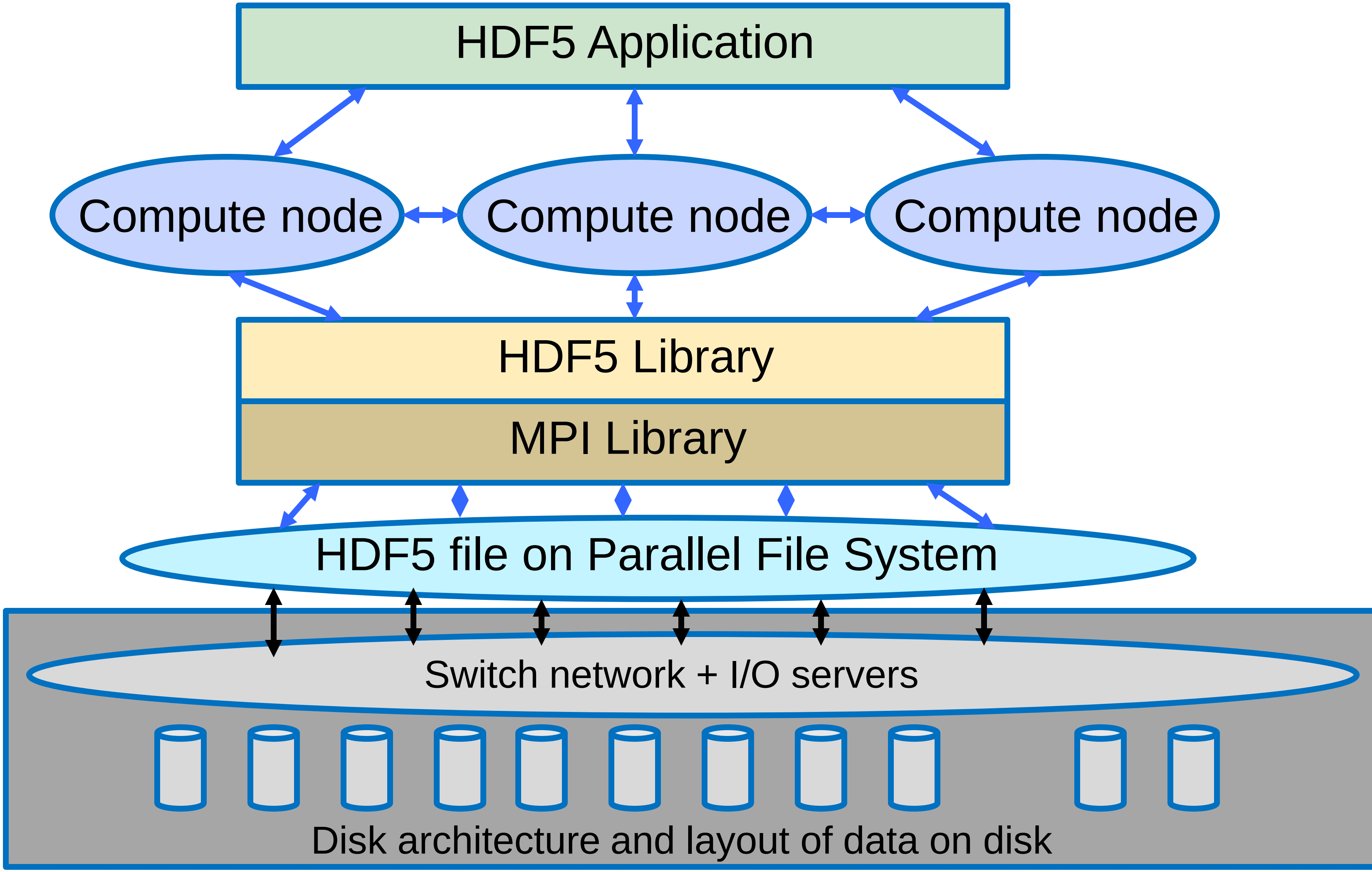
(MPI-)Parallel vs. Serial HDF5

- PHDF5 allows multiple MPI processes in an MPI communicator 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”
- Bottom line: PHDF5 is as user-friendly as HDF5.

Standard HDF5 “Skeleton”

H5Fcreate (H5Fopen)	create (open) File
H5Screate_simple/H5Screate	create dataSpace
H5Dcreate (H5Dopen)	create (open) Dataset
H5Dread, H5Dwrite	**access Dataset**
H5Dclose	close Dataset
H5Sclose	close dataSpace
H5Fclose	close File

PHDF5 Implementation Layers



Example of a PHDF5 C Program

A parallel HDF5 program has a few extra calls

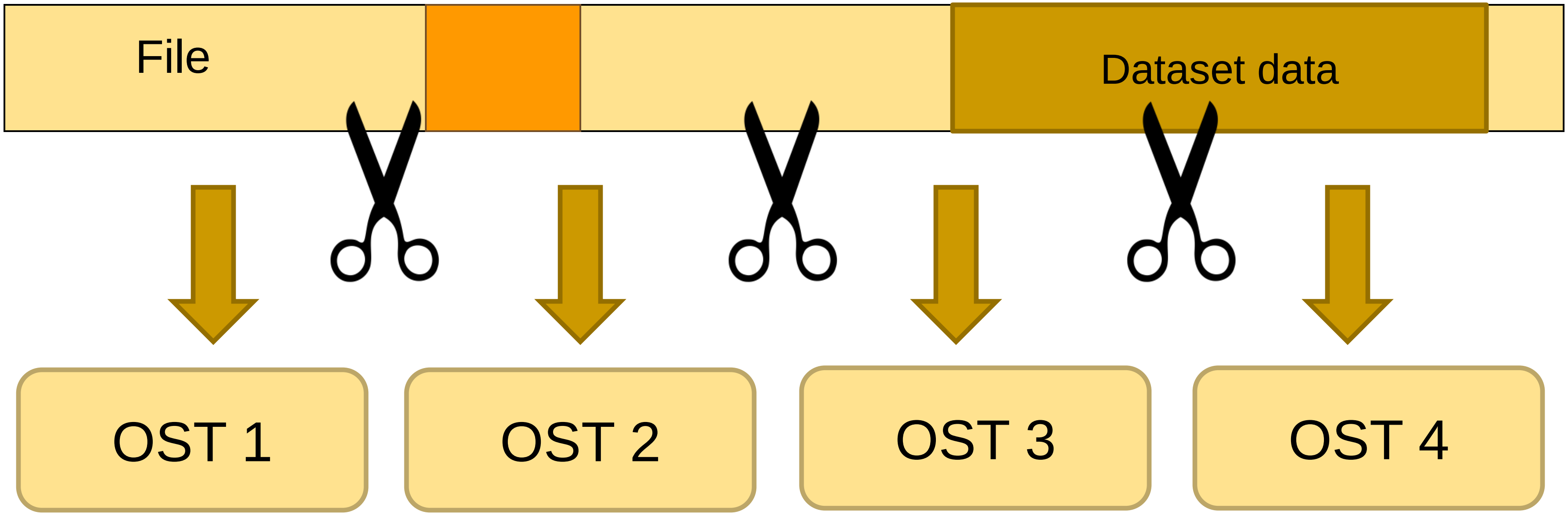
```
MPI_Init(&argc, &argv);

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();
```

PHDF5 Etiquette

- PHDF5 opens a shared file with an MPI communicator
- Returns a file handle
- All future access to the file via that file handle
- All processes must participate in collective PHDF5 APIs
- Different files can be opened via different communicators
- All HDF5 APIs that modify structural metadata are collective! (file ops., object structure and life-cycle)

https://www.hdfgroup.org/HDF5/doc/RM/CollectiveCalls.html

In a Parallel File System

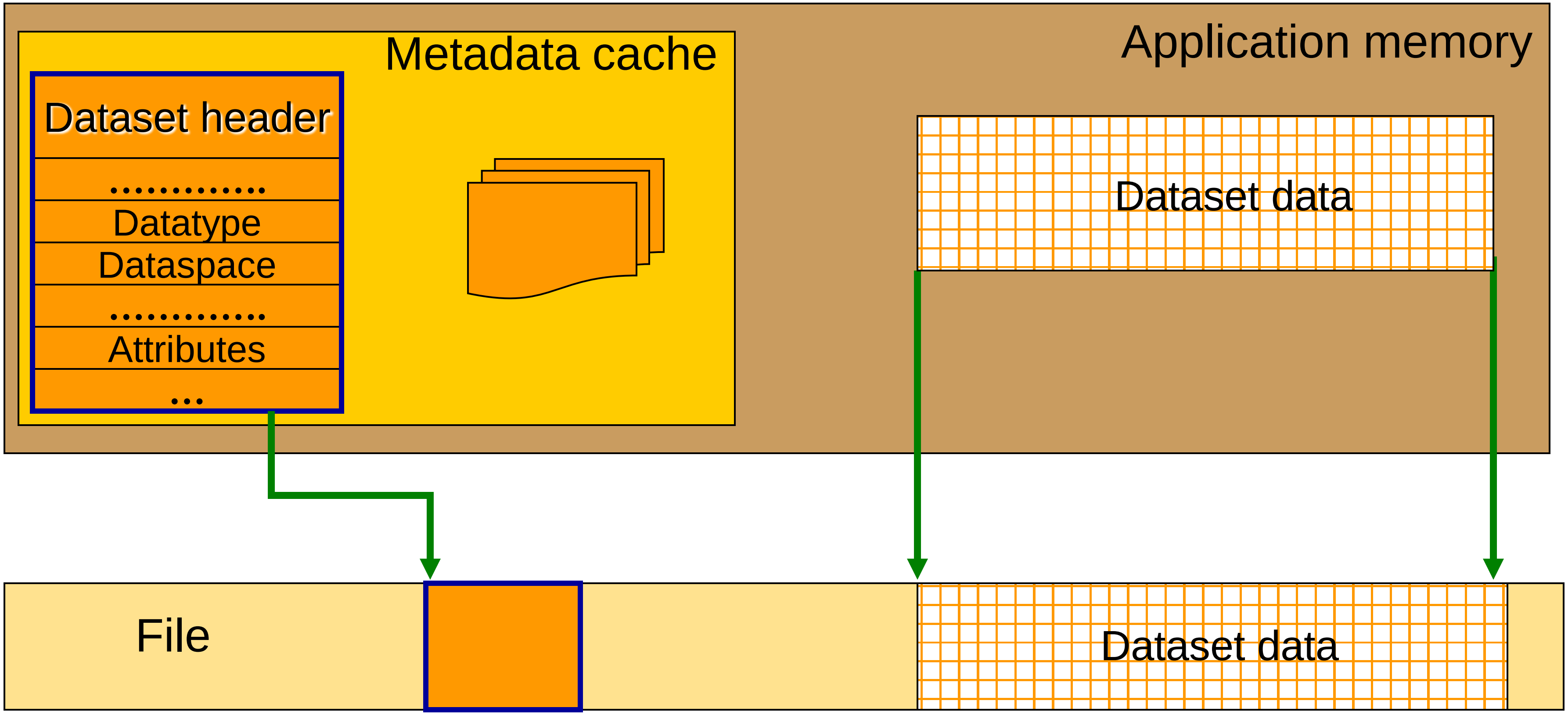


The file is striped over multiple “disks” (Lustre OSTs) depending on the stripe size and stripe count with which the file was created.

And it gets worse before it gets better…

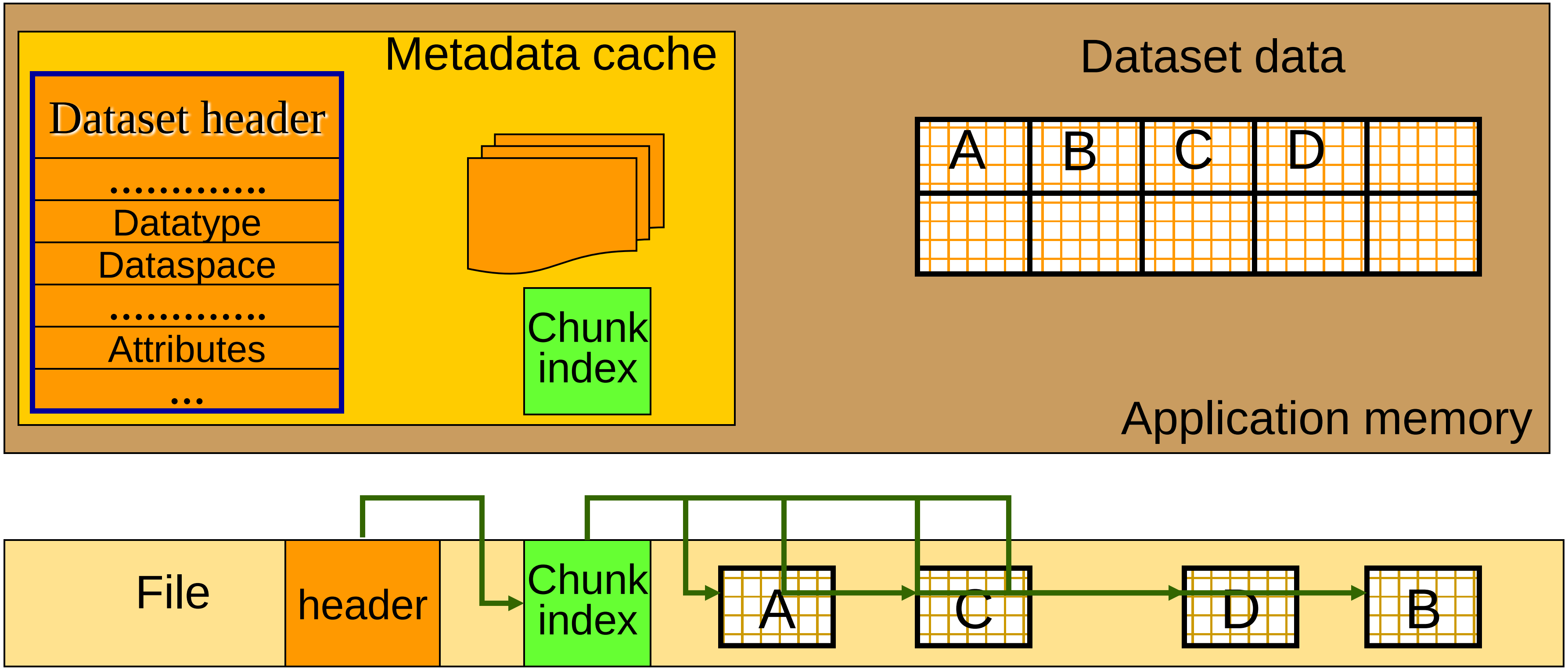
Contiguous Storage

- Metadata header separate from dataset data
- Data stored in one contiguous block in HDF5 file

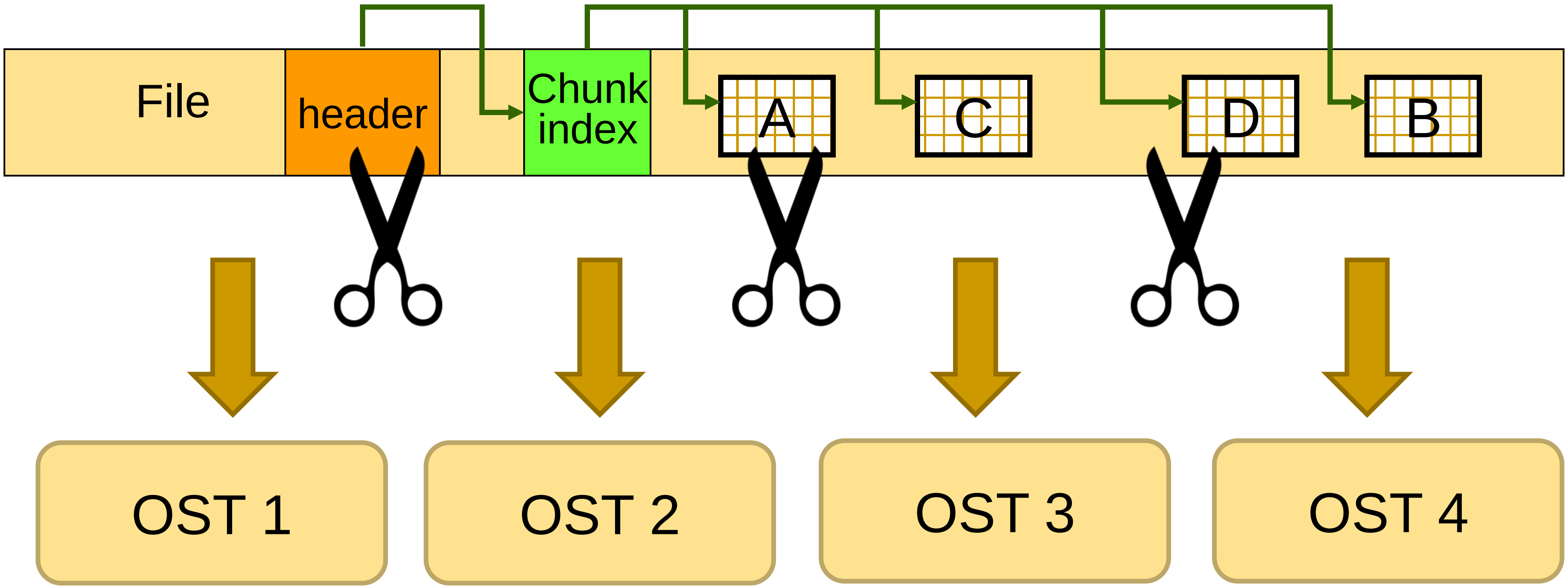


Chunked Storage

- Dataset data is divided into equally sized blocks (chunks).
- Each chunk is stored separately as a contiguous block in HDF5 file.



In a Parallel File System



The file is striped over multiple OSTs depending on the stripe size and stripe count with which the file was created.

Collective vs. Independent I/O

- MPI definition of collective calls:
  - All processes of the communicator must participate in calls in the right order.
    - Process1 Process2
    - call A(); call B(); call A(); call B(); **right**
    - call A(); call B(); call B(); call A(); **wrong**
- Independent means not collective ☺
- Collective is not necessarily synchronous, nor must it require communication
- Neither mode is preferable a priori.

Collective I/O ➔ attempt to combine multiple smaller independent I/O ops into fewer larger ops.

Data and Metadata I/O

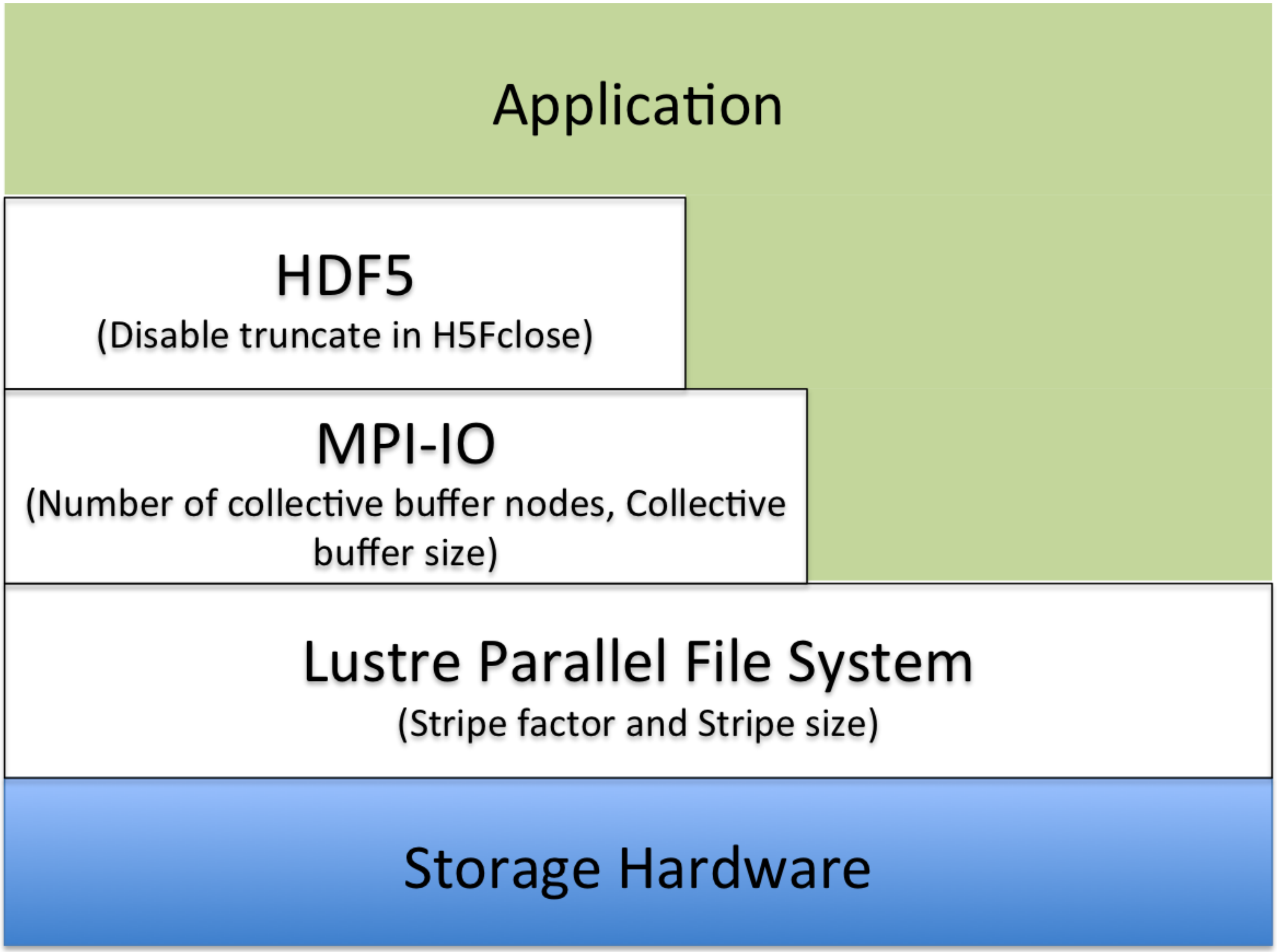
Data

- Problem-sized
- I/O can be independent or collective
- Improvement targets:
  - Avoid unnecessary I/O
  - I/O frequency
  - Layout on disk
    - Different I/O strategies for chunked layout
  - Aggregation and balancing
  - Alignment

Metadata

- Small
- Reads can be independent or collective
- All modifying I/O must be collective
- Improvement targets:
  - Metadata design
  - Use the latest library version, if possible
  - Metadata cache
    - In desperate cases, take control of evictions

Don't Forget: It's a Multi-layer Problem



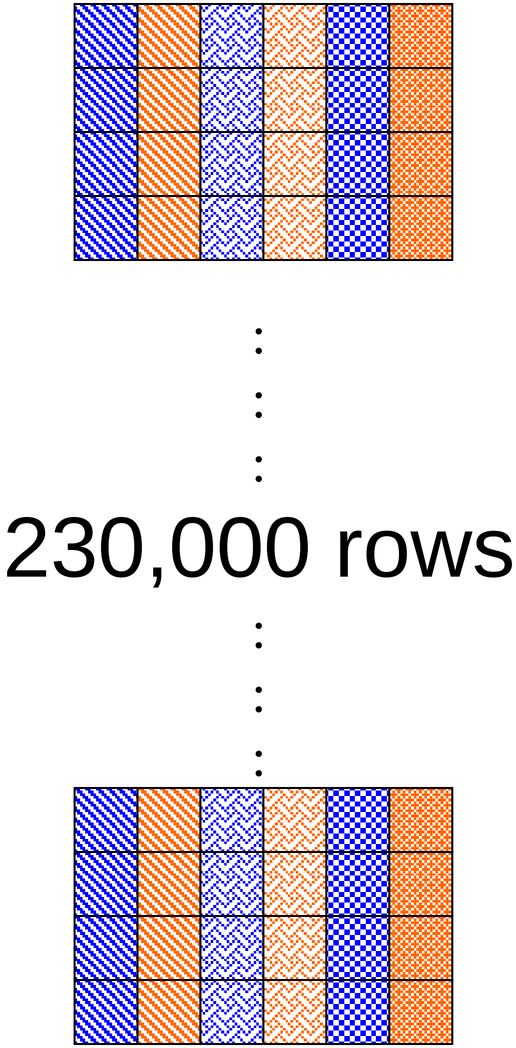
Tools

DIAGNOSTICS AND INSTRUMENTATION

A Textbook Example

User report:

- Independent data transfer mode is much slower than the collective data transfer mode
- Data array is tall and thin: 230,000 rows by 6 columns



Symptoms

Writing to one dataset

- 4 MPI processes ➔ 4 columns
- Datatype is 8-byte floats (doubles)
- 4 processes x 1000 rows x 8 bytes = 32,000 bytes

```
% mpirun -np 4 ./a.out 1000
```

- ➢ Execution time: 1.783798 s.

```
% mpirun -np 4 ./a.out 2000
```

- ➢ Execution time: 3.838858 s. (linear scaling )

- 2 sec. extra for 1000 more rows = 32,000 bytes.

Whopping speed of 16KB/sec ➔ Way too slow!!!

“Poor Man’s Debugging”

- Build a version of PHDF5 with
- `./configure --enable-debug --enable-parallel …`
- This allows the tracing of MPIO I/O calls in the HDF5 library such as `MPI_File_read_xx` and `MPI_File_write_xx`
- Don’t forget to `% setenv H5FD_mpio_Debug “rw”`

- You’ll get something like this…

Independent and Contiguous

```
% setenv H5FD_mpio_Debug ’rw’
```

`% mpirun -np 4 ./a.out 1000` # Indep.; contiguous.

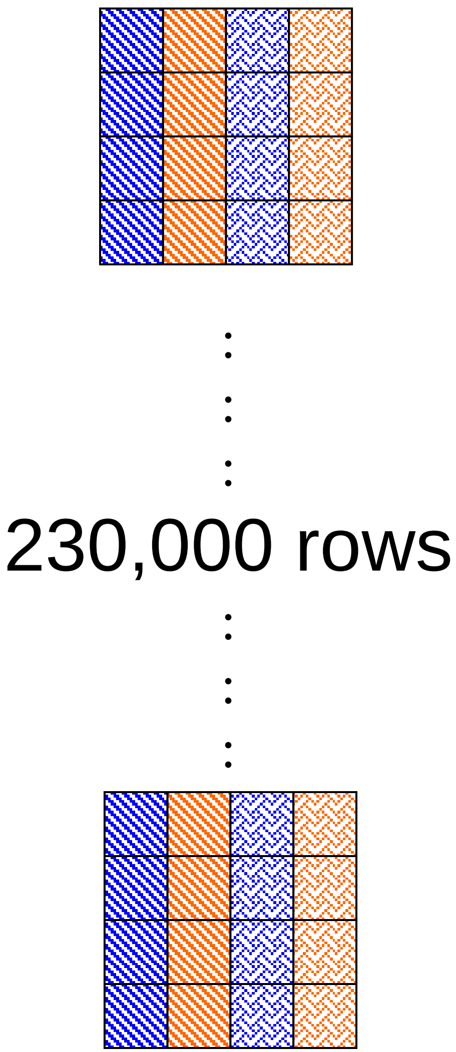
```
in H5FD_mpio_write  mpi_off=0     size_i=96
in H5FD_mpio_write  mpi_off=0     size_i=96
in H5FD_mpio_write  mpi_off=0     size_i=96
in H5FD_mpio_write  mpi_off=0     size_i=96
in H5FD_mpio_write  mpi_off=2056  size_i=8
in H5FD_mpio_write  mpi_off=2048  size_i=8
in H5FD_mpio_write  mpi_off=2072  size_i=8
in H5FD_mpio_write  mpi_off=2064  size_i=8
in H5FD_mpio_write  mpi_off=2088  size_i=8
in H5FD_mpio_write  mpi_off=2080  size_i=8
…
```

- A total of 4000 of these 8 bytes writes == 32,000 bytes.

Plenty of Independent and Small Calls

Diagnosis:

- Each process writes one element of one row, skips to next row, writes one element, and so on.
- Each process issues 230,000 writes of 8 bytes each.



Chunked by Column

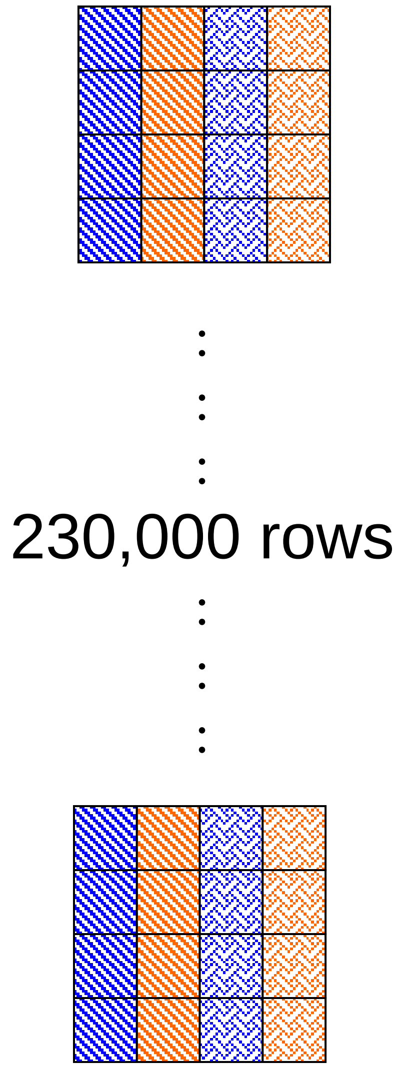
```
% setenv H5FD_mpio_Debug 'rw'
% mpirun -np 4 ./a.out 1000   # Indep., Chunked by column.
in H5FD_mpio_write  mpi_off=0        size_i=96
in H5FD_mpio_write  mpi_off=0        size_i=96
in H5FD_mpio_write  mpi_off=0        size_i=96
in H5FD_mpio_write  mpi_off=0        size_i=96
in H5FD_mpio_write  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
…
```

- Execution time: 0.011599 s.

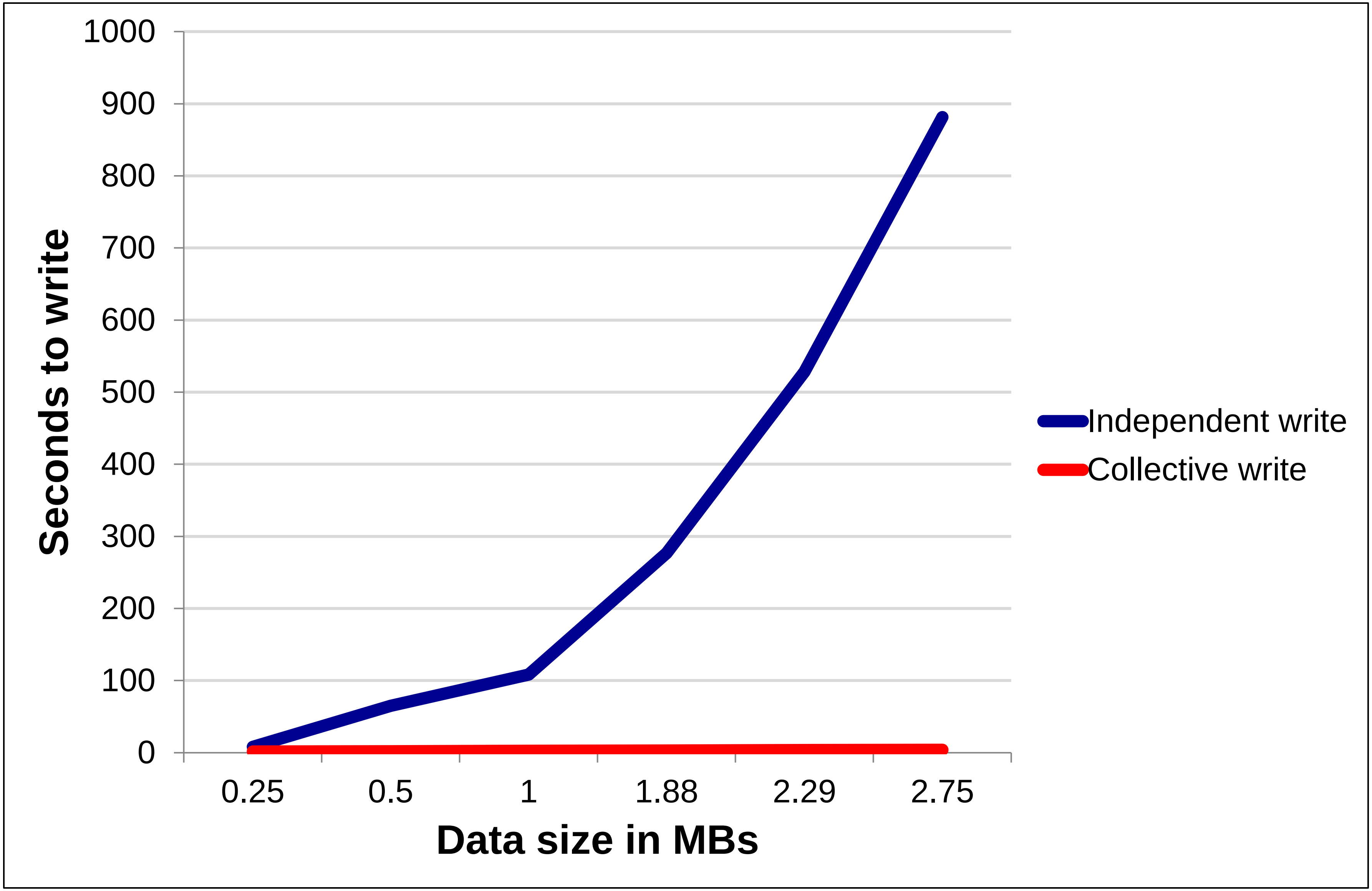
Use Collective Mode or Chunked Storage

Remedy:

- Collective I/O will combine many small independent calls into few but bigger calls
- Chunks of columns speeds up too



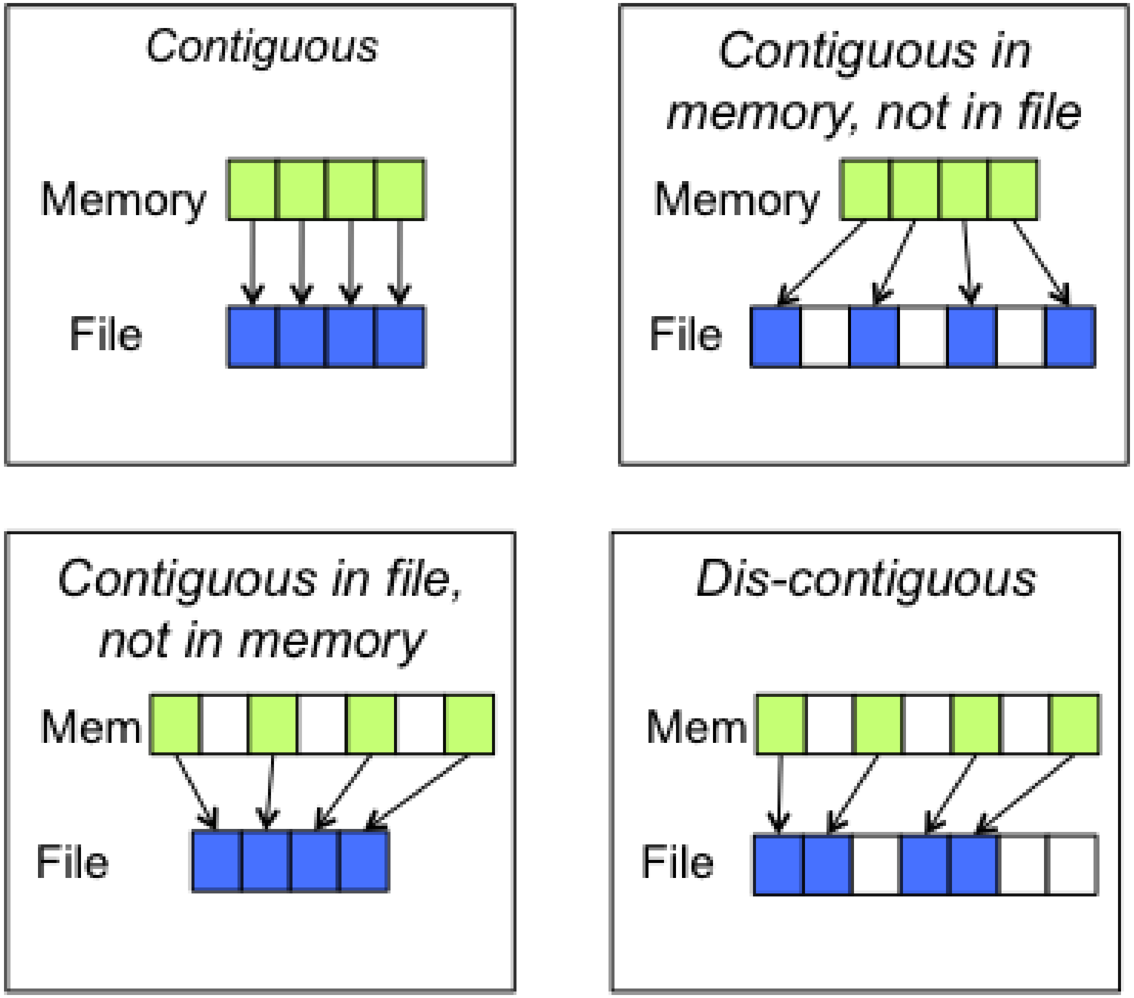
Collective vs. independent write



Back Into the Real World…

- Two kinds of tools:
  - I/O benchmarks for measuring a system's I/O capabilities
  - I/O profilers for characterizing applications' I/O behavior
- Two examples:
  - h5perf (in the HDF5 source code distro)
  - Darshan (from Argonne National Laboratory)
- Profilers have to compromise between
  - A lot of detail → large trace files and overhead
  - Aggregation → loss of detail, but low overhead

I/O Patterns

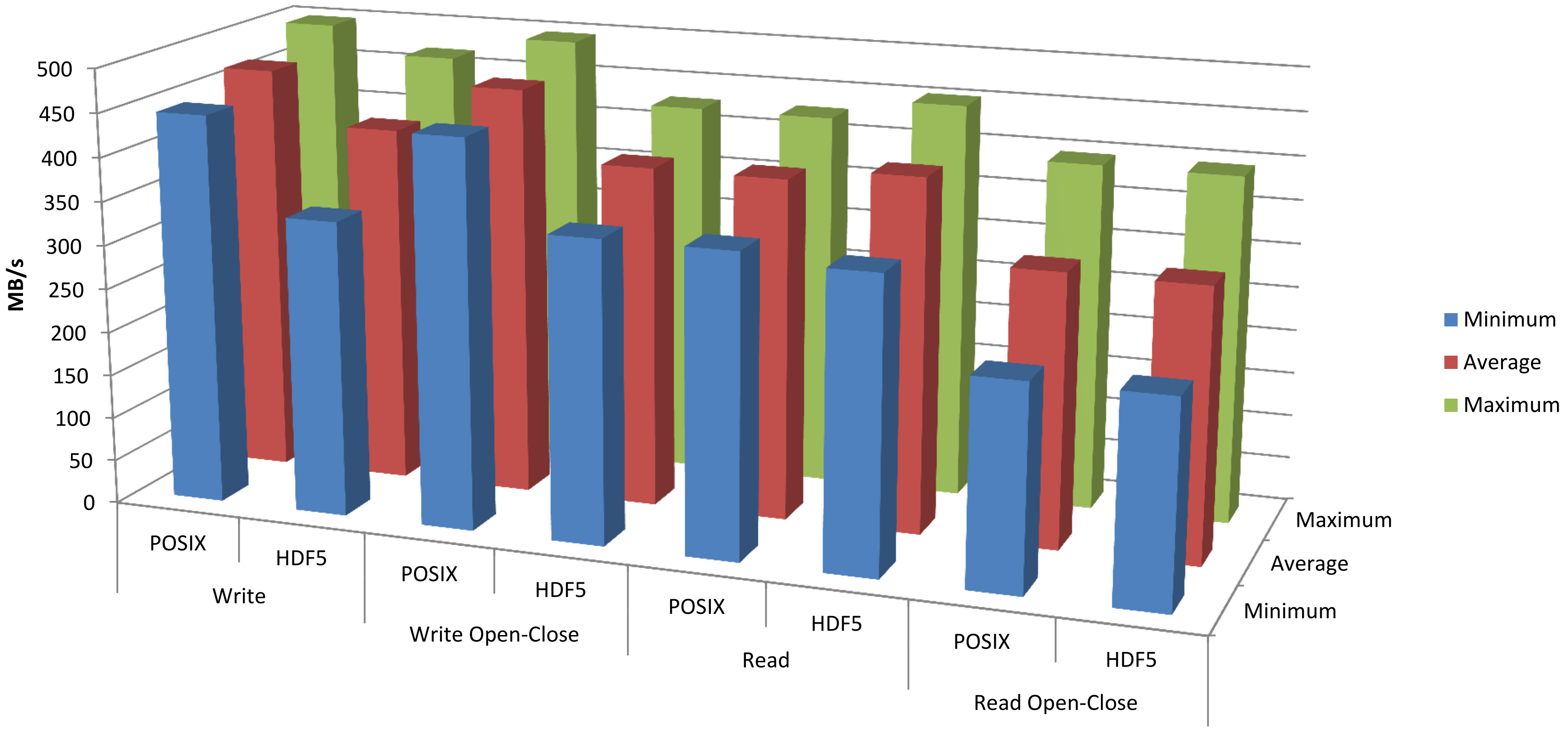

Contiguous
Memory
File
Contiguous in memory, not in file
Memory
File
Contiguous in file, not in memory
Mem
File
Dis-contiguous
Mem
File

h5perf(_serial)

- Measures performance of a filesystem for different I/O patterns and APIs
- Three File I/O APIs for the price of one!
  - POSIX I/O (open/write/read/close…)
  - MPI-I/O (MPI_File_{open,write,read,close})
  - HDF5 (H5Fopen/H5Dwrite/H5Dread/H5Fclose)
- An indication of I/O speed ranges and HDF5 overheads
- Expectation management…

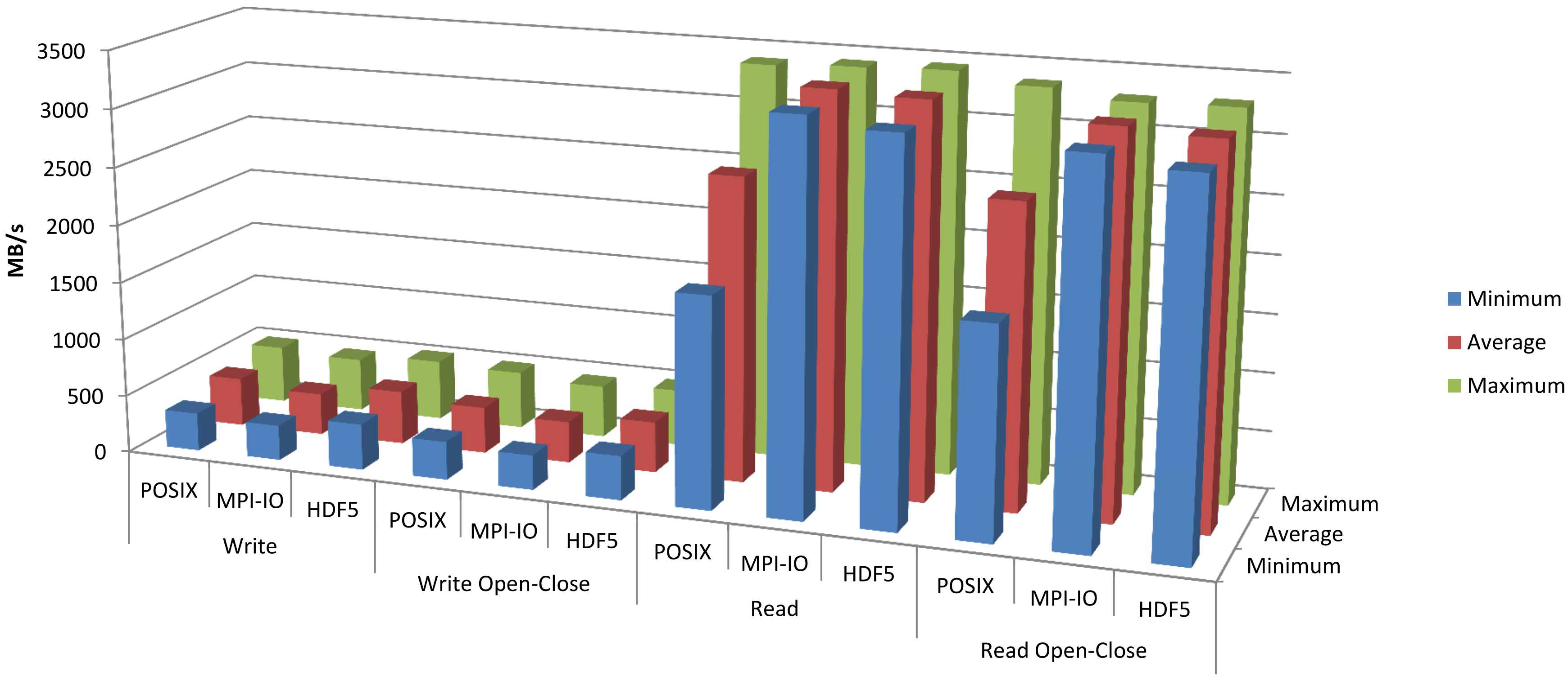
A Serial Run

h5perf_serial, 3 iterations, 1 GB dataset, 1 MB transfer buffer, HDF5 dataset contiguous storage, HDF5 SVN trunk, NCSA BW



A Parallel Run

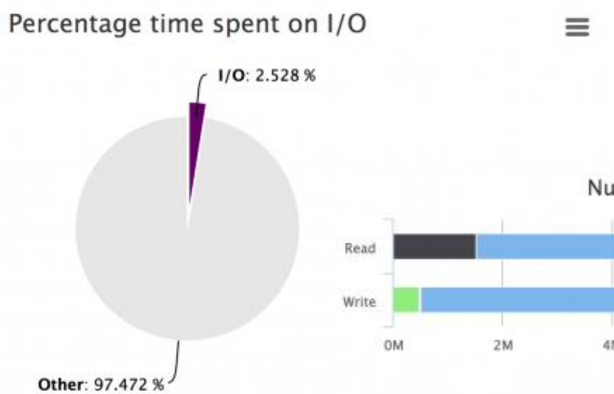
h5perf, 3 MPI processes, 3 iterations, 3 GB dataset (total), 1 GB per process, 1 GB transfer buffer, HDF5 dataset contiguous storage, HDF5 SVN trunk, NCSA BW

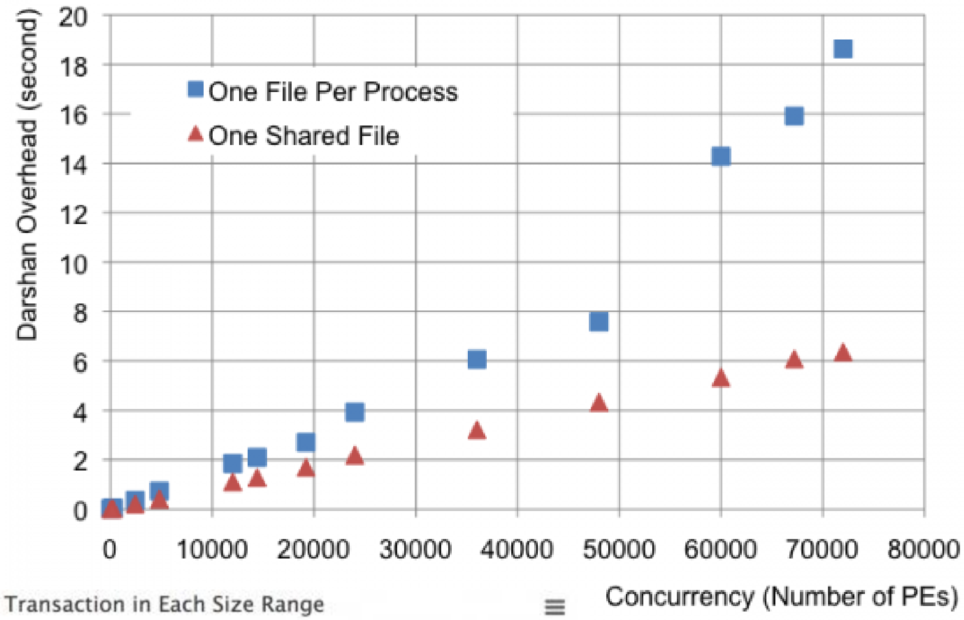


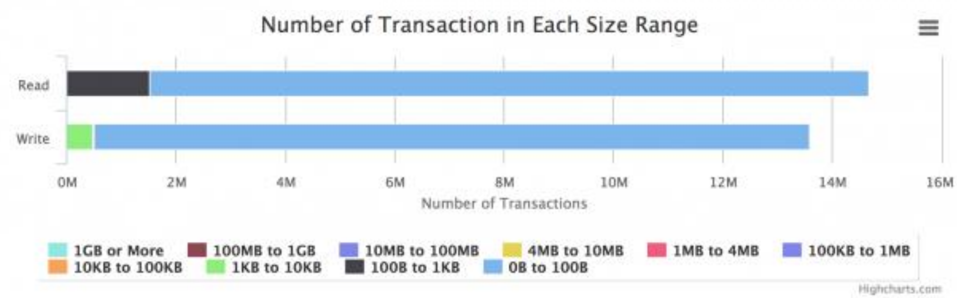
Darshan (ANL)

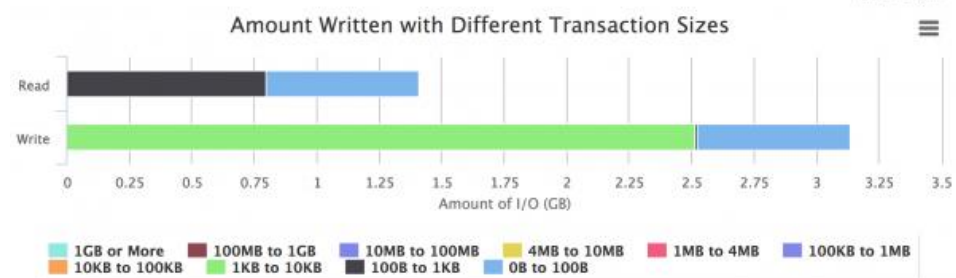
- Design goals:
  - Transparent integration with user environment
  - Negligible impact on application performance
- Provides aggregate figures for:
  - Operation counts (POSIX, MPI-IO, HDF5, PnetCDF)
  - Datatypes and hint usage
  - Access patterns: alignments, sequentiality, access size
  - Cumulative I/O time, intervals of I/O activity
- Does not provide I/O behavior over time
- Excellent starting point, maybe not your final stop

Darshan Sample Output







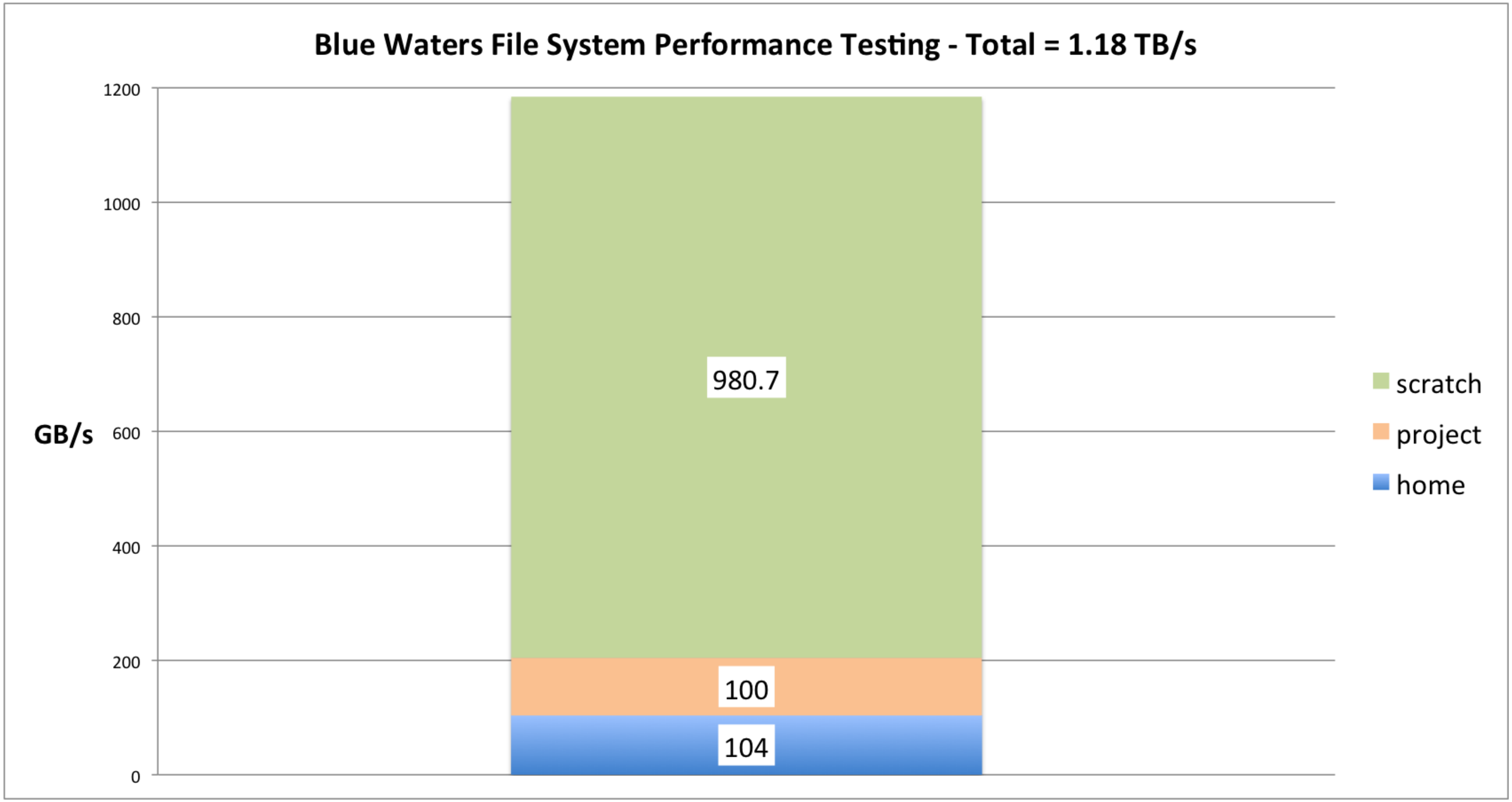


Source: NERSC

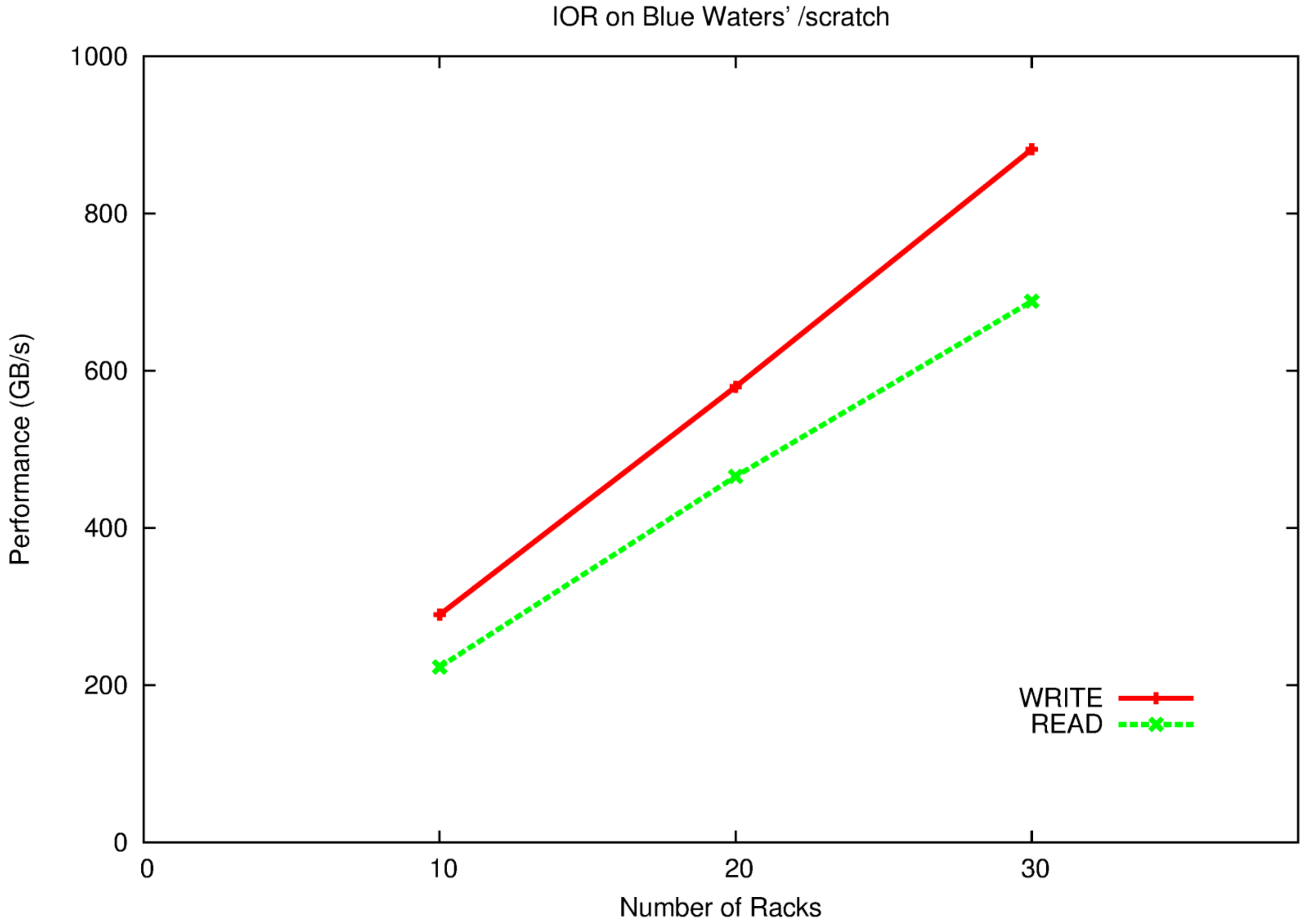
Tools

NCSA BW I/O SYSTEM BASIC FACTS

NCSA BW I/O System 1



NCSA BW I/O System 2



NCSA BW I/O System Facts

- `/scratch` is your main workhorse
  - 22 PB capacity, ~980 GB/s aggregate bandwidth
- Lustre parallel file system
  - Servers “=“ Object Storage Servers (OSS)
  - Disks “=“ Object Storage Targets (OST)
  - Files in Lustre are striped across a configurable number of OSTs
  - Default values: stripe count 2, stripe size1MB
  - `/scratch` has 1,440 OSTs (160 max. for you)

Bottom Line: We can’t blame “the system” for poor I/O performance.

NCSA BW HDF5 Software Setup

- https://bluewaters.ncsa.illinois.edu/software-and-packages
- HDF5 is installed on BW
  - cray-hdf5 xor cray-hdf5-parallel
  - Up to version 1.8.17
- Darshan is installed, but works only with the pre-installed I/O libraries (Still a good start!)
- For adventurers:
  - HDF5 feature branches
  - HDF5 SVN trunk / Git master

EXAMPLES

Standard Questions

- What I/O layers are involved and how much control do I have over them?
- Which ones do I tackle in which order?
  - Are there any low-hanging fruit?
- What's my baseline (for each layer) and what are my metrics?
- Which tool(s) will give me the information I need?
- When do I stop?

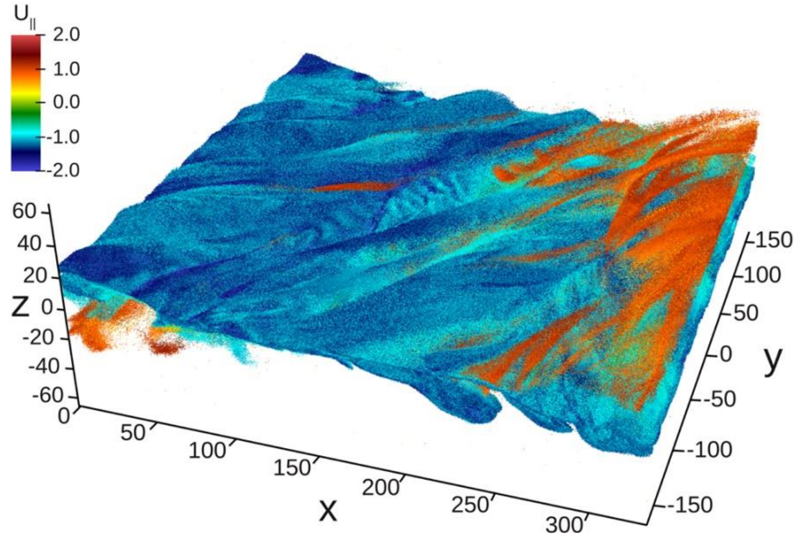
- New information ➔ New answers (maybe) : Need to keep an open mind!

Reference:

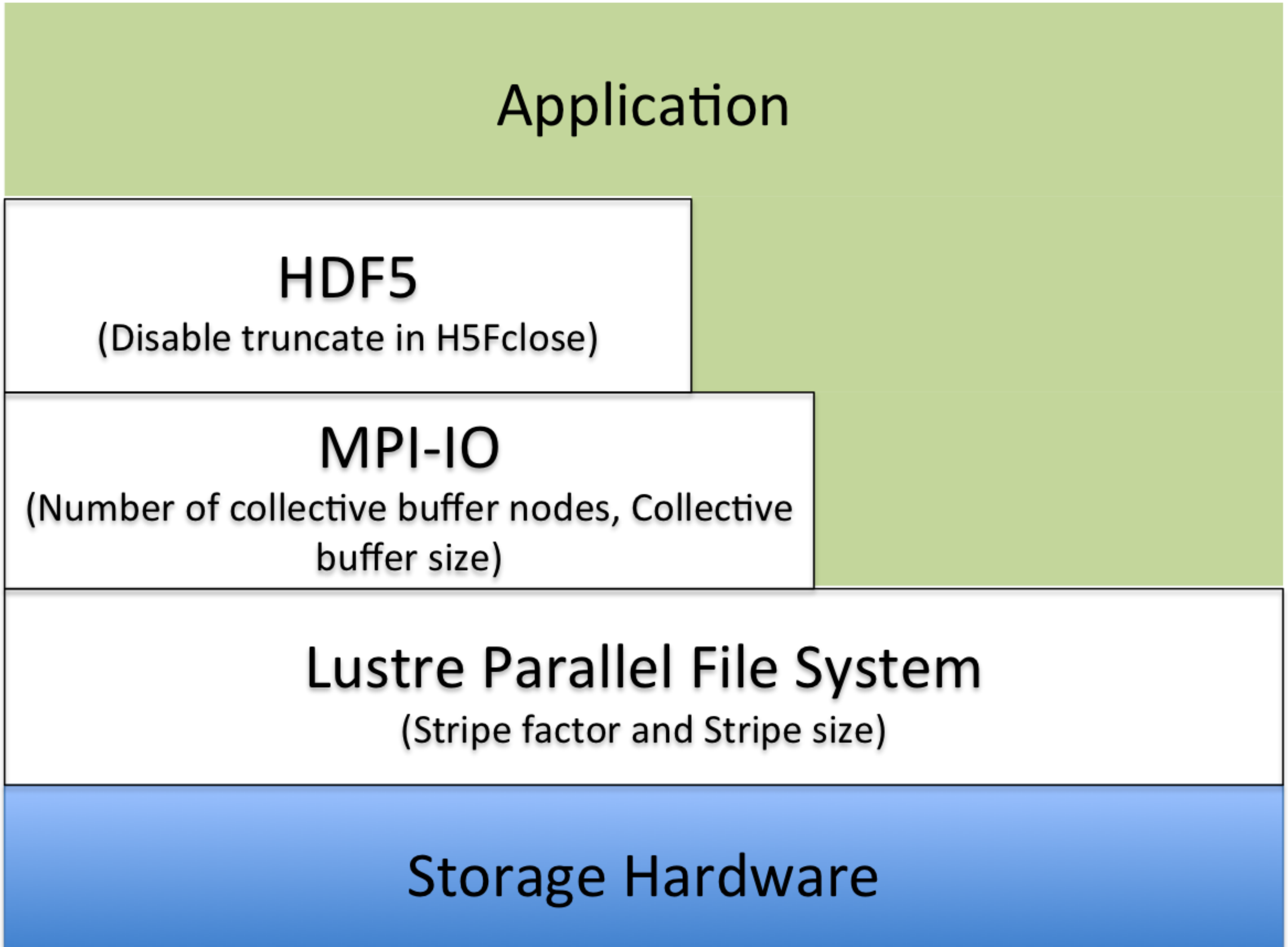
[Trillion Particles, 120,000 cores, and 350 TBs: Lessons Learned from a Hero I/O Run on Hopper](), By Suren Byna (LBNL) et al., 2015.

Examples

VPIC



Layers


Application
HDF5
(Disable truncate in H5Fclose)
MPI-IO
(Number of collective buffer nodes, Collective buffer size)
Lustre Parallel File System
(Stripe factor and Stripe size)
Storage Hardware

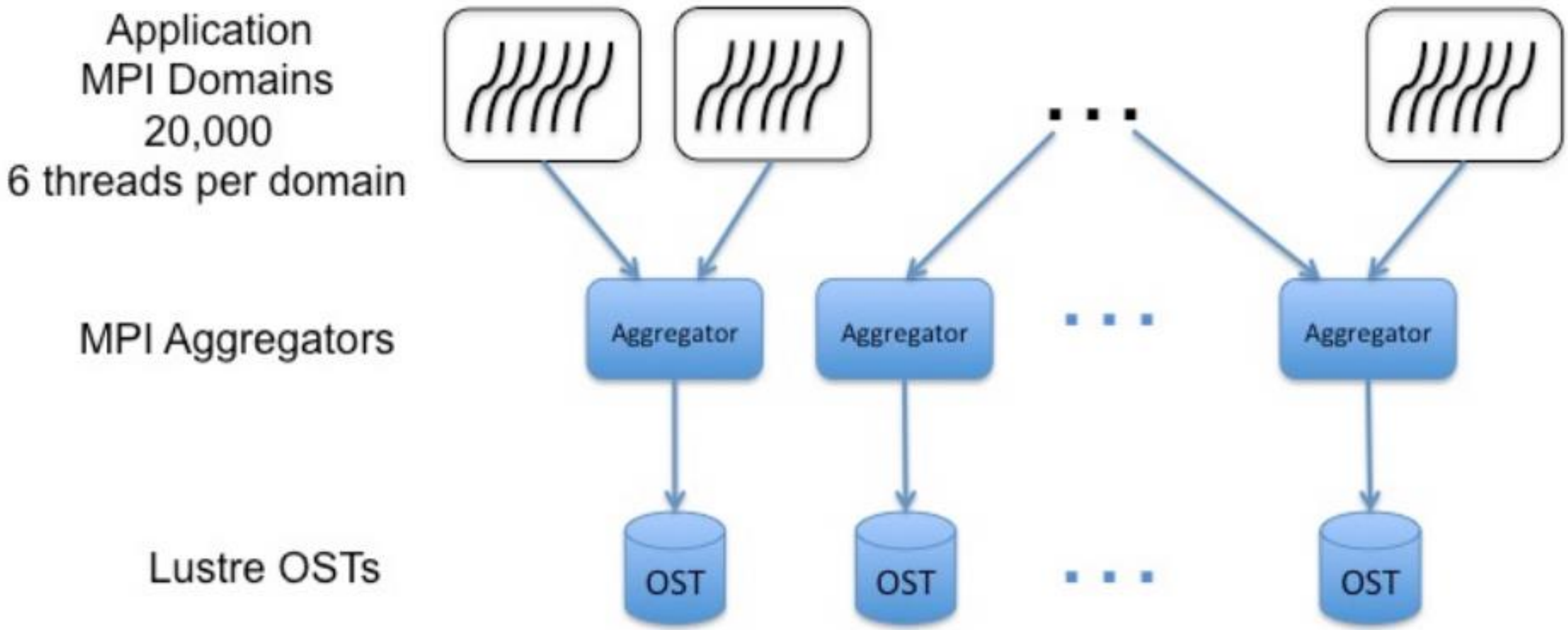
“Application I/O Structure”

- Total control over all layers
- Challenge: large output files
- Metric: write speed (throughput)
- Computationally intensive ➔ Need an I/O kernel
- H5Part multiple dataset writes

```
h5pf = H5PartOpenFileParallel (fname, H5PART_WRITE |
                   H5PART_FS_LUSTRE, MPI_COMM_WORLD);
H5PartSetStep (h5pf, step);
H5PartSetNumParticlesStrided (h5pf, np_local, 8);

H5PartWriteDataFloat32 (h5pf, "dX", Pf);
H5PartWriteDataFloat32 (h5pf, "dY", Pf+1);
H5PartWriteDataFloat32 (h5pf, "dZ", Pf+2);
H5PartWriteDataInt32   (h5pf, "i",  Pi+3);
H5PartWriteDataFloat32 (h5pf, "Ux", Pf+4);
H5PartWriteDataFloat32 (h5pf, "Uy", Pf+5);
H5PartWriteDataFloat32 (h5pf, "Uz", Pf+6);
H5PartWriteDataFloat32 (h5pf, "q", Pf+7);

H5PartCloseFile (h5pf);
```

- “Game plan”:
  - MPI-IO / Lustre tuning
    - Low hanging fruit (relatively)
    - Pair MPI aggregators with Lustre OSTs
    - Match MPI-IO buffer sizes and Lustre stripe size
  - Worry about HDF5 (H5Part)

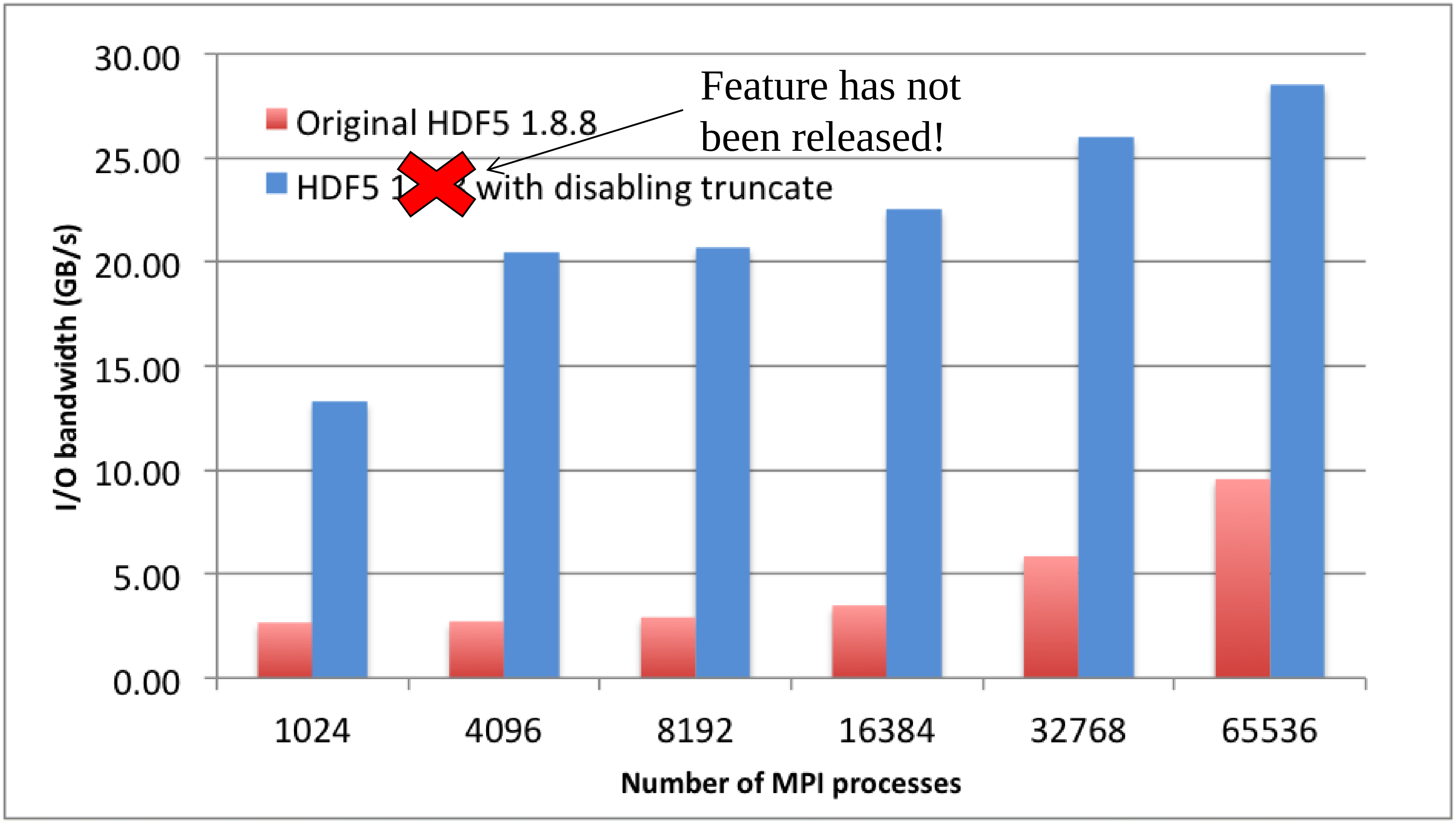
I/O Aggregation



Closing HDF5 File …

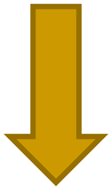
Q: How long does it take to close/flush an HDF5 file?

A: A lot longer than you might expect!



File Truncation (Today)

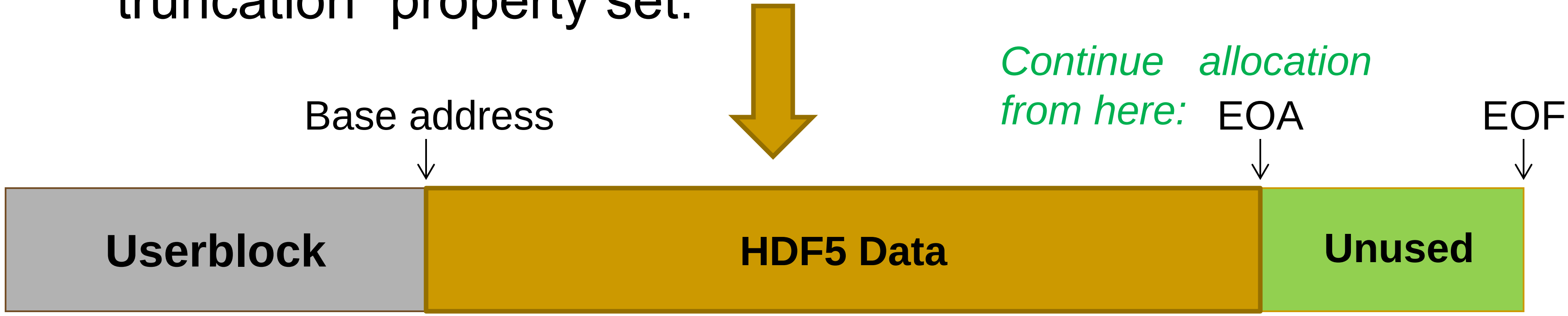
A call to `H5Fflush` or `H5Fclose` triggers a call to `ftruncate` (serial) or `MPI_File_set_size` (parallel), which can be fairly expensive.



*Currently, only **one** number is stored in the file and used for error detection.*

File Truncation (Tomorrow)

A call to `H5Fflush` or `H5Fclose` triggers both values (EOA, EOF) to be saved in the file and **no** truncation takes place, IF the file was created with the “avoid truncation” property set.



Caveat: Incompatible with older versions of the library. Requires HDF5 library version 1.10 or later.

Multi-Dataset I/O - Motivation

- HDF5 accesses elements in one dataset at a time
- Many HPC applications access data in multiple datasets in every time step
- Frequent small-size dataset access → Trouble (≠Big Data)

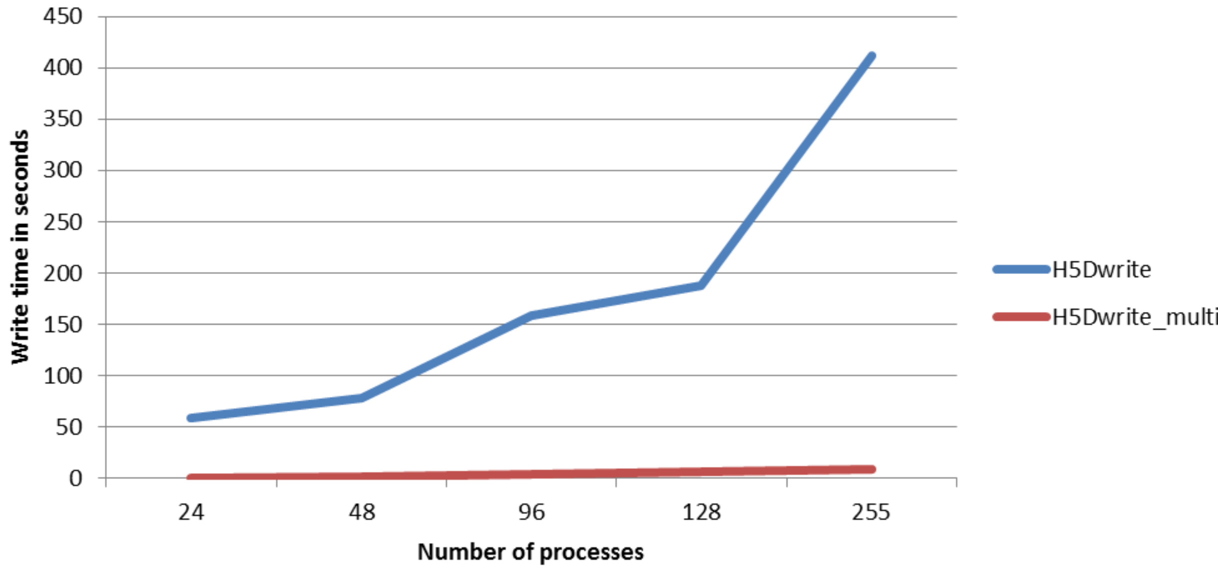
- Parallel file systems tend not to like that.
- **Idea:** Let users to do more I/O per HDF5 call!
- Two New API routines:
  - `H5Dread_multi()`
  - `H5Dwrite_multi()`

Not a new idea: PnetCDF has supported that for some time…

Sample Results

The plot shows the performance difference between using a single `H5Dwrite()` multiple times and using `H5Dwrite_multi()` once on 30 chunked datasets.

(On Hopper @ NERSC, a Cray XE-6 with Lustre file system)



Run	Code	Nodes	Cores	File Size	Stripe Size	Write Time	Total HDF Time	Throughput
Max Throughput	Multiple Dataset	320	5,120	5 TB	1 GB	91.08 s	167.78 s	56.21 GB/s
Code Comparison	Single Dataset	320	5,120	5 TB	128 MB	116.94 s	117.37 s	43.78 GB/s
Hero Run	Single Dataset	9,314	298,048	291 TB	1 GB	5,763.14 s	5,779.89 s	51.81 GB/s

TABLE I
COMPARISON OF VPIC-IO KERNEL PARAMETERS AND OBSERVED IO THROUGHPUT.

Reference:

Parallel and Large-scale Simulation Enhancements to CGNS,
By Scot Breitenfeld, The HDF Group, 2015.

Examples

CGNS

CFD Standard

- 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

Shaping the Future of Aerospace

CGNS Storage Evolution

- CGNS data was originally stored in ADF ('Advanced Data Format')
- ADF lacks parallel I/O or data compression capabilities
- Doesn't have HDF5's support base and tools
- HDF5 superseded ADF as the official storage mechanism
- CGNS introduced parallel I/O APIs w/ parallel HDF5 in 2013
- Poor performance of the new parallel APIs in most circumstances

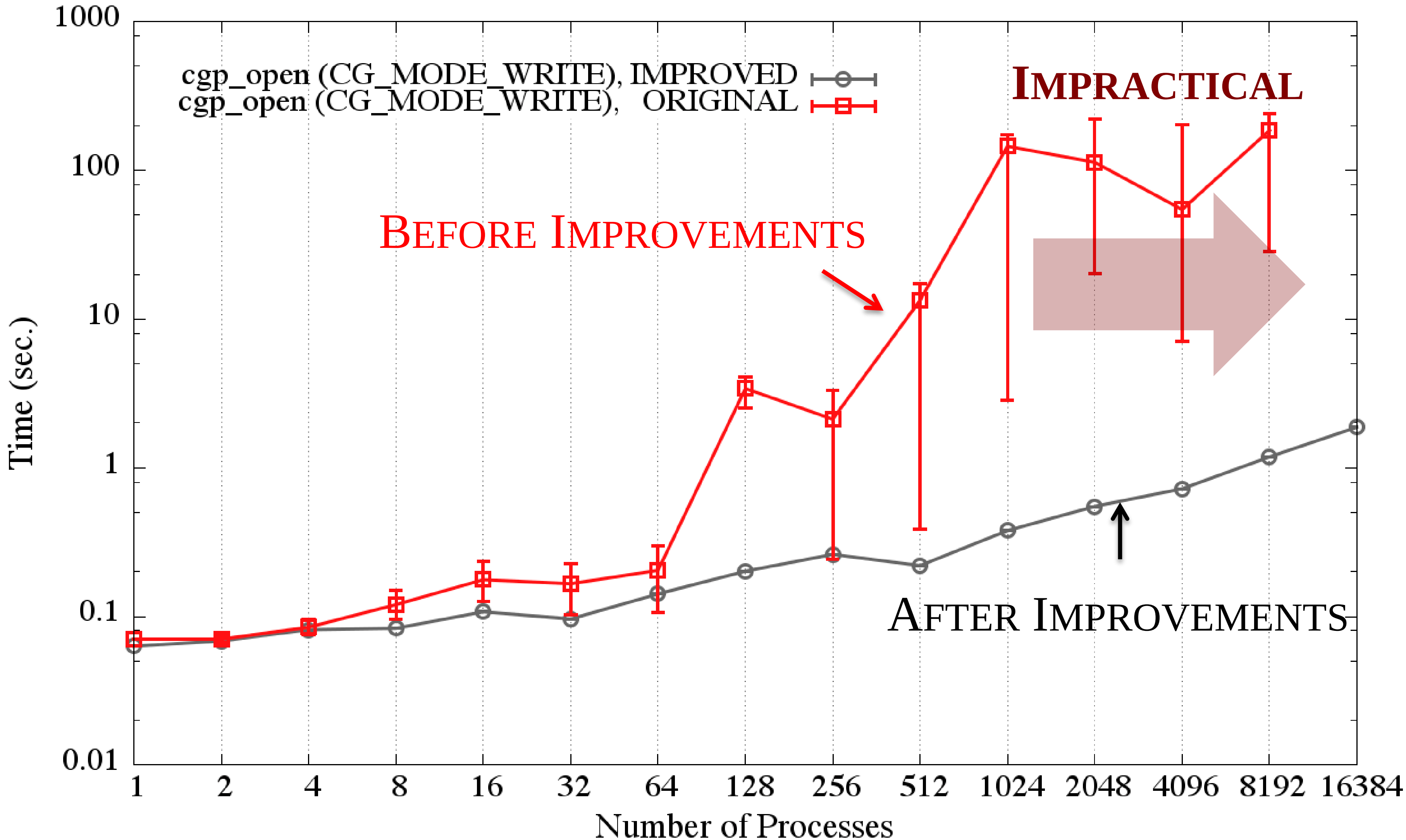
CGNS Performance Problems

- 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"

- Closing a CGNS file
  - Triggers HDF5 flush of a large amount of small metadata entries
  - Implemented as iterative, independent writes, an unsuitable workload for parallel file systems

Opening CGNS File …



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");
```

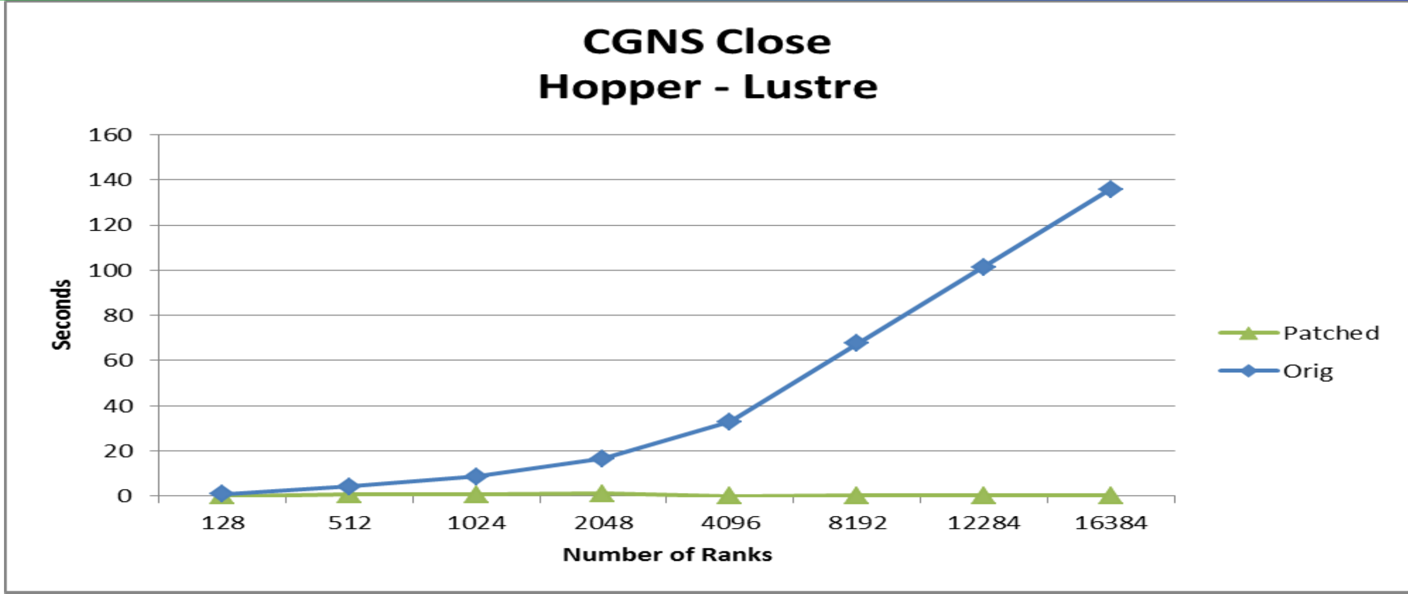
Metadata Read Storm Problem (II)

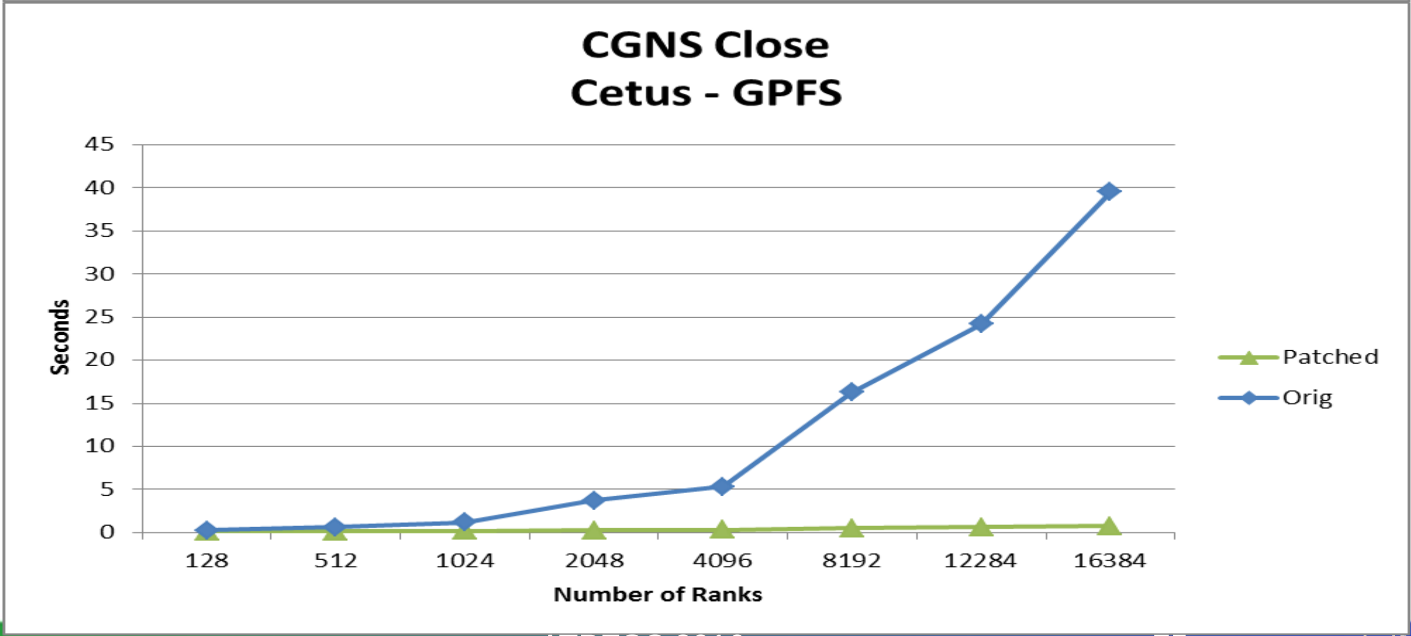
- Metadata read operations are treated by the library as independent read operations.
- Consider a very large MPI job size where all processes want to open a dataset that already exists in the file.
- All processes
  - Call `H5Dopen("/G1/G2/D1");`
  - Read the same metadata to get to the dataset and 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
- 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

Closing a CGNS File …





Write Metadata Collectively!

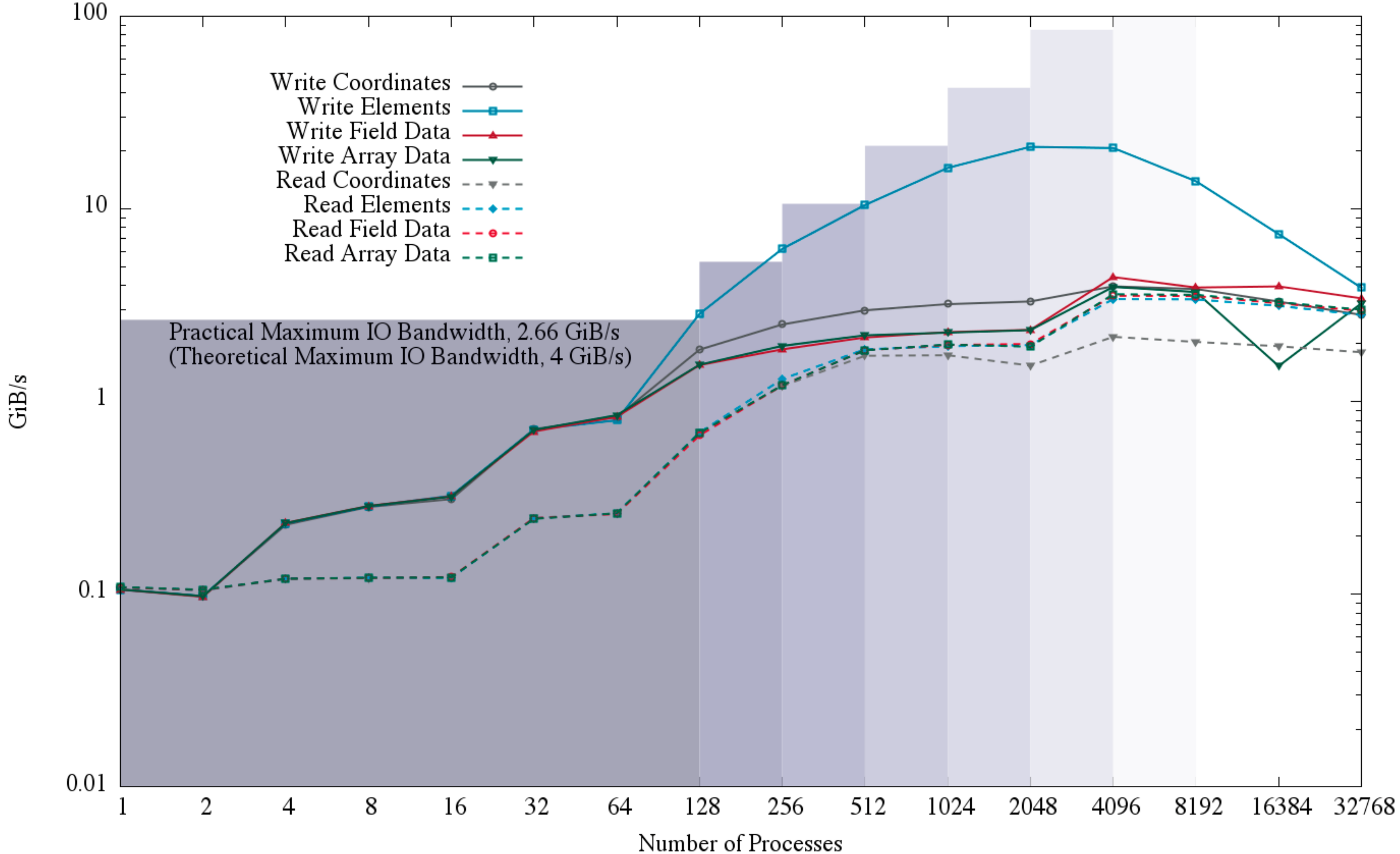
- **Symptoms:** Many users reported that `H5Fclose()` is very slow and doesn't scale well on parallel file systems.

- **Diagnosis:** HDF5 metadata cache issues very small accesses (one write per entry). We know that parallel file systems don't do well with small I/O accesses.

- **Solution:** Gather up all the entries of an epoch, create an MPI derived datatype, and issue a single collective MPI write.

A Benchmark Problem

Computational mesh size: ~33 million elements and ~200 million nodes

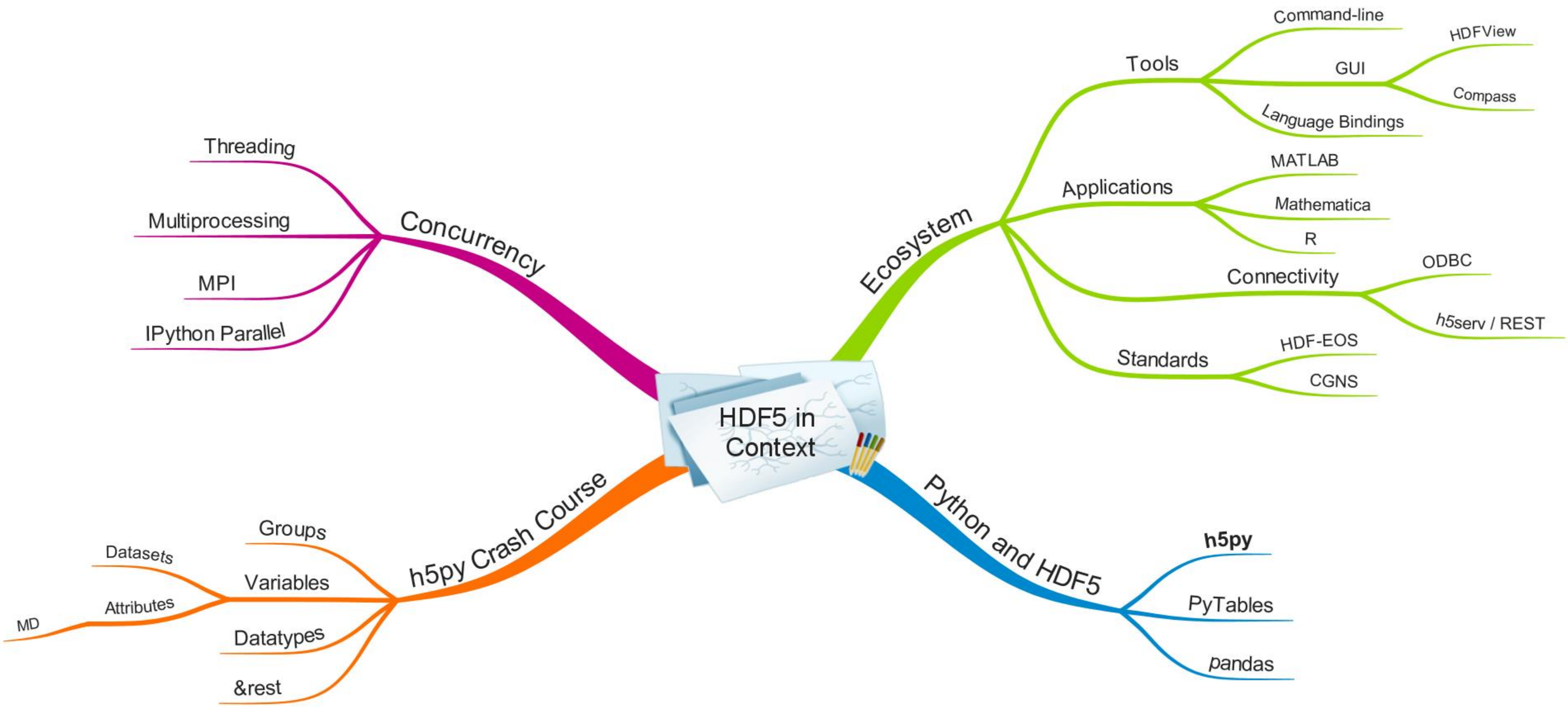


Feature Release Schedule

- HDF5 1.10.0 (March 31, 2016)
  - Metadata cache optimizations
    - Avoiding the metadata “Read Storm”
    - Collective metadata writes
- HDF5 1.10.1 (Q4 2016)
  - Avoid truncation feature
  - Multi-dataset I/O

Doing More With Less Code

PYHTON AND HDF5


HDF5 in Context
Concurrency
Threading
Multiprocessing
MPI
IPython Parallel
Ecosystem
Tools
Command-line
GUI
HDFView
Compass
Language Bindings
Applications
MATLAB
Mathematica
R
Connectivity
ODBC
h5serv / REST
Standards
HDF-EOS
CGNS
h5py Crash Course
Groups
Variables
Datasets
Attributes
MD
Datatypes
&rest
Python and HDF5
h5py
PyTables
pandas

Resources

- HDF Group website www.hdfgroup.org
- HDF Forum
- Helpdesk help@hdfgroup.org
- Priority support