Argonne Training Program on Extreme-Scale Computing

ATPESC 2021

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The HDF Group

Outline

- Foundations of HDF5
  - What is HDF5
  - HDF5 Fundamentals – A Simple Problem
- Intro to HDF5 performance fundamentals
  - Raw data writes with metadata impacts
  - Tuning metadata for parallel HDF5 applications

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What is HDF5?

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What is HDF5?

- Hierarchical Data Format version 5 (**HDF5**)
  - An extensible **data model**
    - Structures for data organization and specification
  - Open-source **software** (I/O library and tools)
    - Performs I/O on data organized according to the data model
    - Works with POSIX and other types of backing store: Object Stores (DAOS, AWS S3, AZURE, Ceph, etc.), memory hierarchies and other storage devices
  - Open **file format** (POSIX storage only)
  - This talk's focus is geared toward traditional file systems

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HDF5 is designed for…

- High volume and complex data
  - HDF5 files of GBs sizes are common
- Every size and type of system (portable)
  - Works on from embedded systems, desktops and laptops to exascale systems
- Flexible, efficient storage and I/O
  - See variety of backing store
- Enabling applications to evolve in their use of HDF5 and to accommodate new models
  - Data can be added, removed and reorganized in the file
- Supporting long-term data preservation
  - Petabytes of remote sensing data, including data for long term climate research is in NASA archives now

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HDF5 Data model

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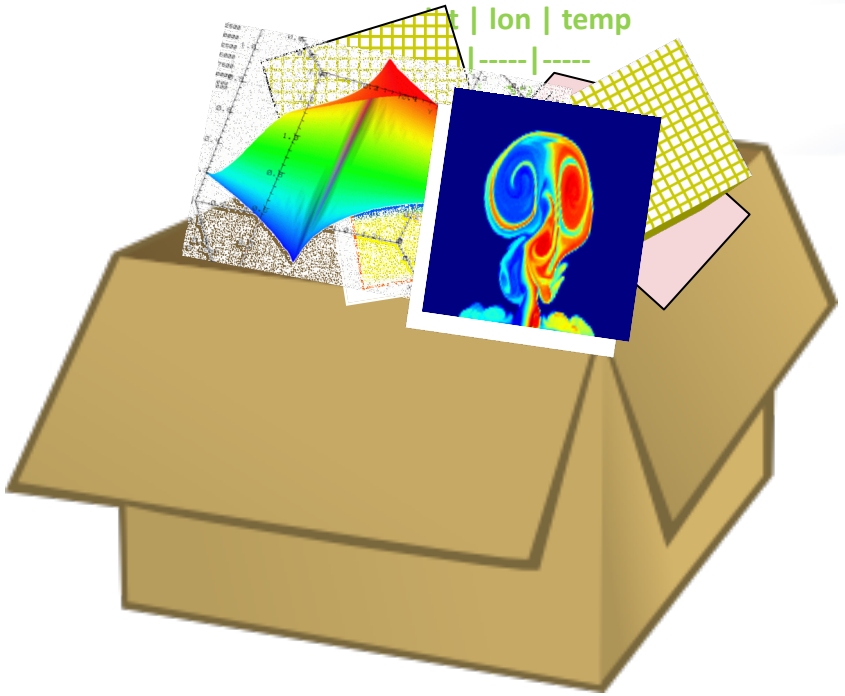
HDF5 File

An HDF5 file is a **structured container** that holds data objects.



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HDF5 Data Model

Dataset –
Organize and contain data elements

Dataspace –
Describes logical layout of the data elements

HDF5 Objects

Attribute –
User-defined metadata

Datatype –
Describes individual data elements

File

Link –
Organize data objects

Group –
Organize data objects

HDF5 Software

HDF5 home page: http://hdfgroup.org/HDF5/

- Latest releases: HDF5 1.10.7 (1.12.1)

HDF5 source code:

- Written in C, and includes optional C++, Fortran, Java APIs, and High-Level APIs
- Contains command-line utilities (h5dump, h5repack, h5diff, ..) and compile scripts

HDF5 pre-built binaries:

- When possible, include C, C++, Fortran, Java, and High-Level libraries. Check ./lib/libhdf5.settings file.
- Built with the SZIP and ZLIB external libraries

3rd party software:

- h5py (Python)
- http://h5cpp.org/ (Contemporary C++ including support for MPI I/O)

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External Help Resources

- Reference manuals, examples
  - https://portal.hdfgroup.org/display/HDF5/HDF5
- The HDF Group Webinars https://www.hdfgroup.org/category/webinar/
  - Past topics covered
    - Introduction to HDF5
    - HDF5 Advanced Features
    - HDF5 VOL connectors
- Direct help from the HDF Group
  - Help desk: help@hdfgroup.org
  - HDF5 office hours: a weekly mini-seminar/Q&A session, Tuesdays 1-1:30 p.m. Central
- Help from the HDF5 Community via the HDF forum

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HDF5 Fundamentals – A Simple Problem

- Writing multiple 2D array variables over time:

ACROSS P processes arranged in a **R x C** process grid
  FOREACH step 1 .. **S**
    FOREACH count 1 .. **A**
      CREATE a double **ARRAY** of size **[X,Y]** | **[R*X,C*Y]** (Strong | Weak)
      (**WRITE** | **READ**) the **ARRAY** (**to** | **from**) an HDF5 file

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Fundamentals – Missing Information

- How are the array variables represented in HDF5?
  - 2D, 3D, 4D datasets
  - Are the extents known a priori?
  - How are the dimensions ordered?
  - Groups?
- What order is the data written, and is the data read the same way?
- What's the storage layout?
  - How many physical files?
  - Contiguous or chunked, etc.
  - Is the data compressible?
- What's the file system or data store?
- Collective vs. independent MPI-IO

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One Kind of Performance Hurdle

- HDF5 has a complex-looking interface
  - Complexity does not necessarily mean difficult to use
  - Users may require such complexity to achieve their goals
    - **Goal**: Self-describing share-friendly data layout
      - Tuning performance and efficiency with the constraint of using a standardized file format (netCDF, CGNS, etc.)
    - **Goal**: Fastest I/O possible
      - Tuning for check-points by minimizing metadata, large write blocks.
  - The complexity of the HDF5 workflow and underlying hardware may make the HDF5 tasks unavoidably complex.

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Other Sources of Performance Variability

- Hardware
- System configuration and activity of other users
- **HDF5 property lists**
  - Nearly 180 APIs
  - Controls storage properties for HDF5 objects
  - Controls in-flight HDF5 behavior
  - About 100 *H5Pset_** functions
    - ≤ $p_1 * \ldots * p_{100}$ combinations!
    - How many are tested?
  - What does *H5P_DEFAULT* mean?
    - (No, you can't control that one)
  - What is the effect of using H5P_DEFAULT?

https://portal.hdfgroup.org/display/HDF5/Property+Lists

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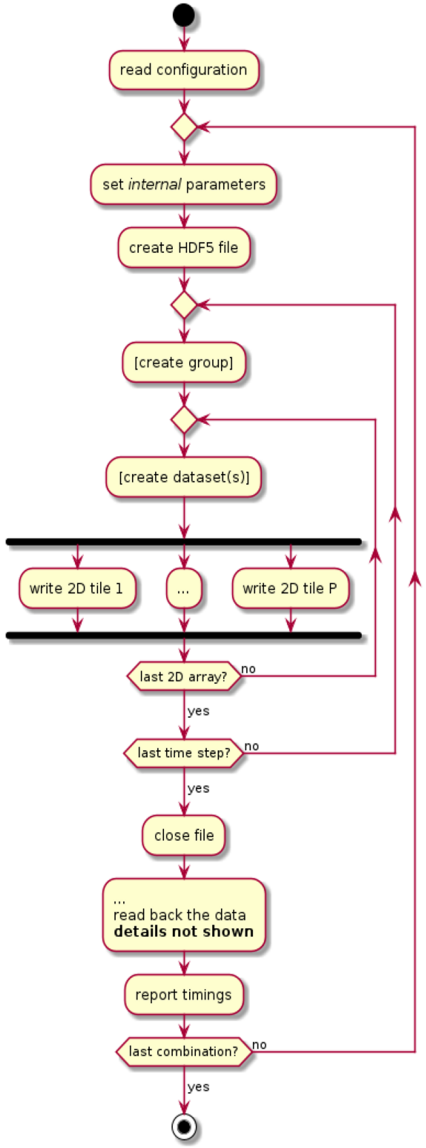
Back to earlier example – Application Model

- Good or bad news:
  - There are *several* different ways to handle the data in HDF5, for example:
    - Many 2D datasets or attributes
    - A few 3D datasets
    - A 4D dataset
  - There are many ways to use HDF5 properties
    - Chunking
    - Data alignment
    - Metadata block size
    - Collective/Independent I/O
  - Ideally, performance would be more or less the same
  - **HDF5 I/O**[1] test explores the HDF5 parameter space



1 https://github.com/HDFGroup/hdf5-iotest

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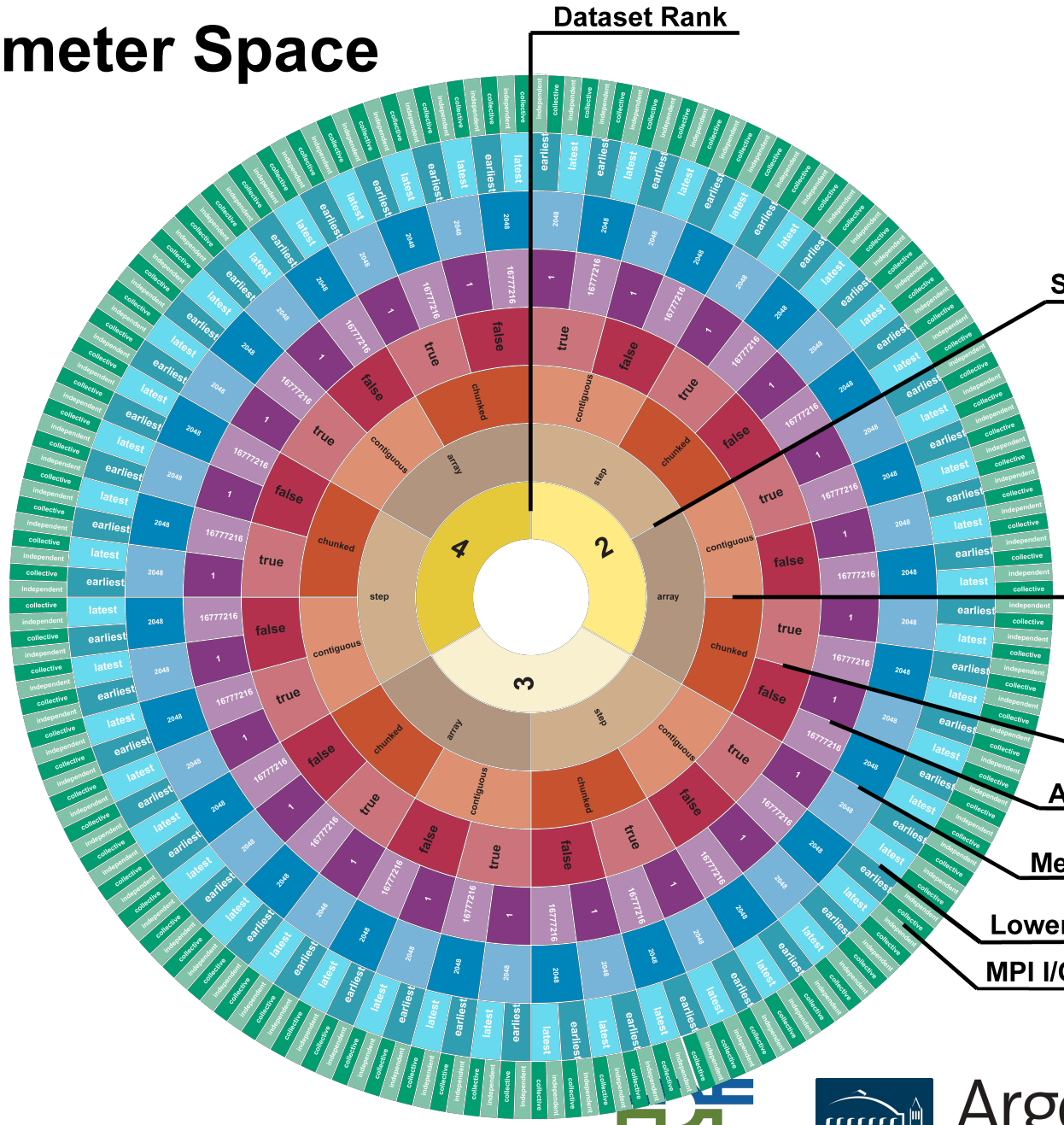
HDF5 Parameter Space



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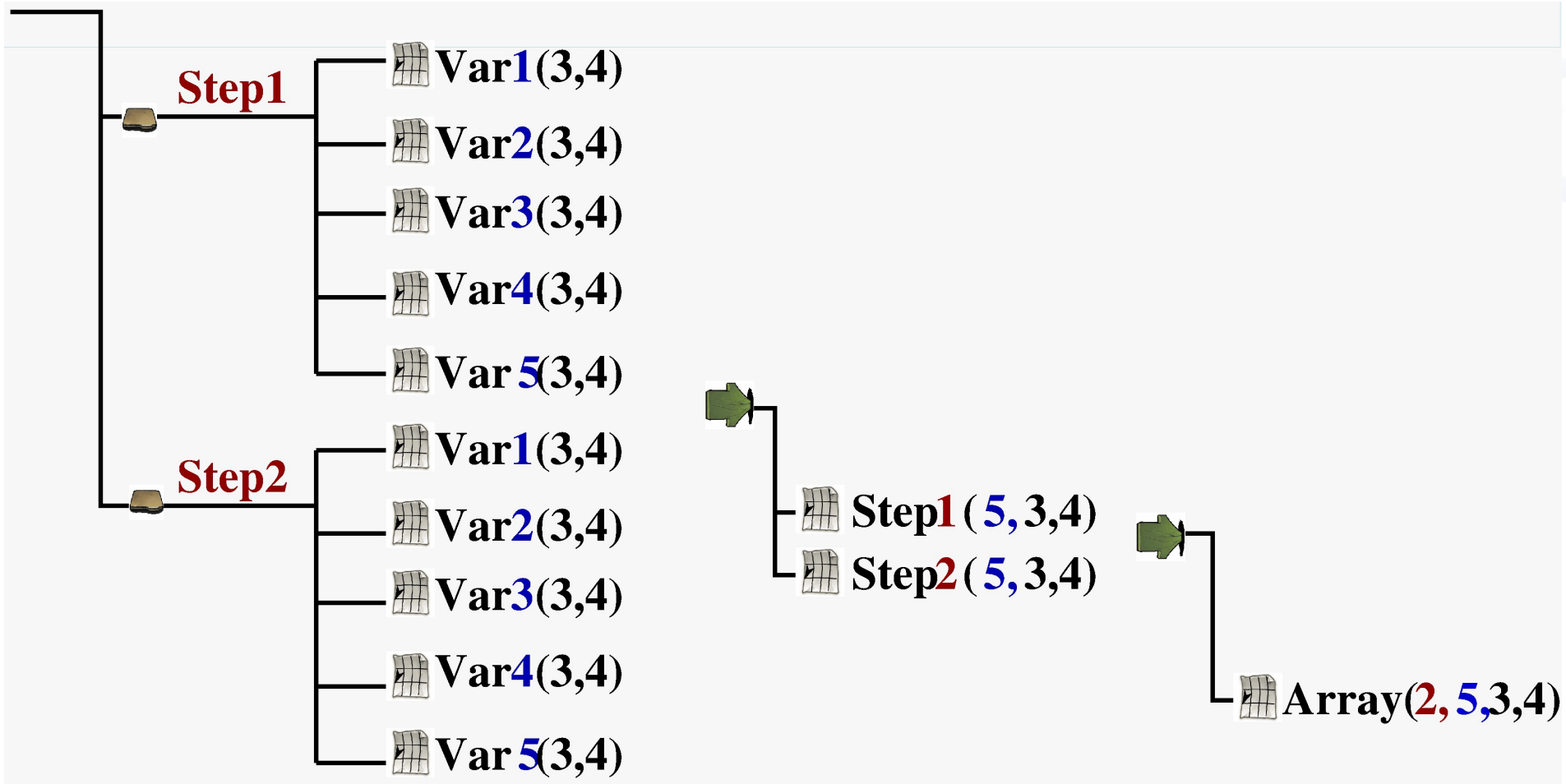
IO Pattern Model

Step based IO Pattern



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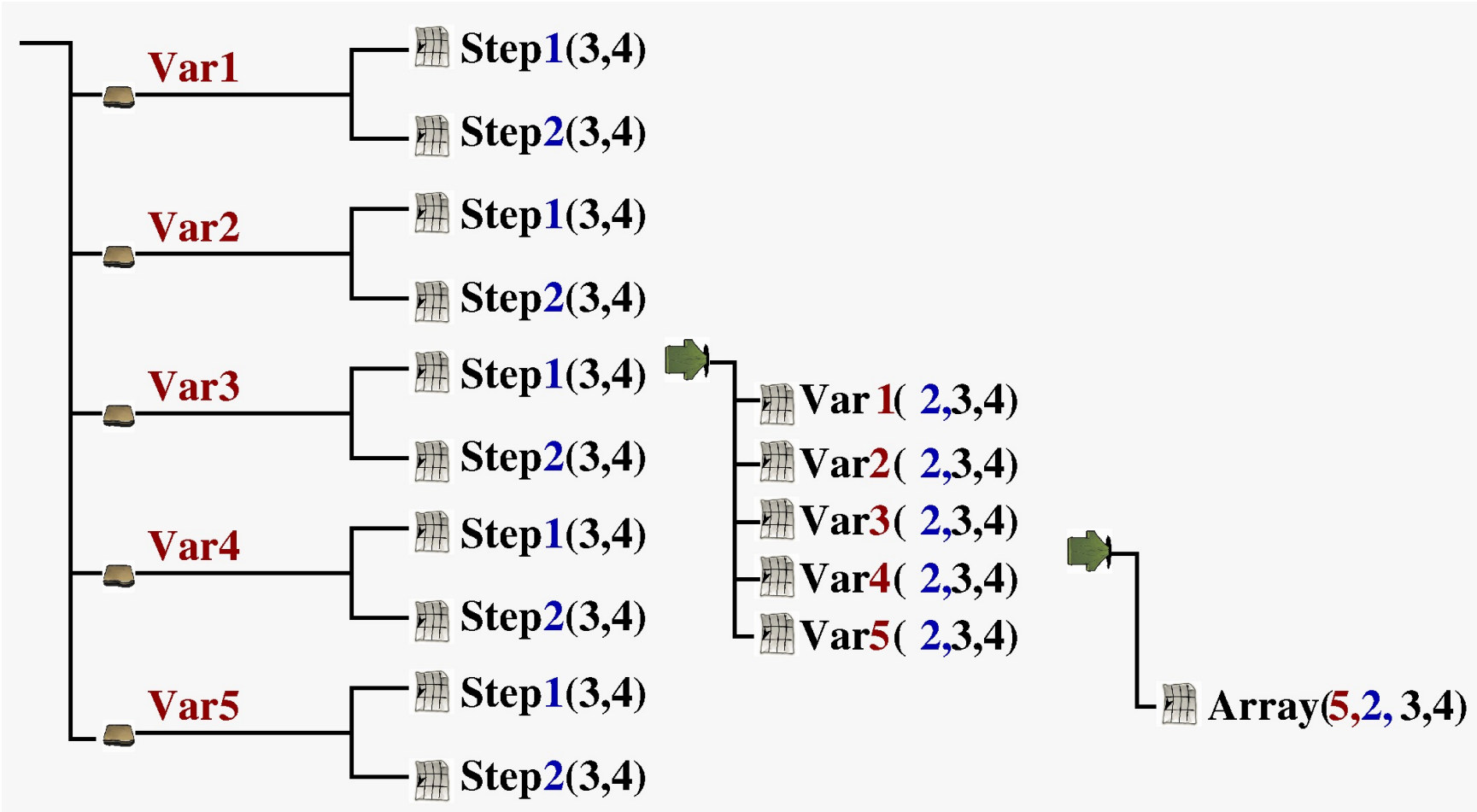
IO Pattern Model

Array based IO Pattern



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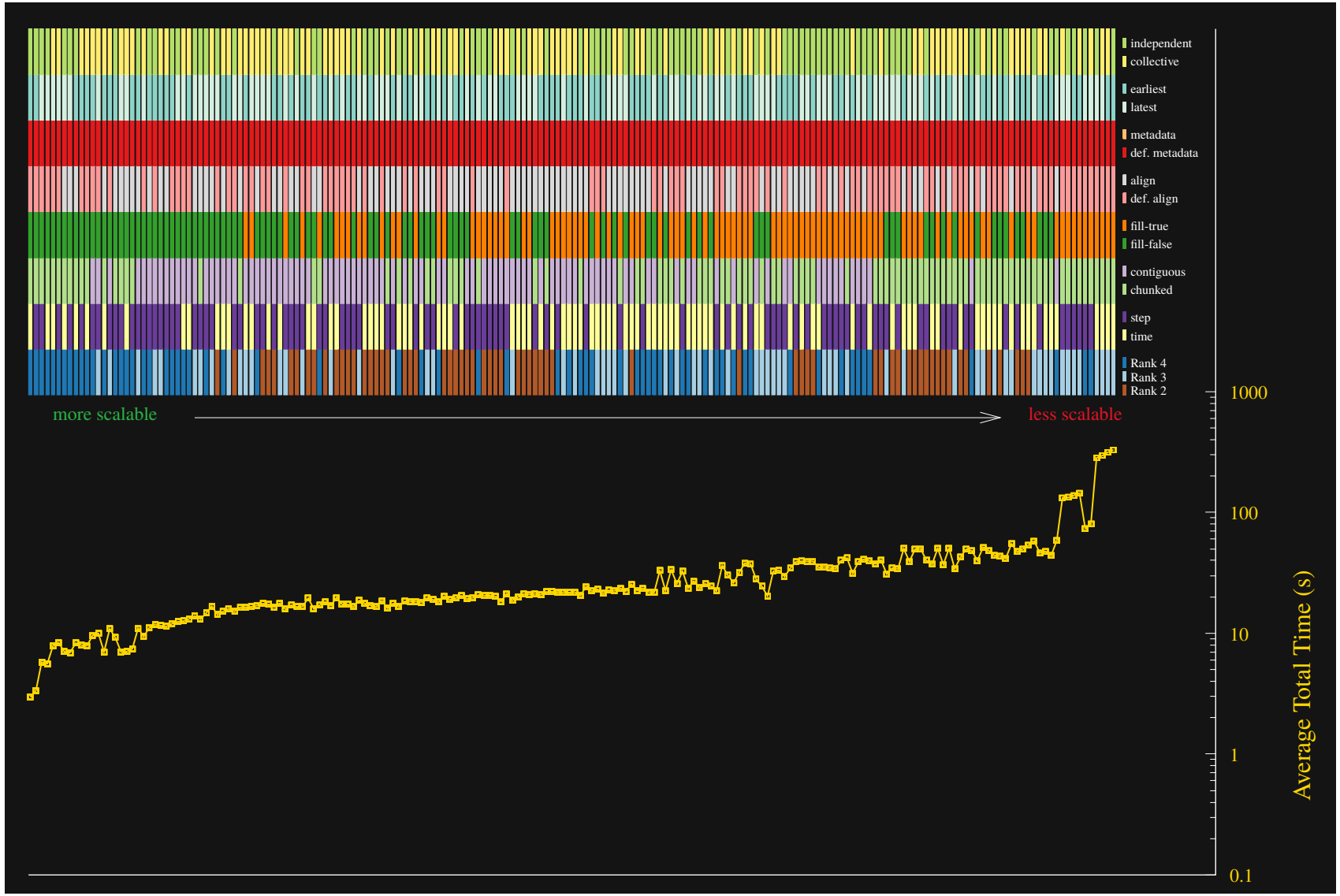
Performance as a function of HDF5 parameter space



- Summit, weak scaling (42 to 2688)
- Best had:
  - four rank array (layout)
  - chunked
  - no fill values
  - default alignment
  - independent I/O

Use Case:
Raw data writes with metadata impacts

Tuning HACC (Hardware/Hybrid Accelerated Cosmology Code)

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HDF5 Metadata

- Describes HDF5 objects in the file
  - Examples:
    - Object headers
      - Contain users' attributes
    - Local and global heaps
    - B-tree nodes
- Small (KBs) comparing to raw data
- Calls for HDF5 metadata can result in many small reads and writes.

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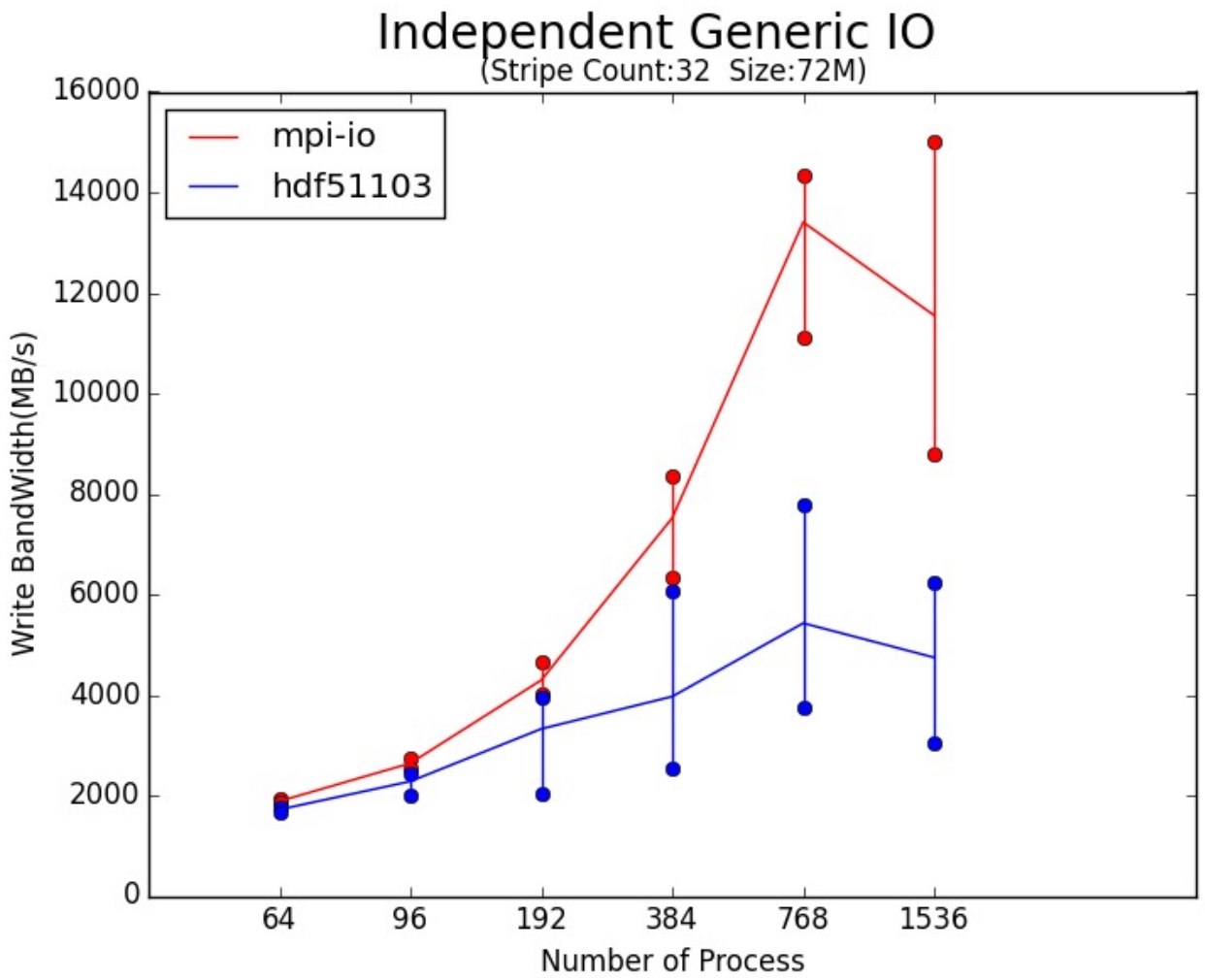
HAAC Performance Results



Includes times for file open and close

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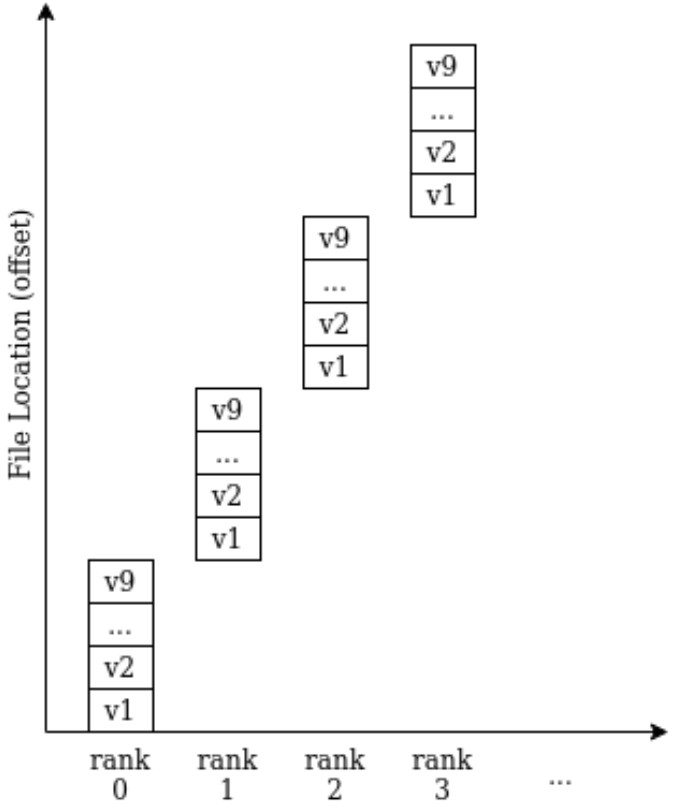
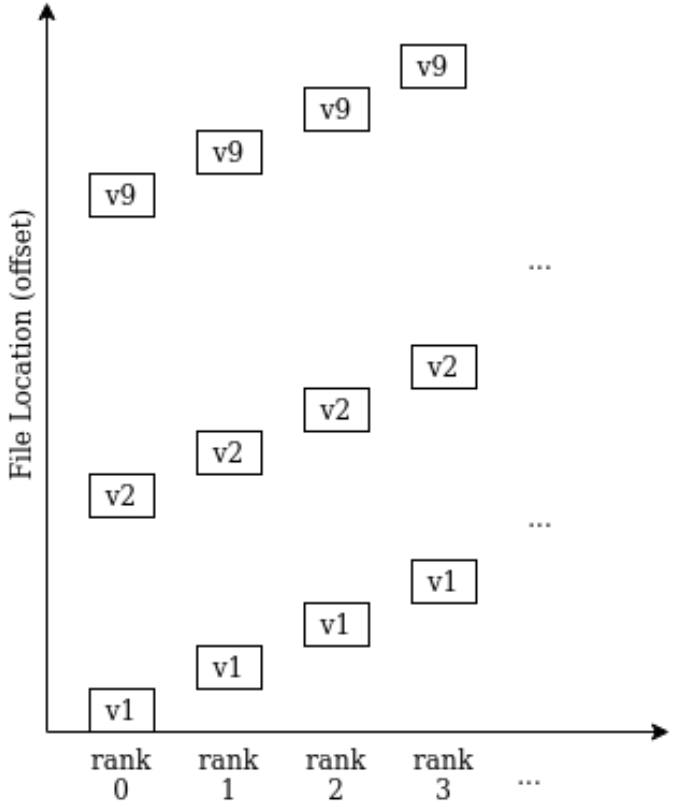
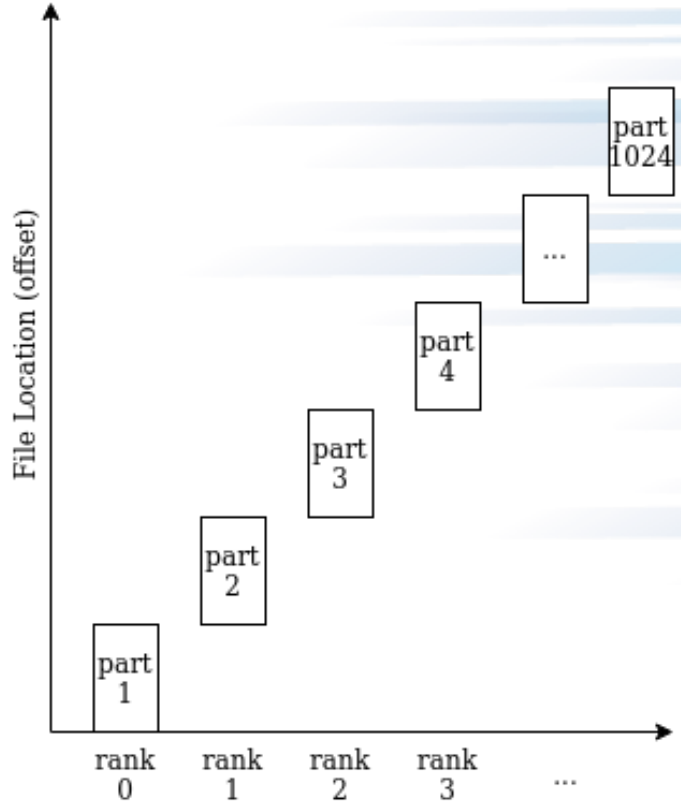
3 Access Patterns



MPI Interleaved = HDF5 Multi



MPI Contiguous = HDF5 Individual



HDF5 Compound

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How to match the pure MPI performance

- First find the best stripe size and stripe count using a pure MPI implementation.
- Decide which data layout gives the best performance
  - On Lustre, MPI Contiguous (HDF5 Individual) is better
  - On GPFS, MPI Interleaved (HDF5 Multi) is better
- **Tune HDF5 to match the performance of MPI implementation**

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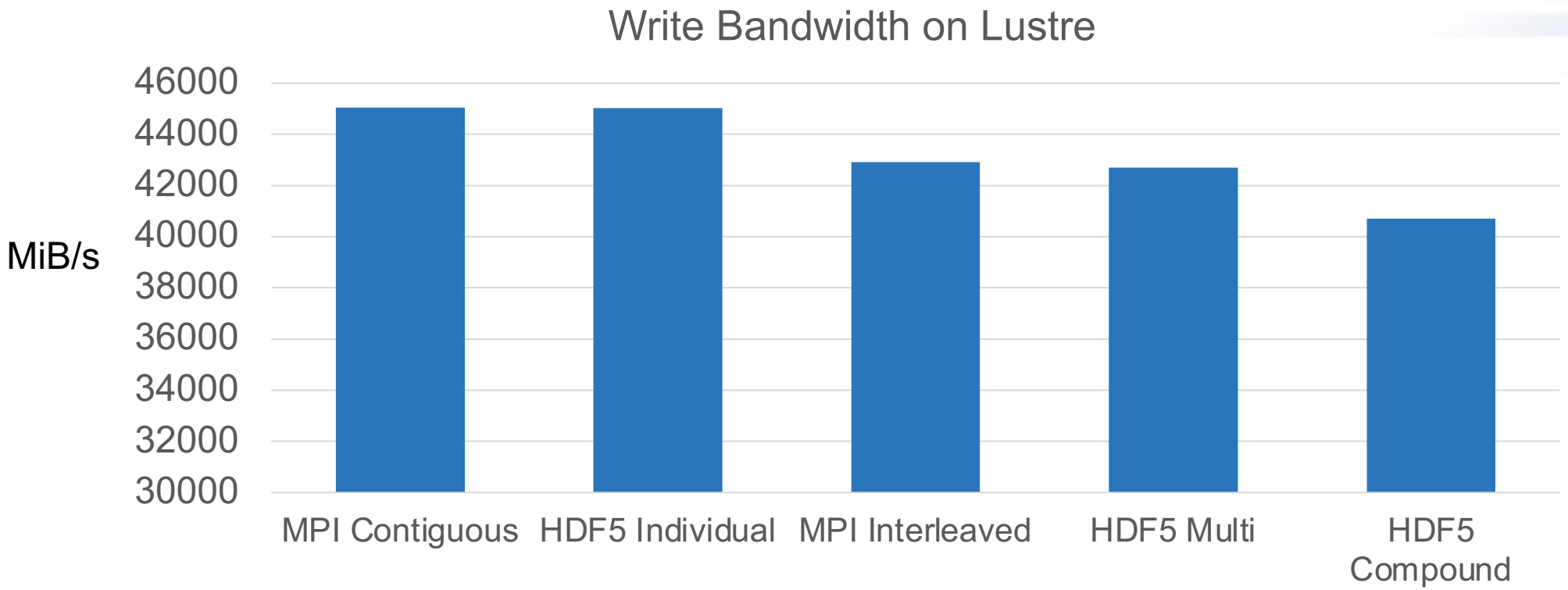
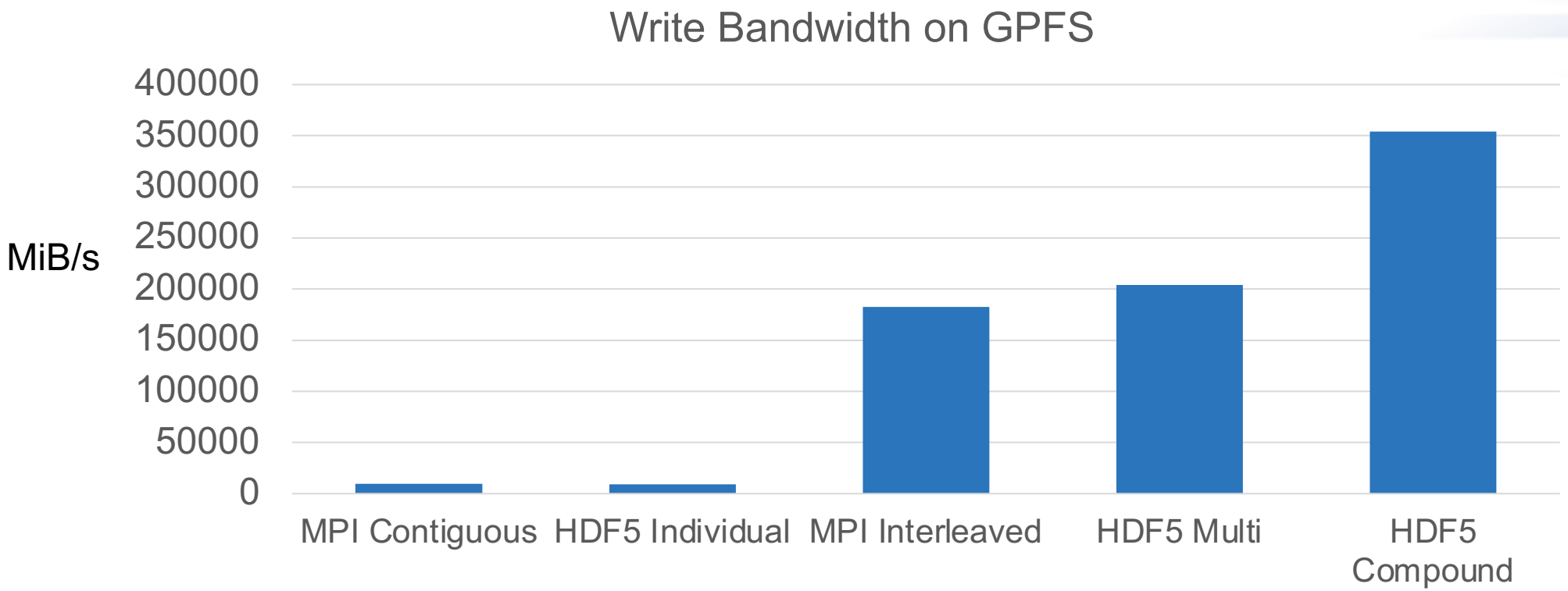
How to match the pure MPI performance

- **Tune HDF5 to match the performance of MPI implementation**
  - **H5Pset_meta_block_size(8MB) on Lustre**



How to match the pure MPI performance

- **Tune HDF5 to match the performance of MPI implementation**
  - **H5Pset_meta_block_size(32MB) on GPFS**



Conclusions

- Current version of HDF5 doesn't have a way to match the MPI-Interleaved access pattern. HDF5_Multi achieves the same pattern.
- Collective I/O does not help since the request size is already very big.
- MPI_Interleaved (HDF5_Multi) is better on GPFS.
  - Because the stripe size is small and users can not change it.
- MPI_Contiguous (HDF5_Individual) is better on Lustre.
  - Because we use a big stripe size (128M)
  - For smaller stripe sizes (e.g. < 36M), MPI_Interleaved is better.

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Tuning Metadata for parallel HDF5 applications

Features for Metadata tuning performance

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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.

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Collective Metadata I/O Functions

H5P_SET_COLL_METADATA_WRITE	Establishes I/O mode property setting, collective or independent, for metadata writes
H5P_GET_COLL_METADATA_WRITE	Retrieves I/O mode property setting for metadata writes
H5P_SET_ALL_COLL_METADATA_OPS	Establishes I/O mode, collective or independent, for metadata read operations
H5P_GET_ALL_COLL_METADATA_OPS	Retrieves I/O mode for metadata read operations

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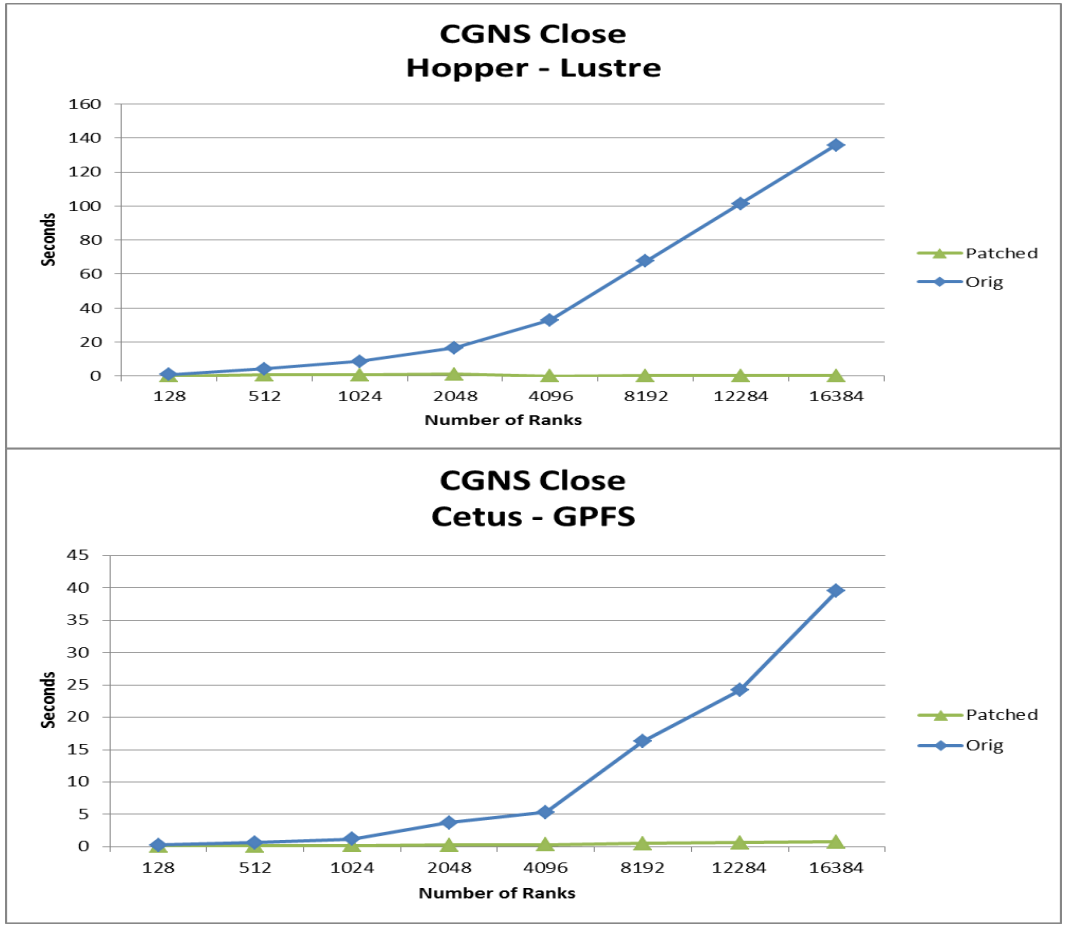
Closing a CGNS File …



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