ARGONNE
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EXTREME-SCALE COMPUTING

Performant HDF5

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Talk Outline

Foundations of HDF5

- Introduction to
  - HDF5 data model, software, and architecture
  - HDF5 programming model
- Overview of general best practices

Overview of parallel HDF5

- Introduction to HDF5 parallel I/O
- New features, general best practices and methods which affect parallel performance

Why HDF5?

- Have you ever asked yourself:
  - How do I organize and share my data?
  - How can I use visualization and other tools with my data?
  - What will happen to my data if I need to move my application to another system?
  - How will I deal with one-file-per-processor in the exascale era?
  - Do I need to be an “MPI I/O and Lustre, or Object Store, etc.” pro to do my research?

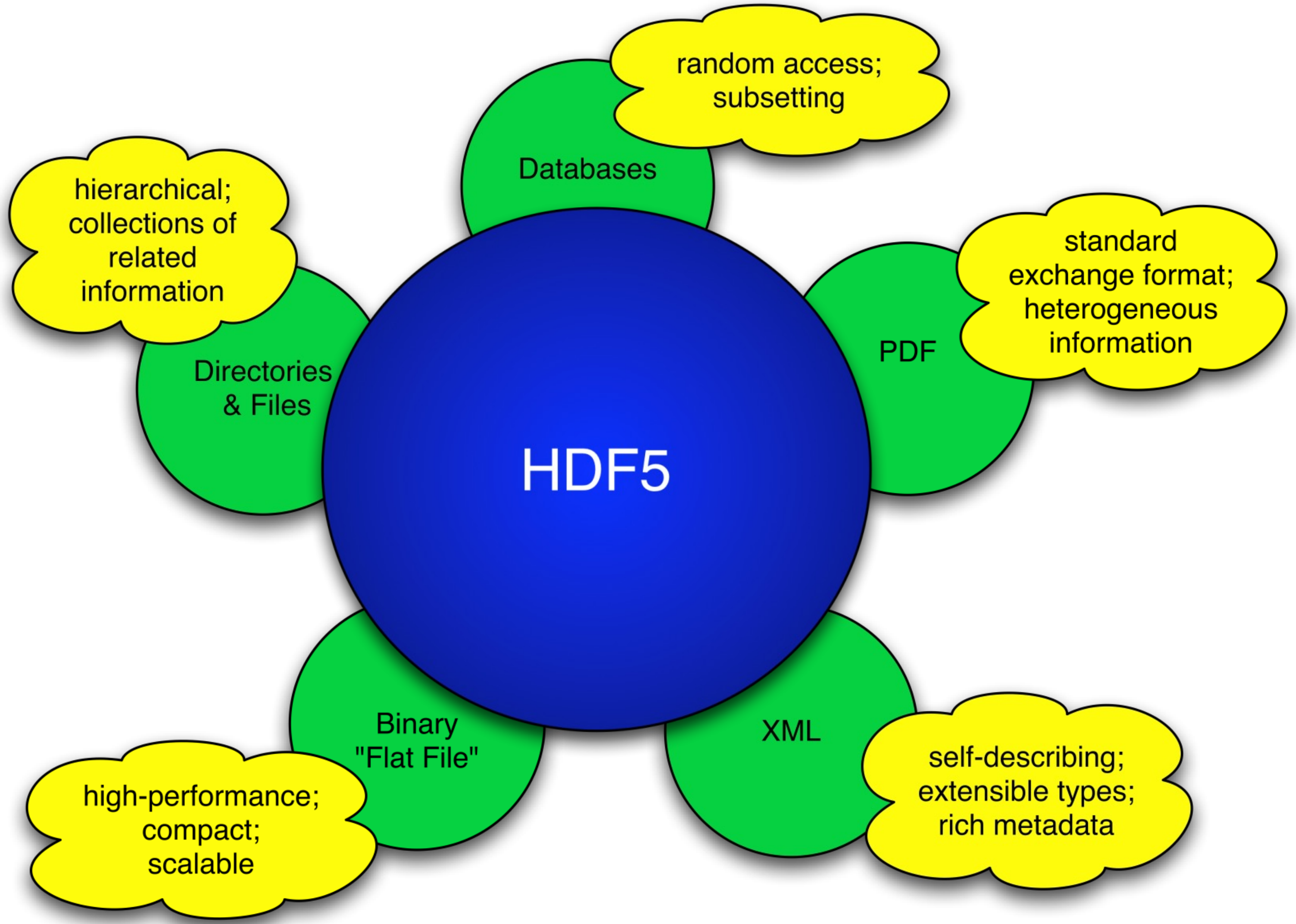
HDF5 is an answer to the questions above and can hide all complexity so you can concentrate your research

What is HDF5?

Hierarchical **D**ata **F**ormat version 5 (**HDF5**)

1. An extensible **data model**
   - Uses structures for data organization and specification
2. 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
3. Open **file format** (POSIX storage only)

HDF5 is like …



HDF5
Databases
random access; subsetting
Directories & Files
hierarchical; collections of related information
PDF
standard exchange format; heterogeneous information
Binary "Flat File"
high-performance; compact; scalable
XML
self-describing; extensible types; rich metadata

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

- Works for a variety of backing storage

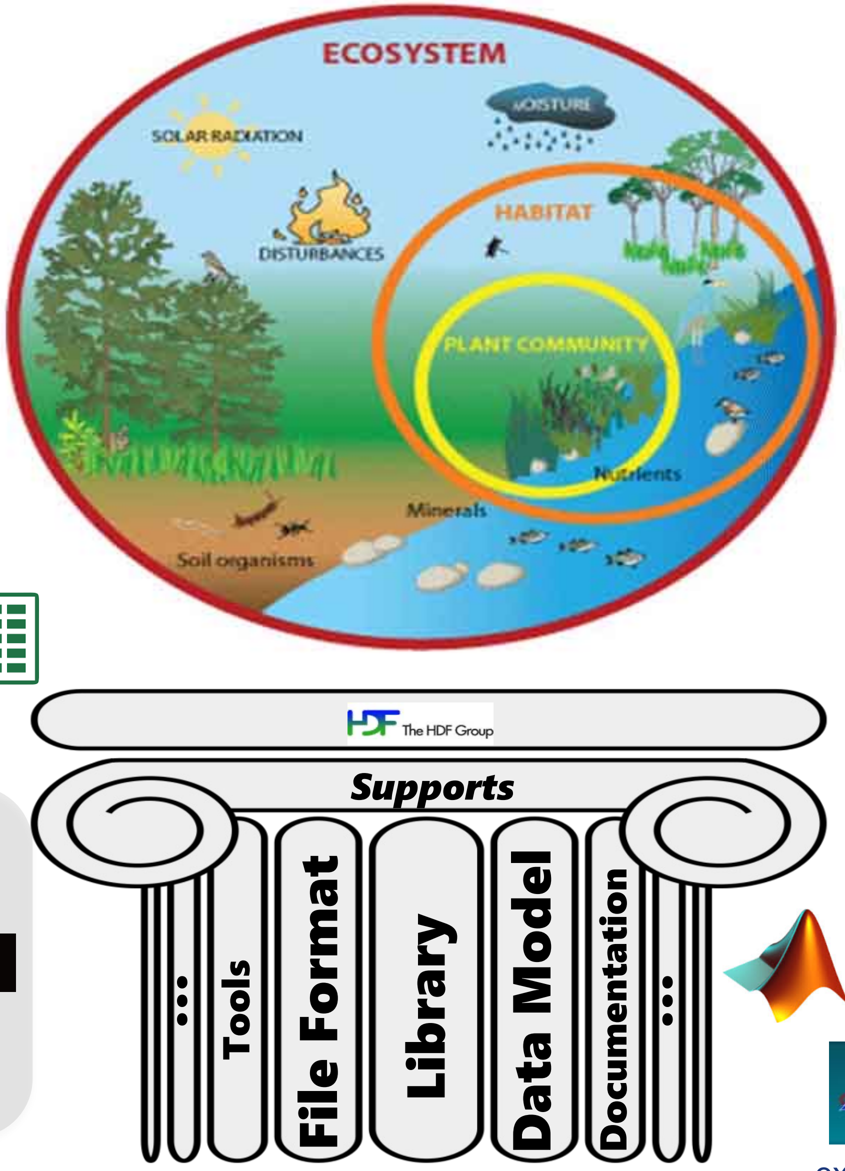
Enabling applications to evolve in their use of HDF5 and to accommodate new models

- 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 in NASA archives now

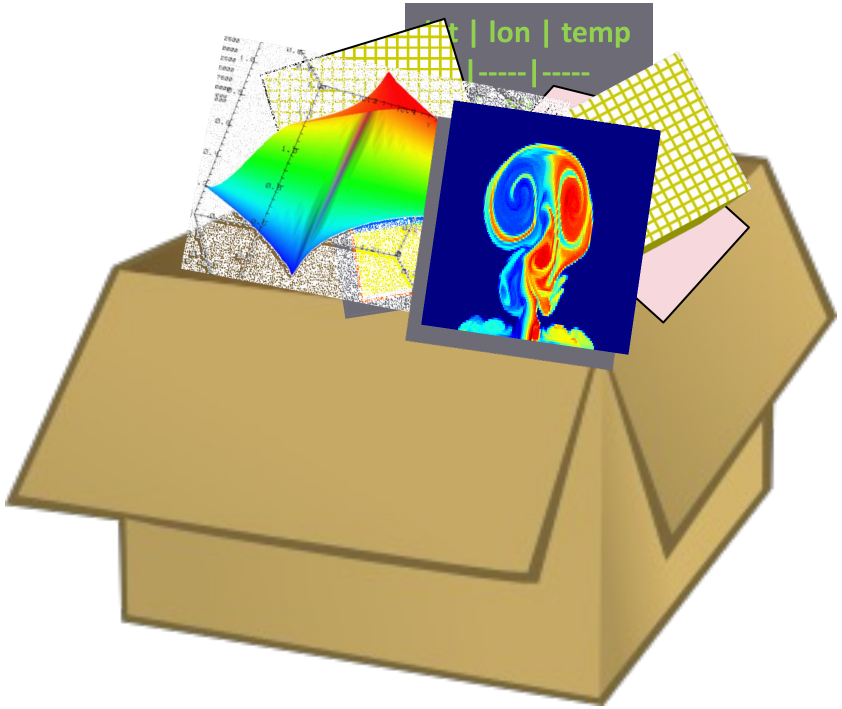
HDF5 Ecosystem



HDF5 Data model

HDF5 File

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



HDF5 Data Model

Dataset –
Organize and contain data elements

Dataspace –
Describes logical layout of the data elements

Attribute –
User-defined metadata

HDF5 Objects

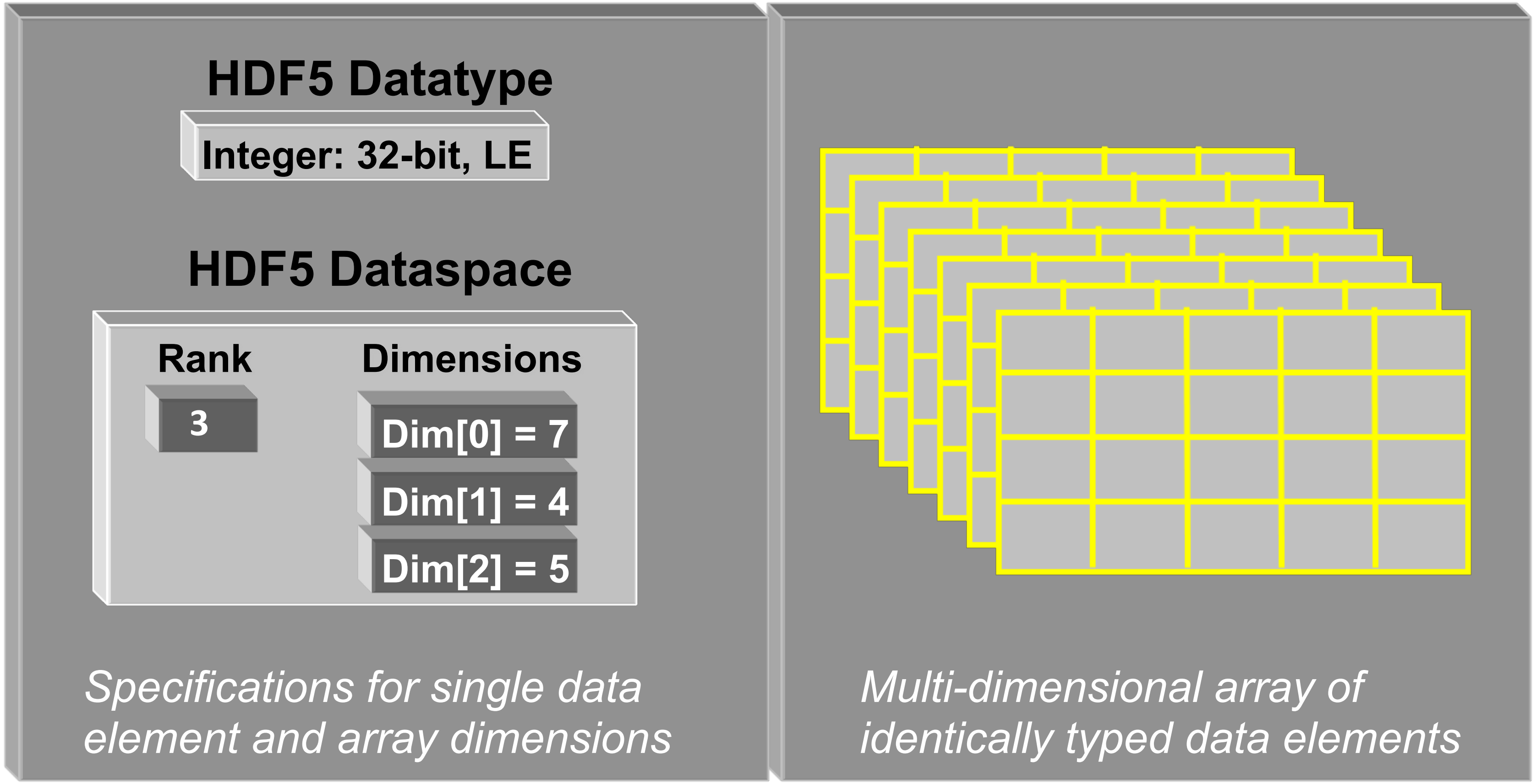
File

Datatype –
Describes individual data elements

Link –
Organize data objects

Group –
Organize data objects

HDF5 Dataset



- HDF5 datasets **organize and contain** data elements
  - HDF5 datatype describes individual data elements
  - HDF5 dataspace describes the logical layout of the data elements

HDF5 Dataspace

Two roles:

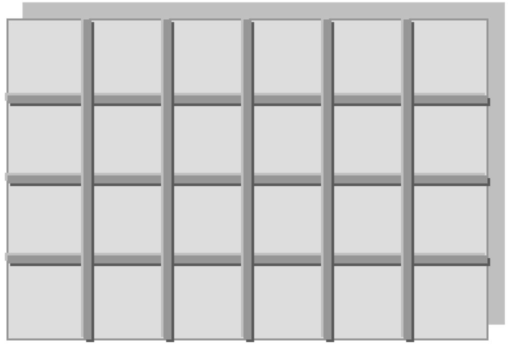
(1) Spatial information for Datasets and Attributes

Empty sets and scalar values

Multidimensional arrays

Rank and dimensions

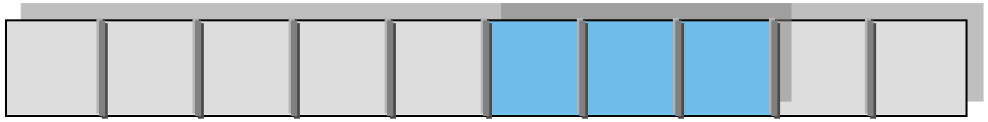
A permanent part of object definition



Rank = 2

Dimensions = 4 x 6

(2) Partial I/O: Dataspace and subset describe the application’s data buffer and data elements participating in I/O



Rank = 1

Dimension = 10

How to describe a subset in HDF5?

Before writing and reading a subset of data, one must describe it to the HDF5 Library.

The HDF5 APIs and documentation refer to a subset as a "***selection***," for example "*hyperslab* selection."

If specified, HDF5 performs I/O on a selection *only* and <u>not</u> on all dataset elements.

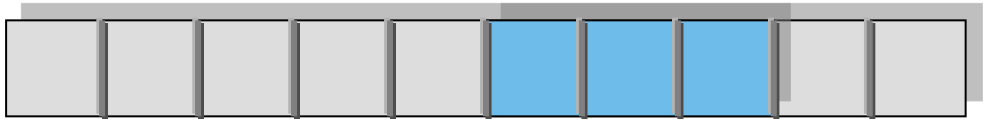
Describing elements for I/O: HDF5 Hyperslab

Everything is "measured" in the number of elements; 0-based

Example 1-dim:

Start - starting location of a hyperslab (5)

Block - block size (3)

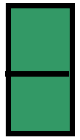


Example 2-dim:

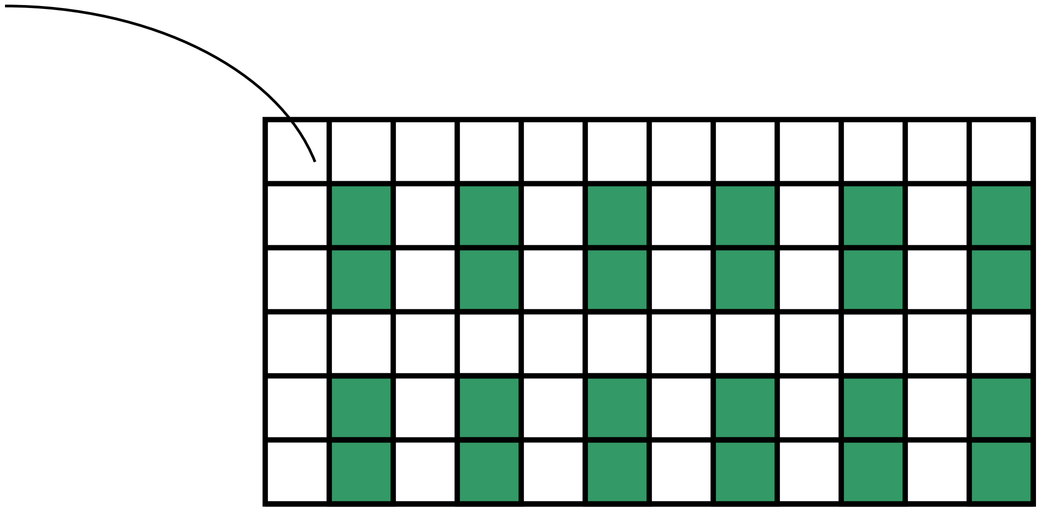
Start - starting location of a hyperslab (1,1)

Stride - number of elements that separate each block (3,2)

Block - block size (2,1)



Count - number of blocks (2,6)



All other selections are built using set operations

HDF5 Datatypes

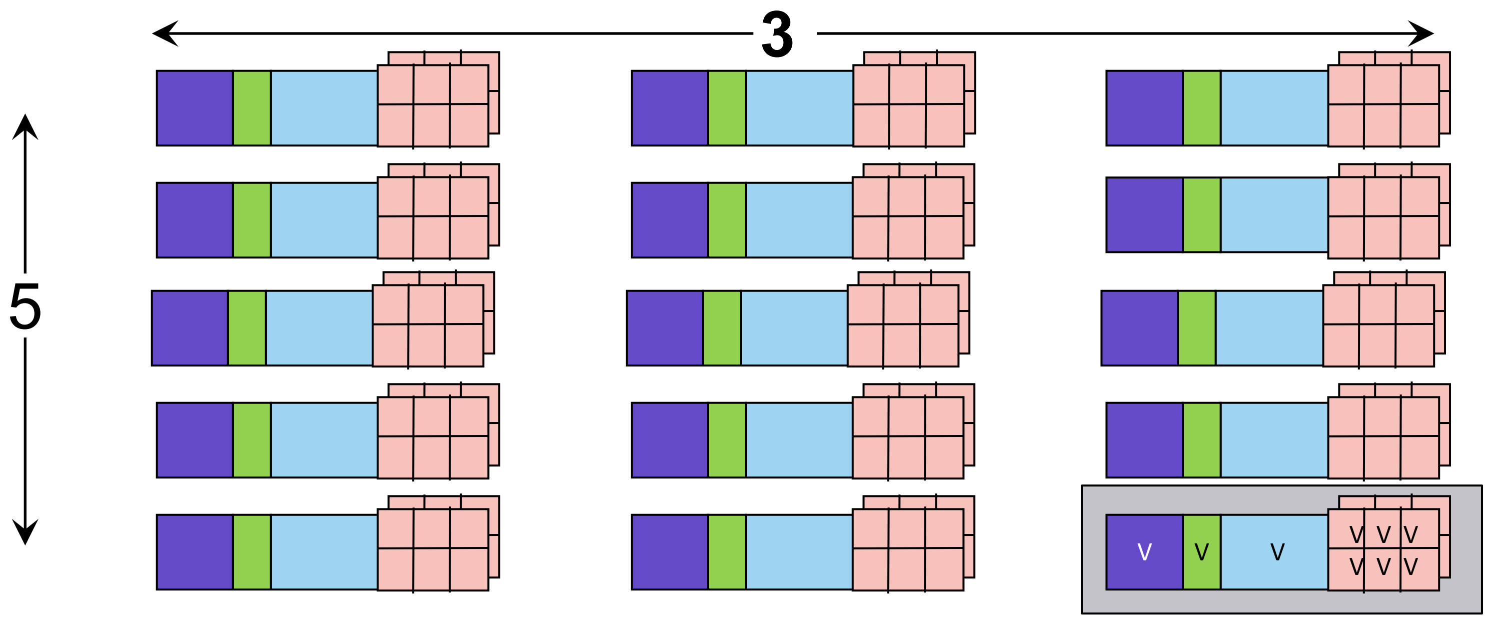
Describe individual data elements in an HDF5 dataset

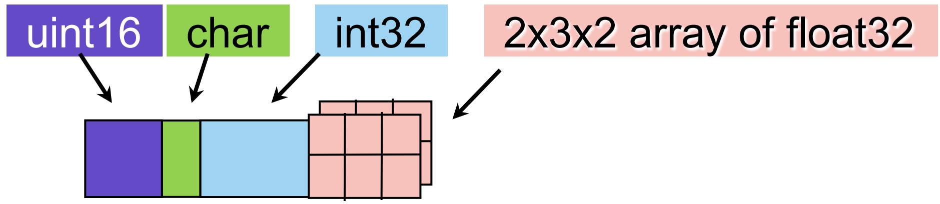
A wide range of datatypes is supported

- Atomic types: integer, floats
- User-defined (e.g., 12-bit integer, 16-bit float)
- Enum
- References to HDF5 objects and selected elements of datasets
- Variable-length types (e.g., strings, vectors)
- Compound (similar to C's structures or Fortran's derived types)
- Array (similar to matrix)

HDF5 library provides predefined symbols to describe atomic datatypes

HDF5 Dataset with Compound Datatype



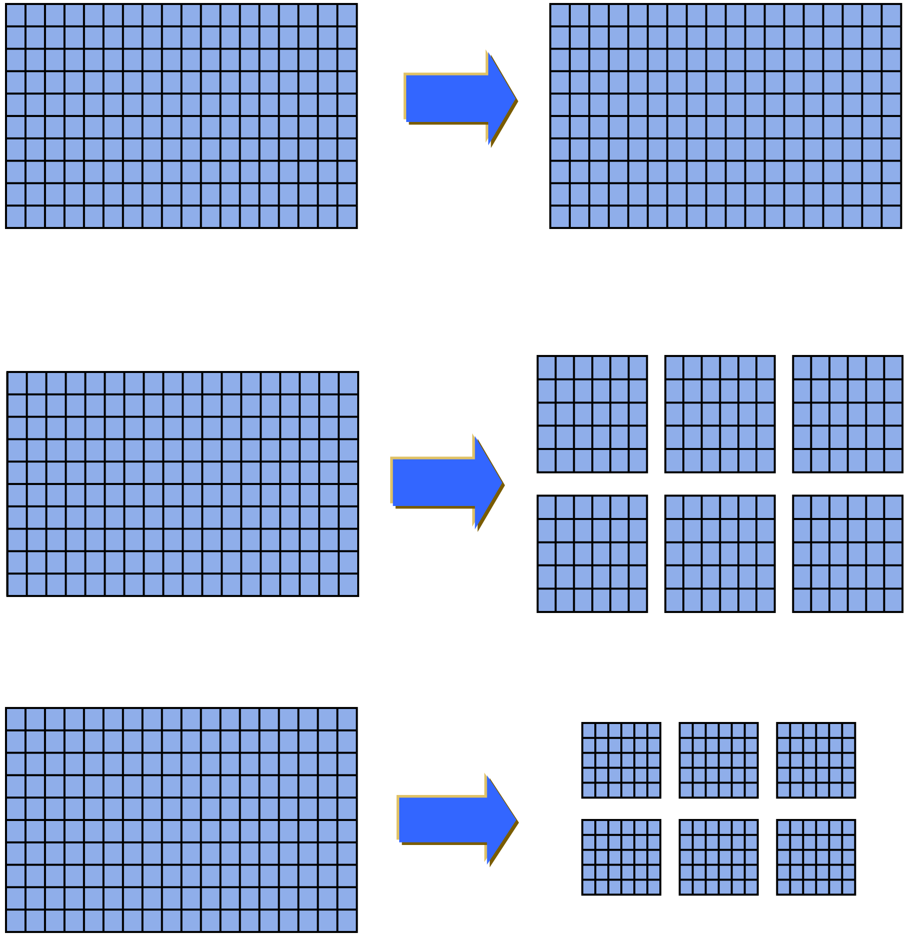


Compound Datatype:

Dataspace: Rank = 2
Dimensions = 5 x 3

How are data elements stored? (1/2)

Buffer in memory | Data in the file



Contiguous (default) — **Data elements stored physically adjacent to each other**

Chunked — **Better access time for subsets; extendible**

Chunked & Compressed — **Improves storage efficiency, transmission speed**

Compression and filters in HDF5

GZIP and SZIP (free version is available from German Climate Computing Center)

Other compression methods registered with The HDF Group at https://portal.hdfgroup.org/display/support/Contributions#Contributions-filters

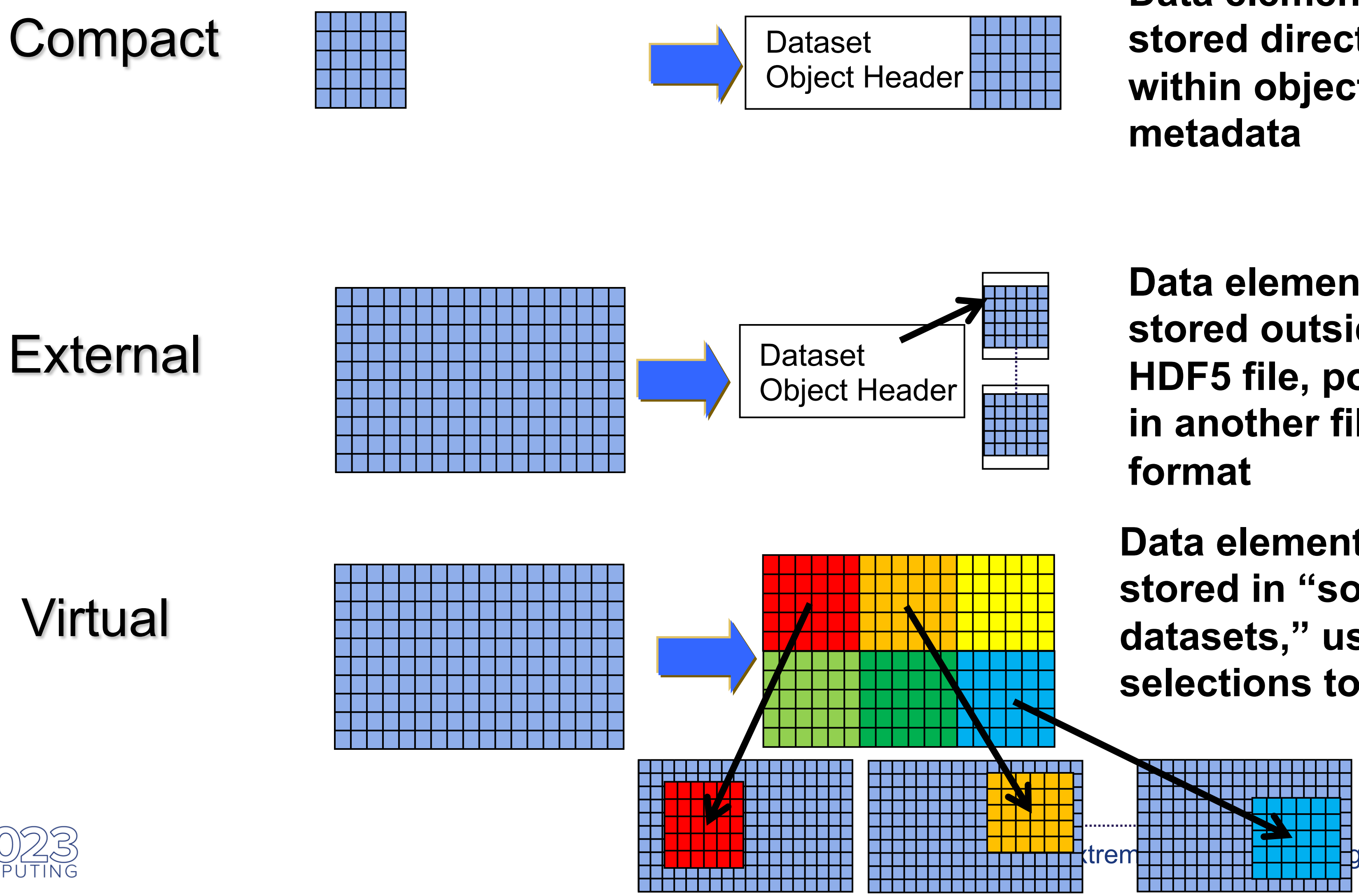
- BZIP2, JPEG, LZF, BLOSC, MAFISC, LZ4, Bitshuffle, SZ and ZFP, etc.
  - The listed above are available as dynamically loaded plugins

Filters:

- Fletcher32 (checksum)
- Shuffle
- Scale+offset
- n-bit

How are data elements stored? (2/2)

Buffer in memory | Data in the file



Compact: Data elements stored directly within object's metadata

External: Data elements stored outside the HDF5 file, possibly in another file format

Virtual: Data elements are stored in "source datasets," using selections to map

HDF5 Attributes

Attributes "decorate" HDF5 objects

Contain *user-defined* metadata

Similar to Key-Values:

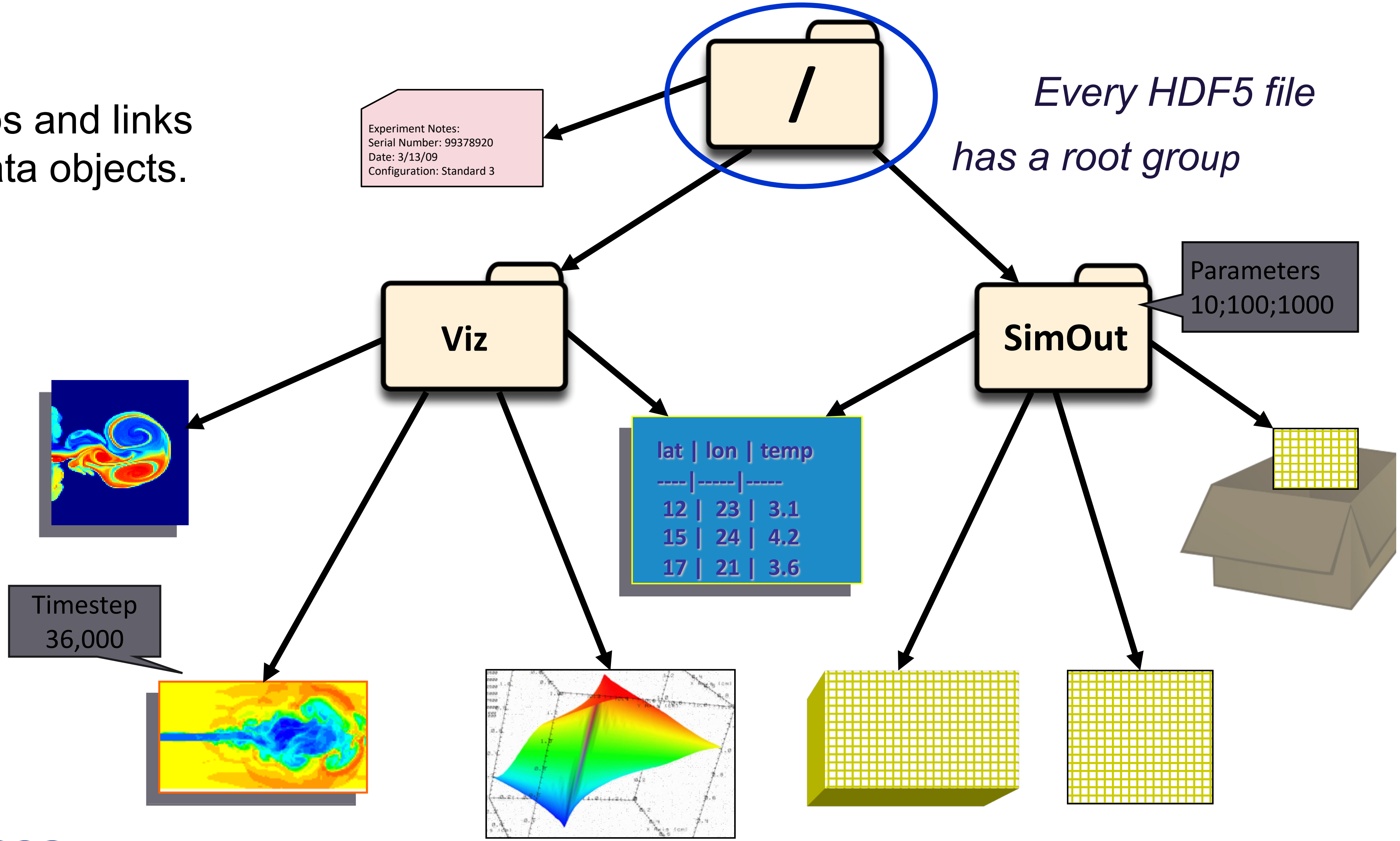
- Have a unique name (for that object) and a value

Analogous to a dataset

- "Value" is described by a datatype and a dataspace
- **Do not** support partial I/O operations; nor can they be compressed or extended

HDF5 Groups and Links

HDF5 groups and links **organize** data objects.



HDF5 software and architecture

HDF5 Software

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

Latest releases: HDF5 1.8.23,1.10.10, 1.12.2, 1.14.1

HDF5 source code:

Available on GitHub: https://github.com/HDFGroup/hdf5

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:

Include C, C++, Fortran, Java, and High-Level libraries when possible. 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)

Useful Tools For New Users

h5dump

Tool to "dump" or display contents of HDF5 files

Scripts to compile applications:

h5cc, h5c++, h5fc (*h5pcc, h5pfc – parallel variants*)

HDFView:

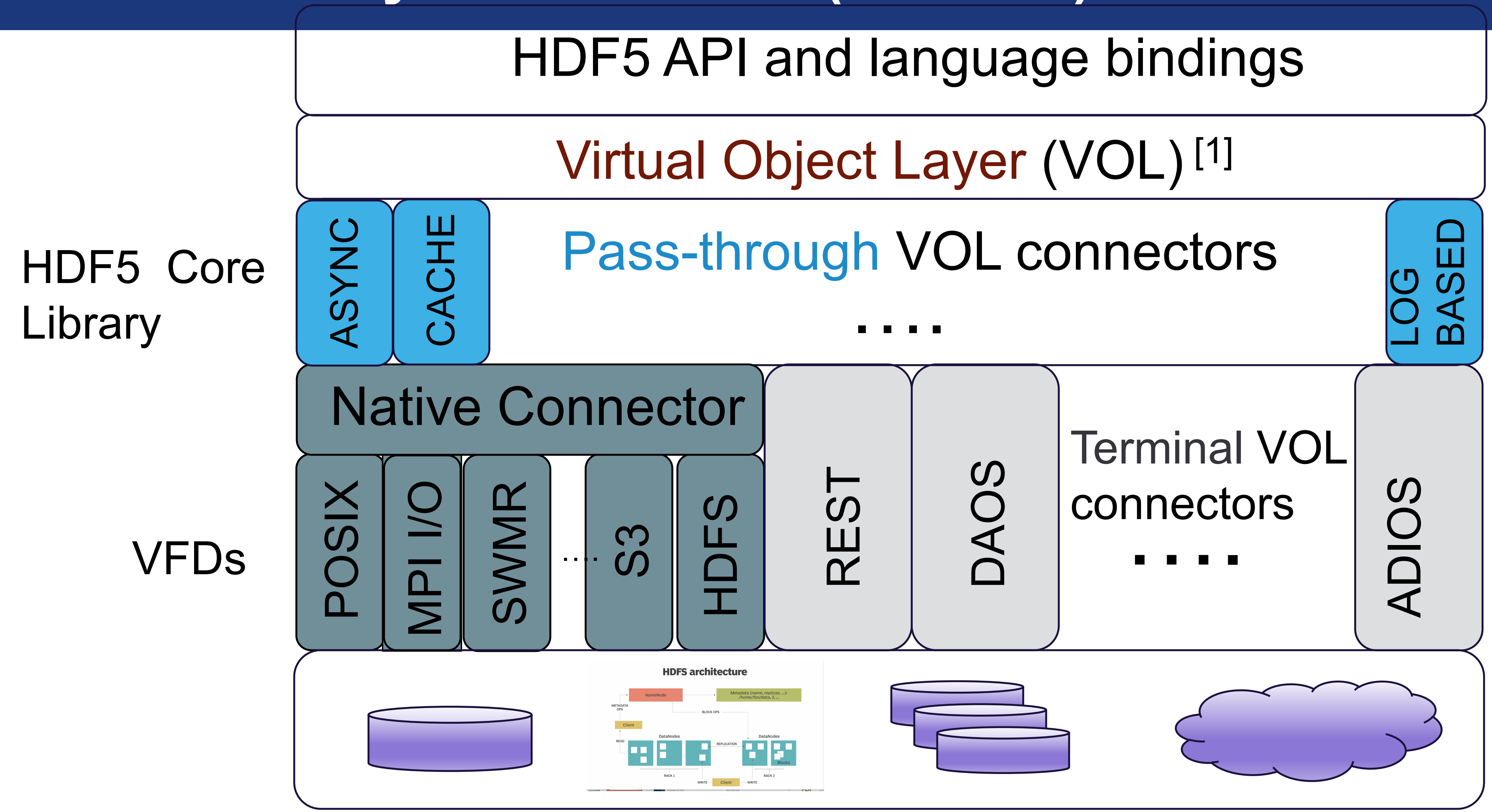
Java browser to view HDF5 file

https://portal.hdfgroup.org/display/HDFVIEW/HDFView

HDF5 Examples (C, Fortran, Java, Python, Matlab, ...)

https://portal.hdfgroup.org/display/HDF5/HDF5+Examples

HDF5 Library Architecture (1.12.0 +)



[1] https://portal.hdfgroup.org/display/support/Registered+VOL+Connectors

HDF5 Programming model and API

The General HDF5 API

C, FORTRAN, Java, and C++

C routines begin with the prefix: H5?

? corresponds to the type of object the function acts on

Example Functions:

H5D : **D**ataset interface *e.g.,* **H5Dread**

H5F : **F**ile interface *e.g.,* **H5Fopen**

H5S : data**S**pace interface *e.g.,* **H5Sclose**

The language wrappers follow the same trend

There are more than 300 APIs – but one can start with less than 50

General Programming Paradigm

Object is opened or created

- Creation properties applied
- Access properties applied
- Supporting objects are defined (datatype, dataspace)

Object is accessed possibly many times

- Access property can be changed

Object is closed

Properties (H5**P**) of an object are optionally defined

- Creation properties (e.g., use chunking storage)
- Access properties (e.g., using MPI I/O driver to access file)

H5**F**create (H5**F**open)	create (open) File
H5**S**create_simple/H5**S**create	create dataSpace
H5**D**create (H5**D**open)	create (open) Dataset
H5**D**read, H5**D**write	**access Dataset**
H5**D**close	close Dataset
H5**S**close	close dataSpace
H5**F**close	close File

General best practices

HDF5 Dataset I/O

Issue large I/O requests

At least as large as the file system block size

Avoid **datatype conversion** ⓘ

Use the same data type in the file as in memory

If conversion is necessary, increase datatype conversion buffer size (default 1MB) with *H5Pset_buffer()*

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

Use **contiguous storage** if no data will be added and compression is not used

- HDF5 will not cache data

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

Chunking is required when using extendibility and/or compression and other filters

I/O is always performed **on a whole chunk**

- Make your chunks the "right" size
  - Goldilocks Principle: Not too big, nor too small

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)?
- Do you need to adjust chunk cache size (1 MB default; can be set up per file or per dataset), *H5Pset_chunk_cache()*?
- `H5Pset_chunk_cache` sets raw data chunk cache parameters for a dataset
  - `–H5Pset_chunk_cache (dapl, …);`
- `H5Pset_cache` sets raw data chunk cache parameters for all datasets in a file
  - `–H5Pset_cache (fapl, …);`
- •Investigate other parameters to control chunk cache

Terminology

DATA – "problem-size" data, e.g., large arrays

METADATA – is an overloaded term

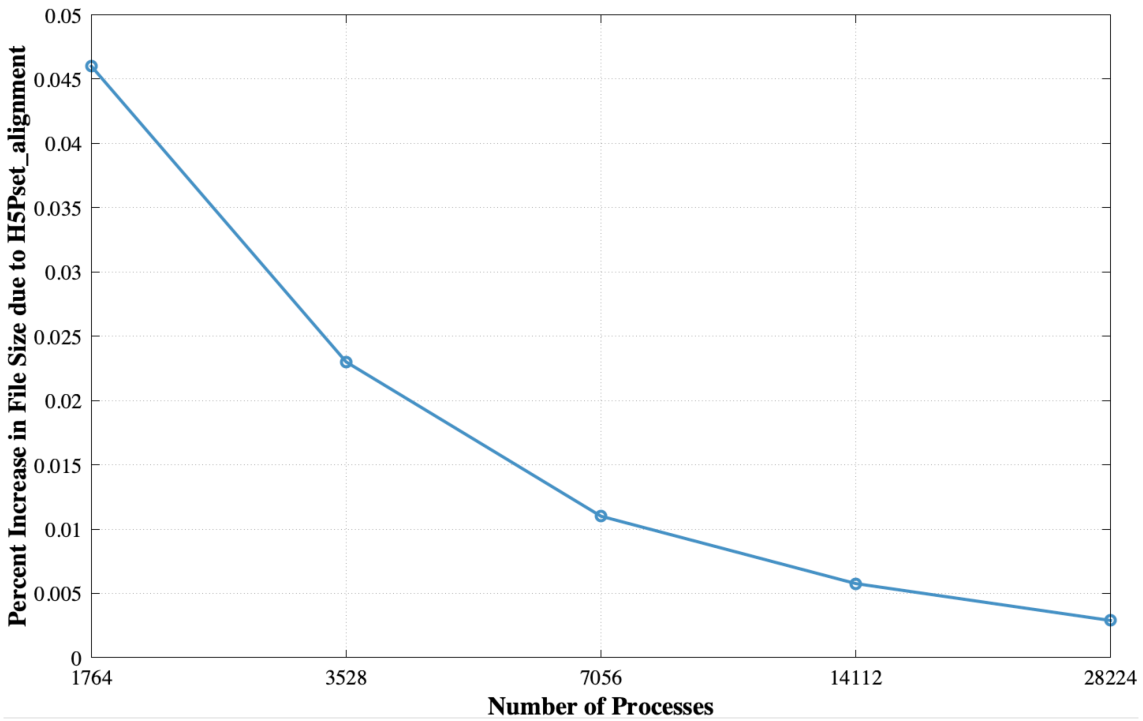
In this presentation:

- 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
  - Chunk indices, heaps to store group links and indices to look them up, object headers, etc.

General HDF5 Efficiency

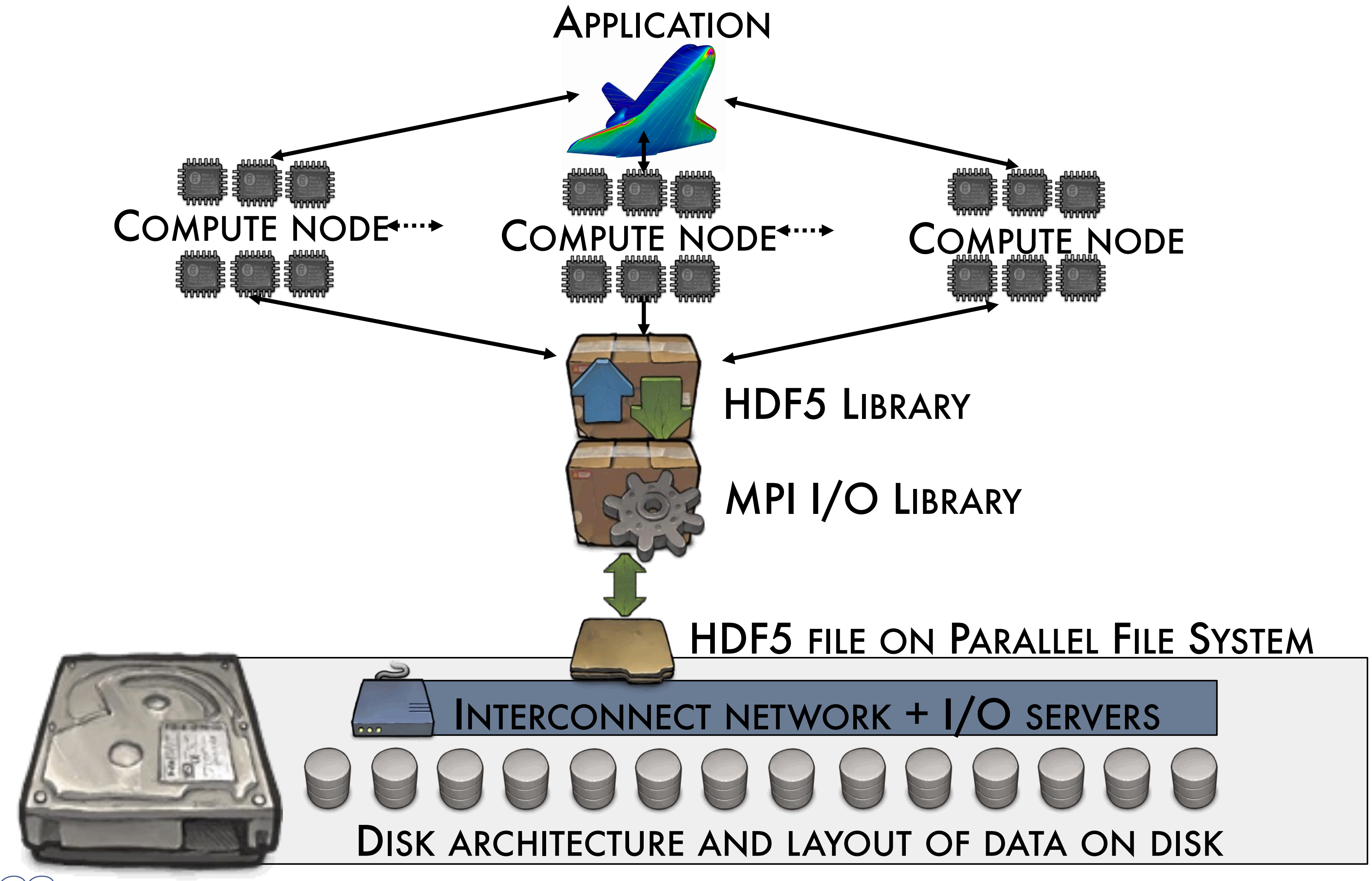
Faster HDF5 Performance: **Metadata**

- Use the “latest” file format features
  - *H5Pset_libver_bounds()*
- Increase the size of metadata data structures
  - *H5Pset_istore_k(), H5Pset_sym_k(), etc.*
- Aggregate metadata into larger blocks
  - *H5Pset_meta_block_size()*
- Align objects in the file
  - *H5Pset_alignment()*
- Control metadata cache
- Paged allocation and page buffering
  - Aggregate and align metadata and small data, perform I/O in aligned pages
  - See File Space Management Documentation https://portal.hdfgroup.org/display/HDF5/File+Space+Management

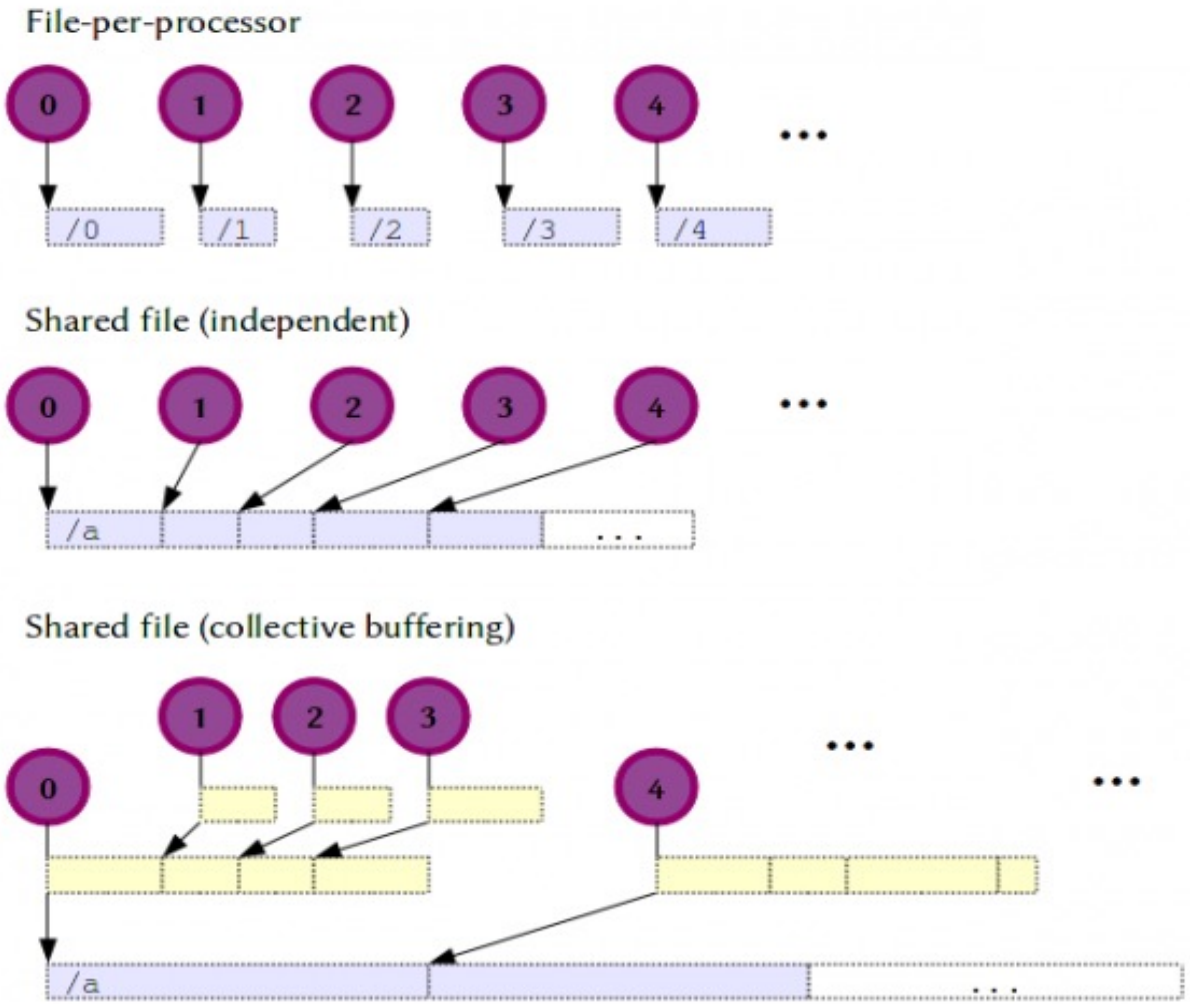


Parallel I/O with HDF5

PHDF5 implementation layers



Types of Application I/O to Parallel File Systems



Why Parallel HDF5?

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

Maintained code base, performance and data portability

- Rely on HDF5 to optimize for the underlying storage system

Parallel HDF5 (PHDF5) vs. Serial HDF5

PHDF5 allows multiple MPI processes in an MPI application to perform I/O to a single HDF5 file

PHDF5 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 “schema”

Parallel HDF5 Schema

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

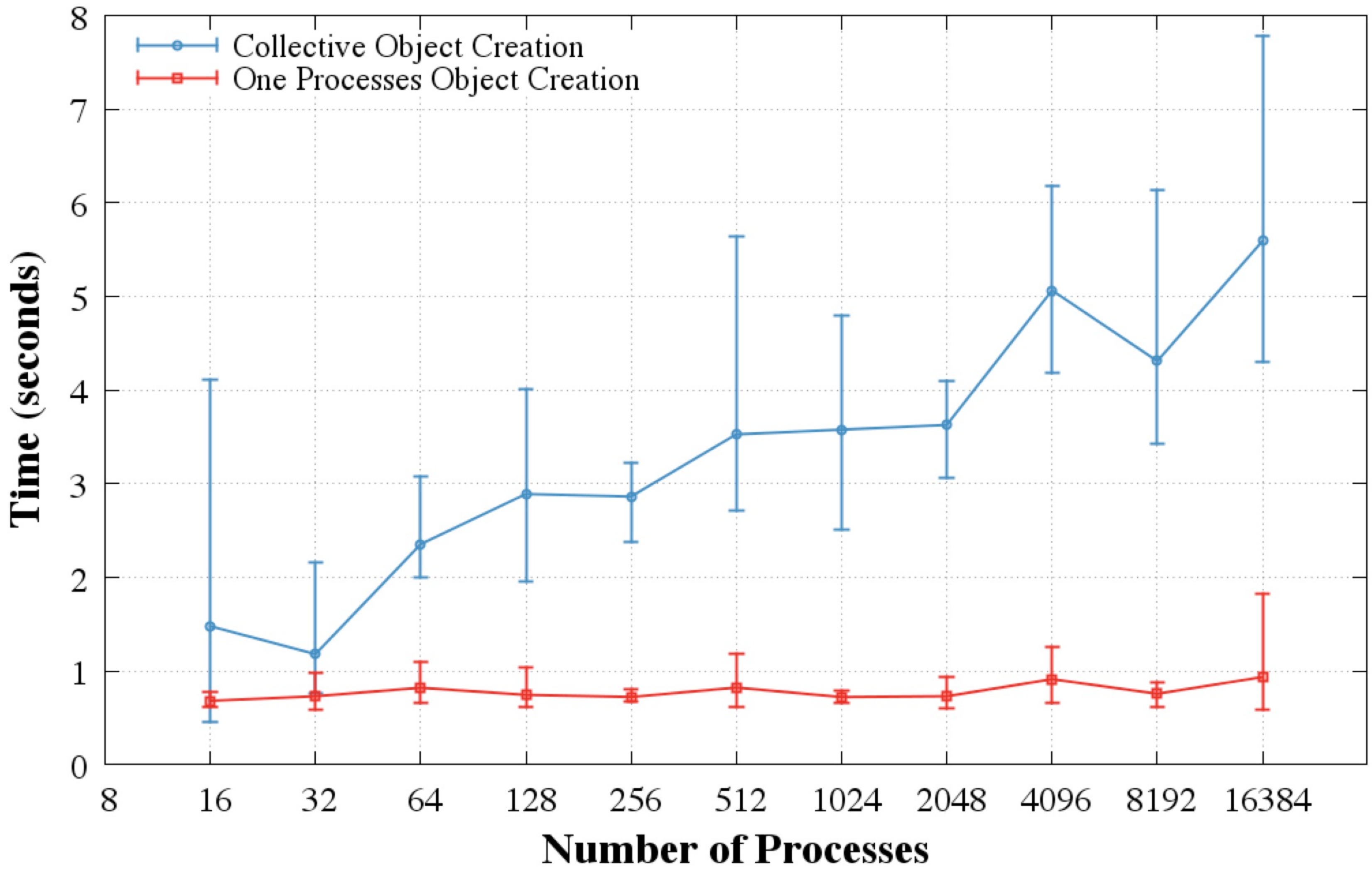
All processes must participate in collective PHDF5 APIs

All HDF5 APIs that modify the HDF5 namespace and structural metadata are collective!

- File ops., group structure, dataset dimensions, object life-cycle, etc.
- Raw data operations can either be collective or independent
  - For collective, all processes must participate, but they don't need to read/write data.

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

Object Creation (Collective vs. Single Process)



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 I/O attempts to combine multiple smaller independent I/O ops into fewer larger ops; neither mode is preferable *a priori*

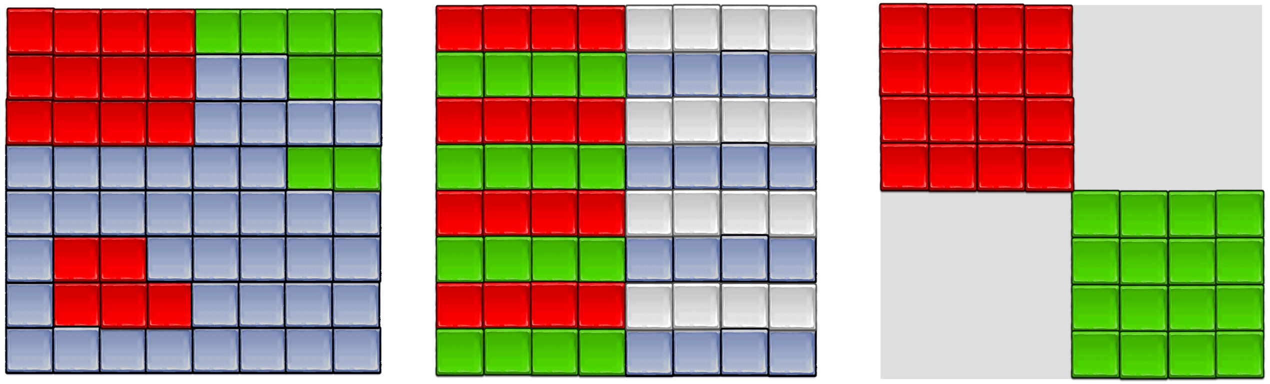
General HDF5 Programming Parallel Model for raw data I/O

Distributed memory model: data is split among processes

Each process defines selections in memory and in file (aka HDF5 hyperslabs) using `H5Sselect_hyperslab`

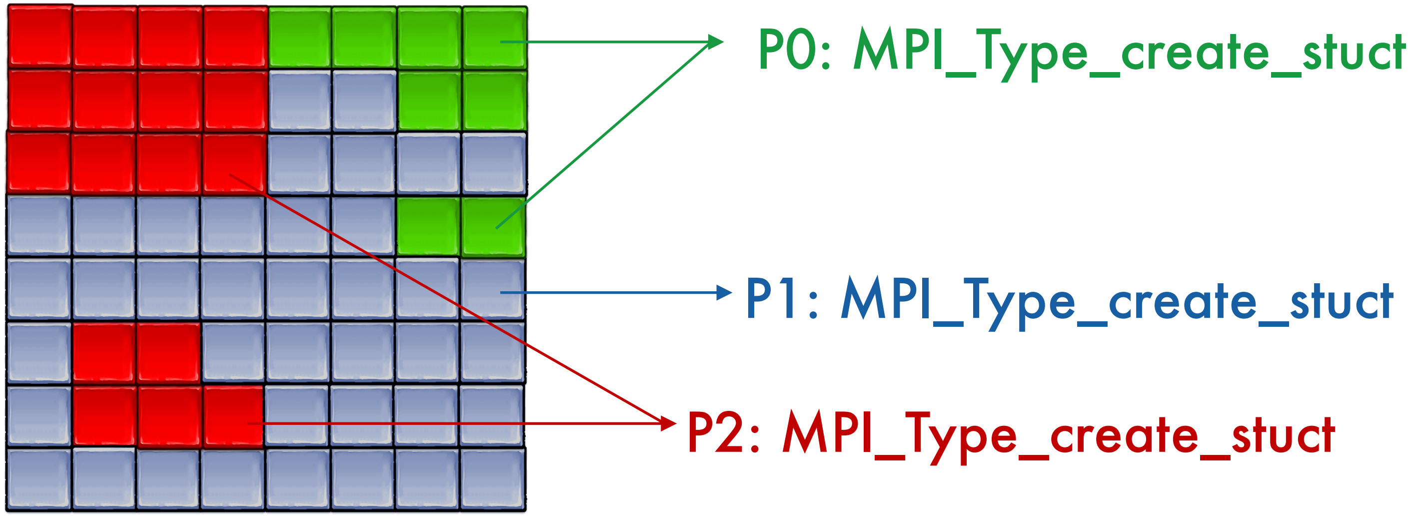
The hyperslab parameters define the portion of the dataset to write to

- Contiguous hyperslab, Regularly spaced data (column or row), Pattern, or Blocks



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

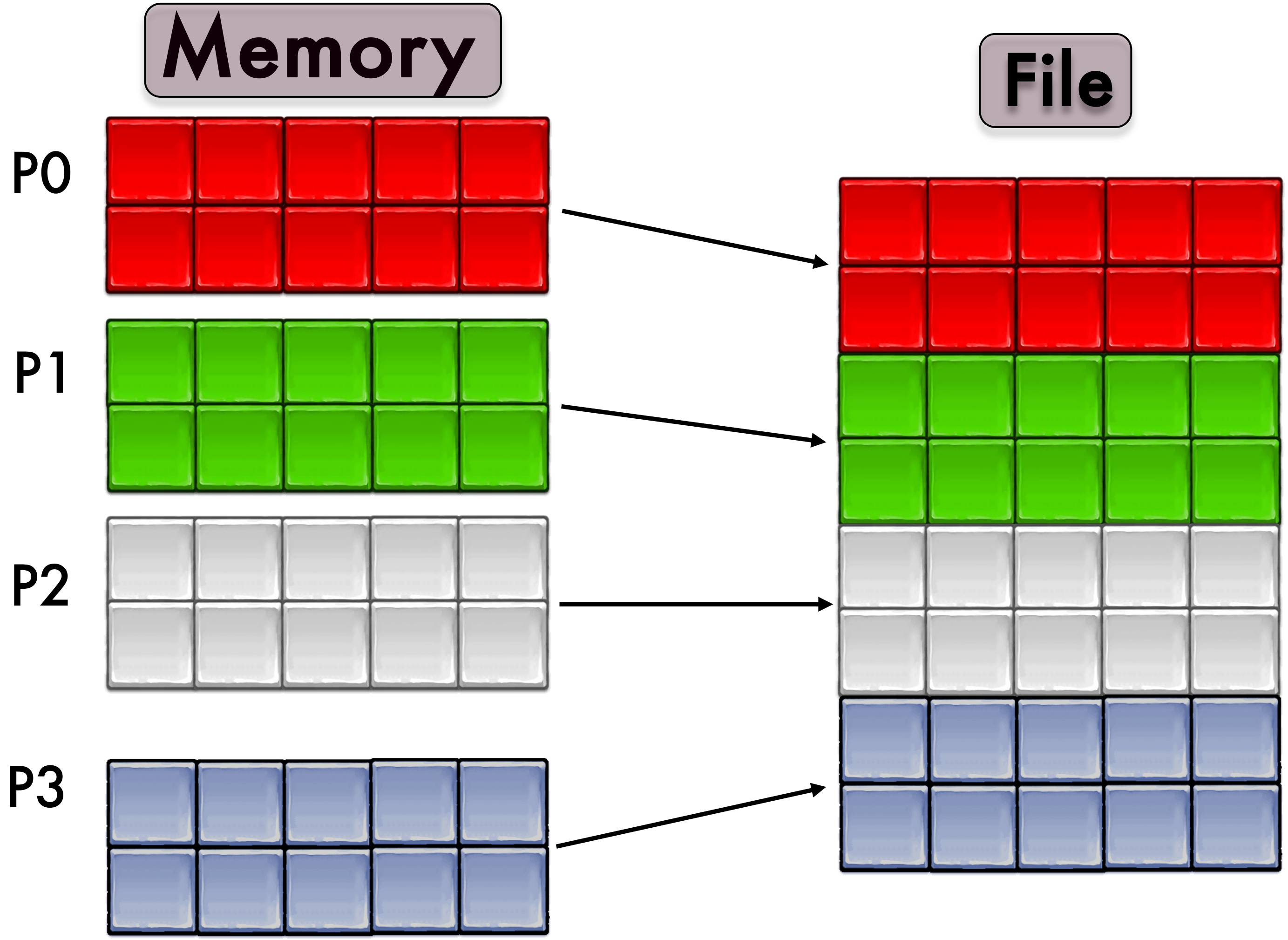
Examples of irregular selection



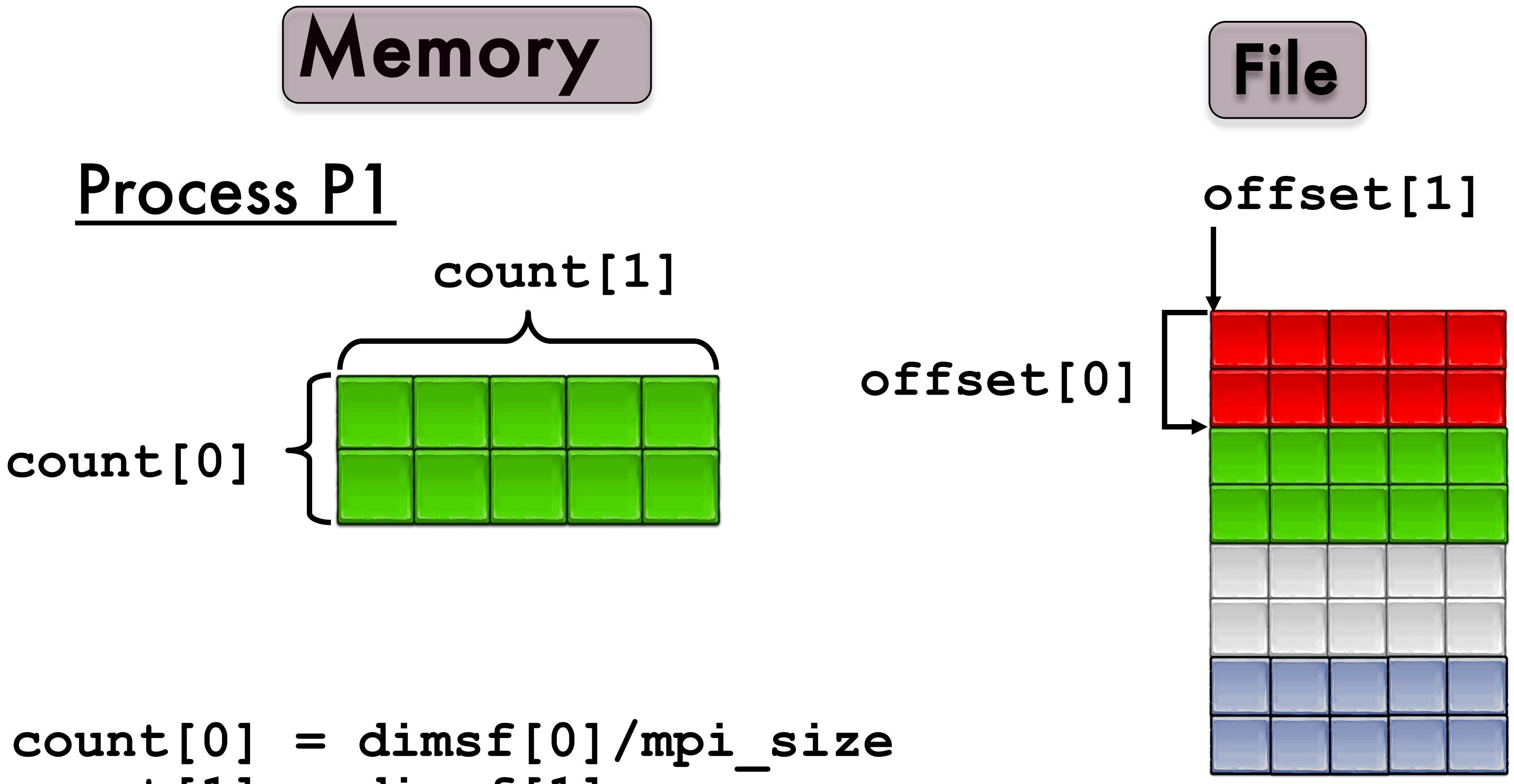
Internally…

1. The HDF5 library creates an MPI datatype for each lower dimension in the selection
2. It then combines those types into one large structured MPI datatype

Example 1: Writing dataset by rows



Example 1: *Writing dataset by rows*




```
count[0] = dimsf[0]/mpi_size
count[1] = dimsf[1];
offset[0] = mpi_rank * count[0];  /* = 2 */
offset[1] = 0;
```

Example 1: *Writing dataset by rows*

```
/*
 * Each process defines dataset in memory and
 * writes it to the hyperslab
 * in the file.
 */
 count[0] = dimsf[0]/mpi_size;
 count[1] = dimsf[1];
 offset[0] = mpi_rank * count[0];
 offset[1] = 0;
 memspace = H5Screate_simple(RANK,count,NULL);

/*
 * Select hyperslab in the file.
 */
 filespace = H5Dget_space(dset_id);
 H5Sselect_hyperslab(filespace,
     H5S_SELECT_SET,offset,NULL,count,NULL);
```

C Example: Collective write and read

```
/*
 * Create property list for collective dataset write.
 */
plist_id = H5Pcreate(H5P_DATASET_XFER);
H5Pset_dxpl_mpio(plist_id, H5FD_MPIO_COLLECTIVE);

status = H5Dwrite(dset_id, H5T_NATIVE_INT,
                  memspace, filespace, plist_id, data);
```

```
/*
 * Collective dataset read.
 */

status = H5Dread(dset_id, H5T_NATIVE_INT,
                        memspace, filespace, plist_id, data);

```

Writing by rows: *Output of h5dump*

```
HDF5 "SDS_row.h5" {
GROUP "/" {
   DATASET "IntArray" {
      DATATYPE  H5T_STD_I32BE
      DATASPACE  SIMPLE { ( 8, 5 ) / ( 8, 5
) }
      DATA {
         10, 10, 10, 10, 10,
         10, 10, 10, 10, 10,
         11, 11, 11, 11, 11,
         11, 11, 11, 11, 11,
         12, 12, 12, 12, 12,
         12, 12, 12, 12, 12,
         13, 13, 13, 13, 13,
         13, 13, 13, 13, 13
      }
   }
}
```

General HDF5 Best Practices and Case Studies for Parallel Performance

PHDF5 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

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

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.

Other Sources of Performance Variability

Hardware

System configuration and activity of other users

<u>HDF5 property (H5P) lists</u>

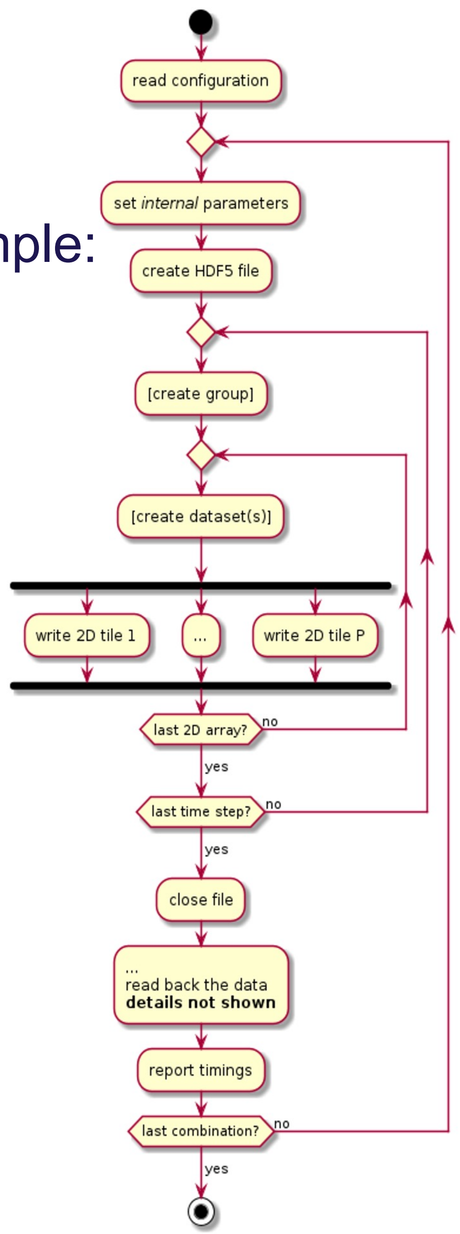
- Nearly 180 APIs
- Controls storage properties for HDF5 objects
- Controls in-flight HDF5 behavior
- About 100 *H5Pset_** functions
  - $\leq p_1 * \ldots * p_{100}$ combinations!
  - How many are tested?
- What does *H5P_DEFAULT* mean?
- What is the effect of using H5P_DEFAULT?

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

Back to earlier example – Application Model

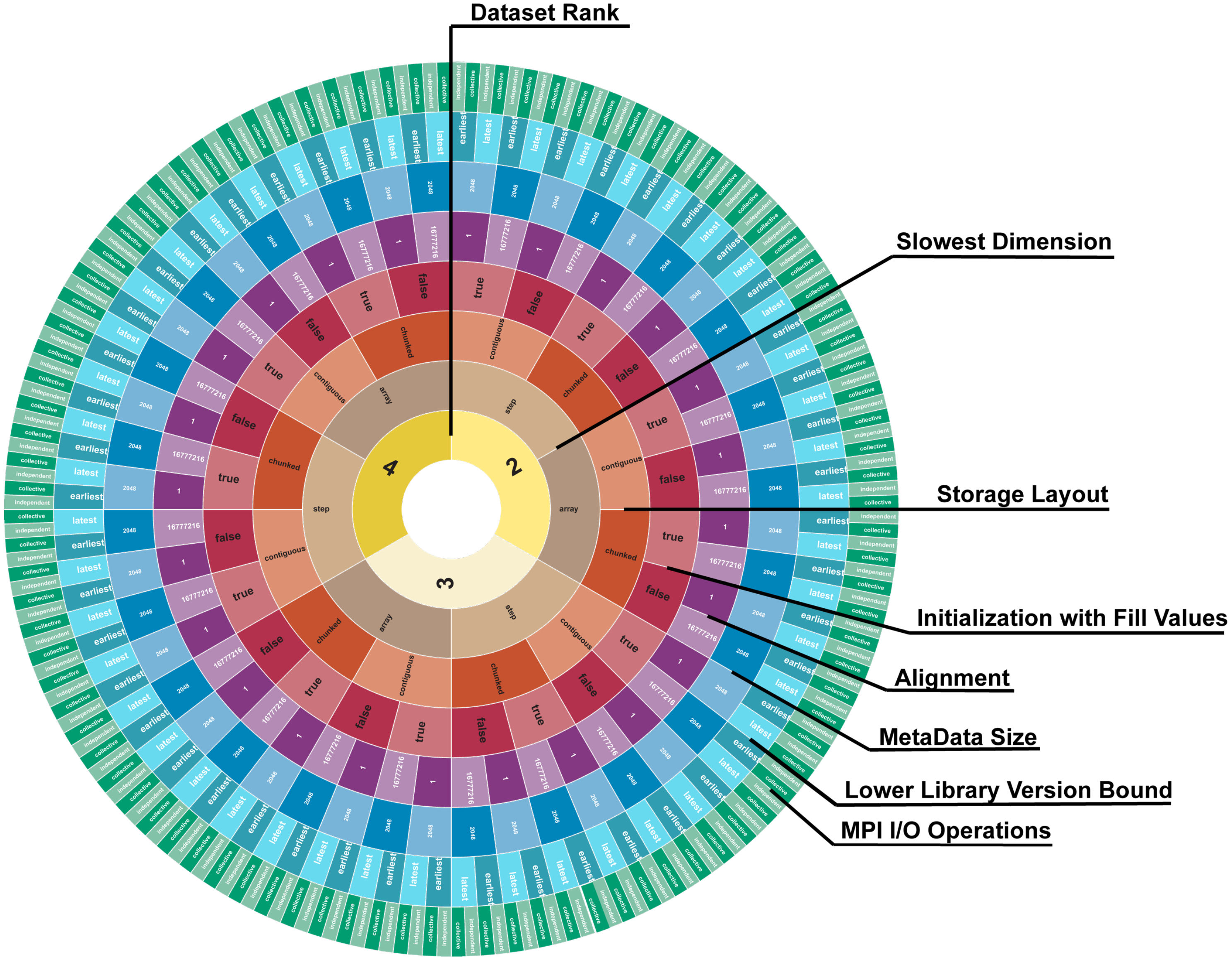
Good or bad news:

- 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



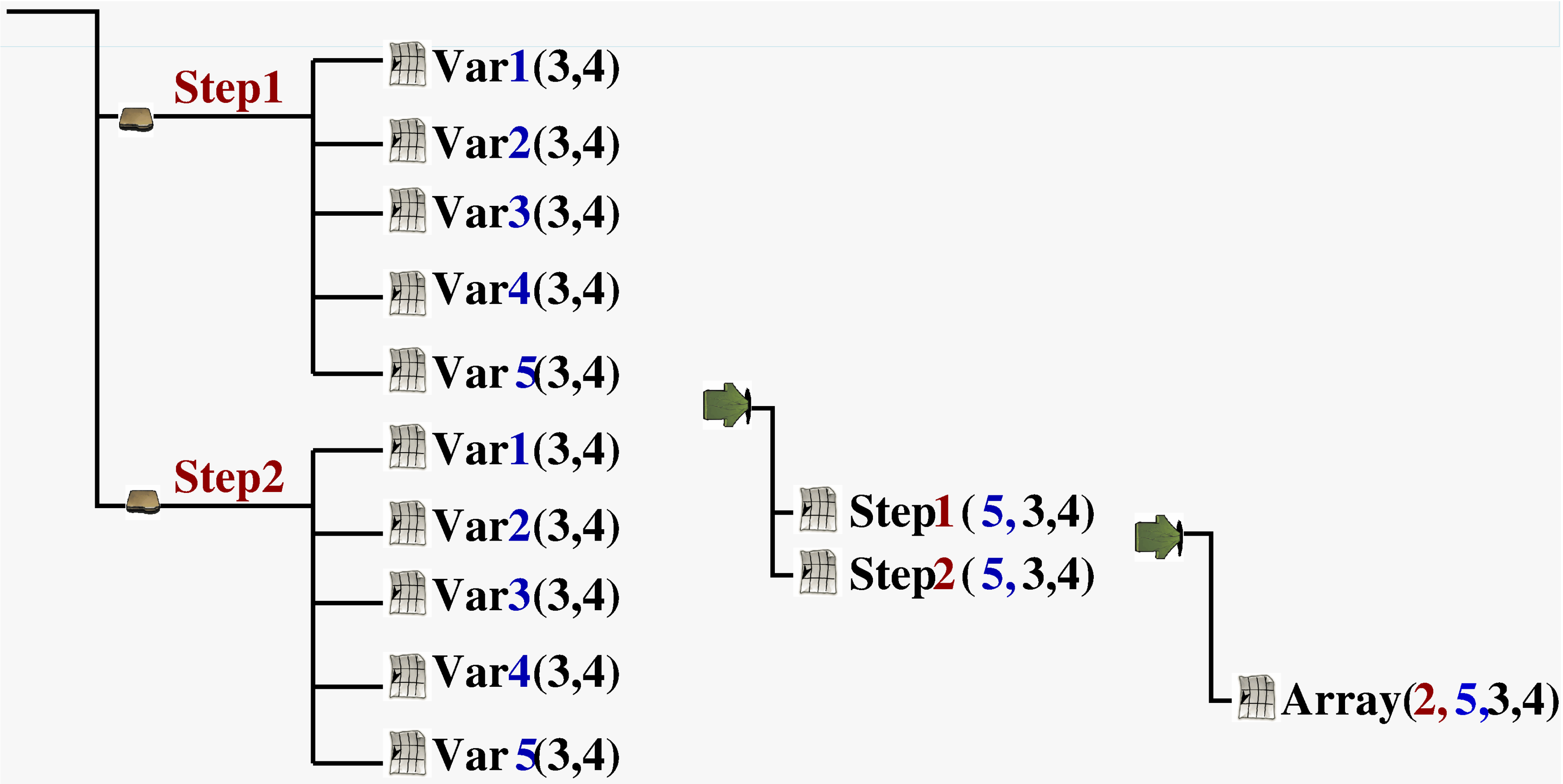
1 https://github.com/HDFGroup/hdf5-iotest

HDF5 Parameter Space



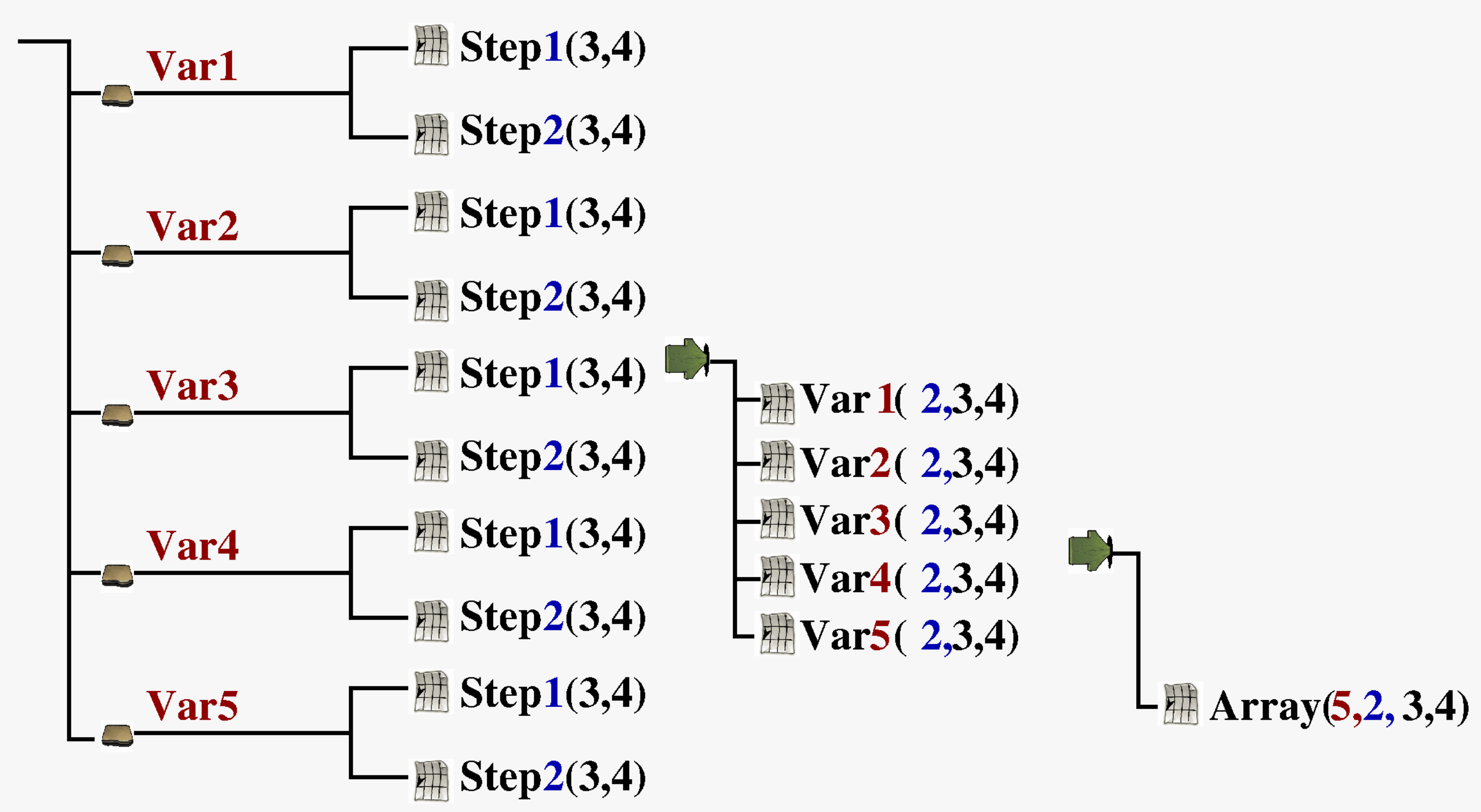
IO Pattern Model

Step based IO Pattern

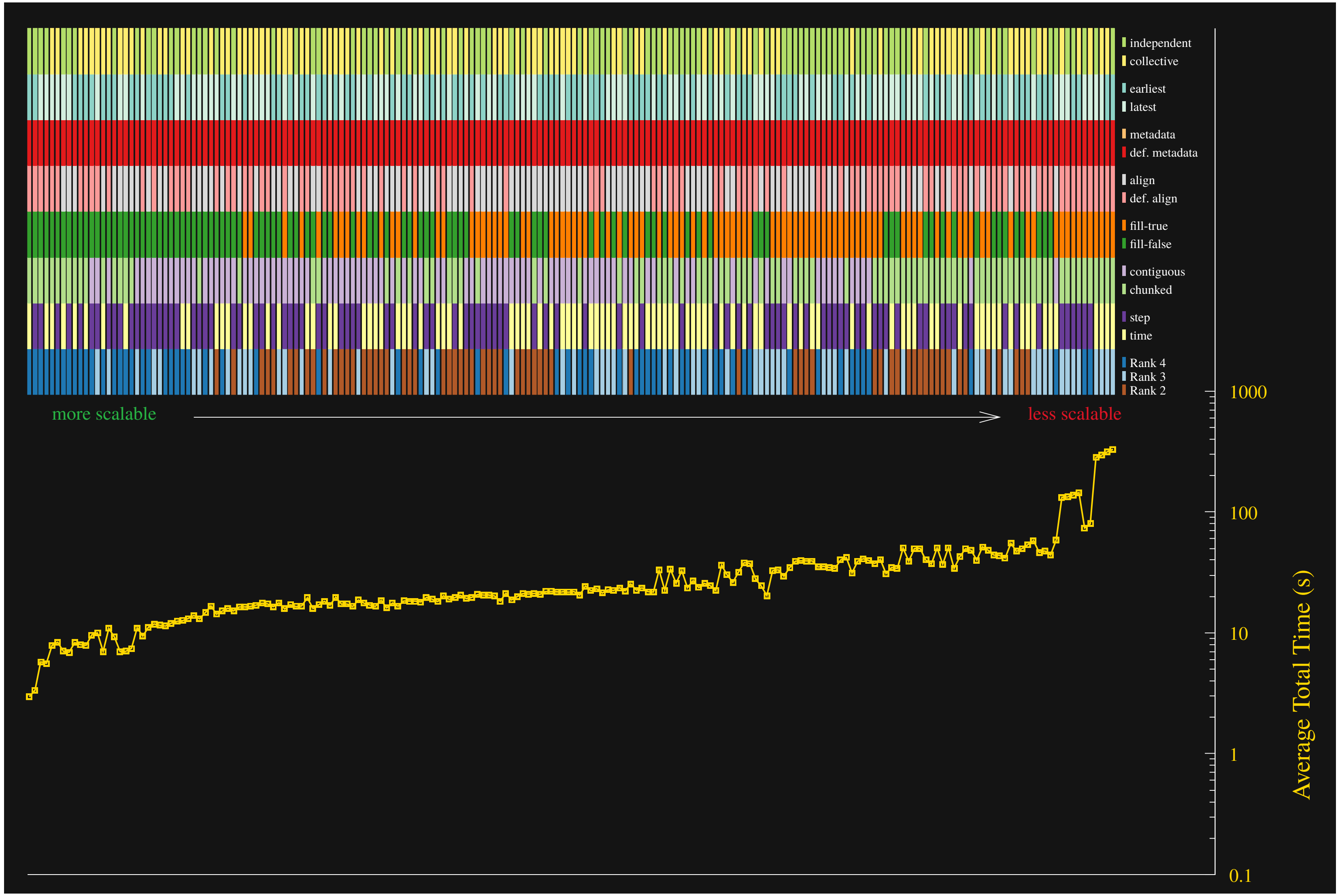


IO Pattern Model

Array based IO Pattern



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

Strongly Recommended Options

- Hint that metadata access is done collectively

  `H5Pset_coll_metadata_write, H5Pset_all_coll_metadata_ops`

  A property on an access property list

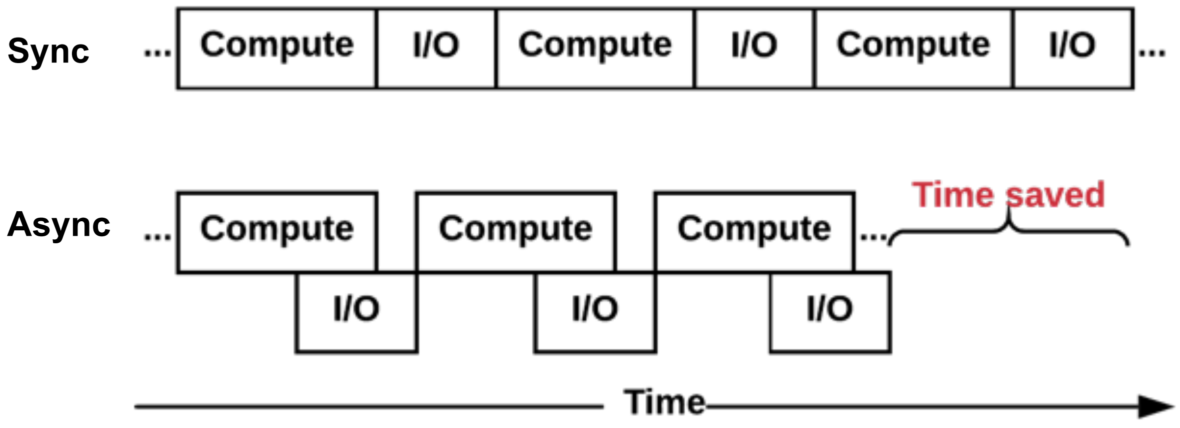
  If set on the file access property list, then all metadata read operations will be required to be collective

  Can be set on individual object property list

  When set, MPI rank 0 will issue the read for a metadata entry to the file system and broadcast to all other ranks

- Set HDF5 to never fill chunks (H5Pset_fill_time with H5D_FILL_TIME_NEVER)

Features: Asynchronous I/O



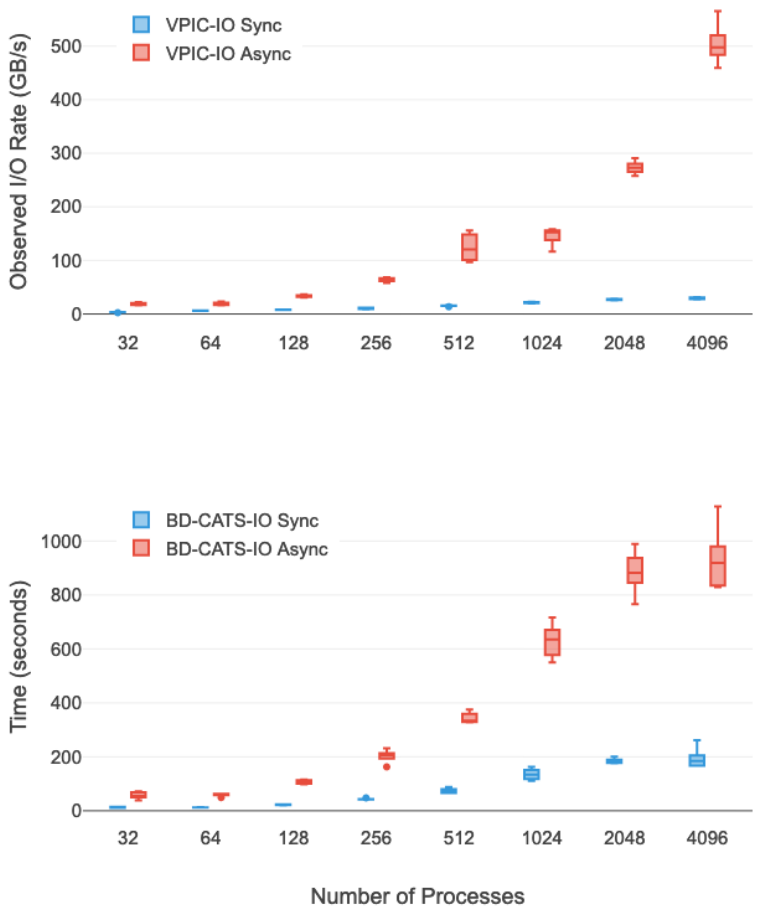
- Allows asynchronous operations for HDF5 applications:
  - Applications use the _*async* versions for the **H5** APIs
  - Return “request tokens” to applications to track I/O tasks.
- Requires a VOL (async or DAOS) which supports asynchronous I/O, otherwise defaults to synchronous I/O.

Asynchronous HDF5 Operations VOL Connector

- Implemented as a pass-through VOL connector w/background threads, using Argobots
- Transparent from the application, no major code changes
- Execute I/O operations in the background thread
- Lightweight and low overhead for all I/O operations
- No need to launch and maintain extra server processes

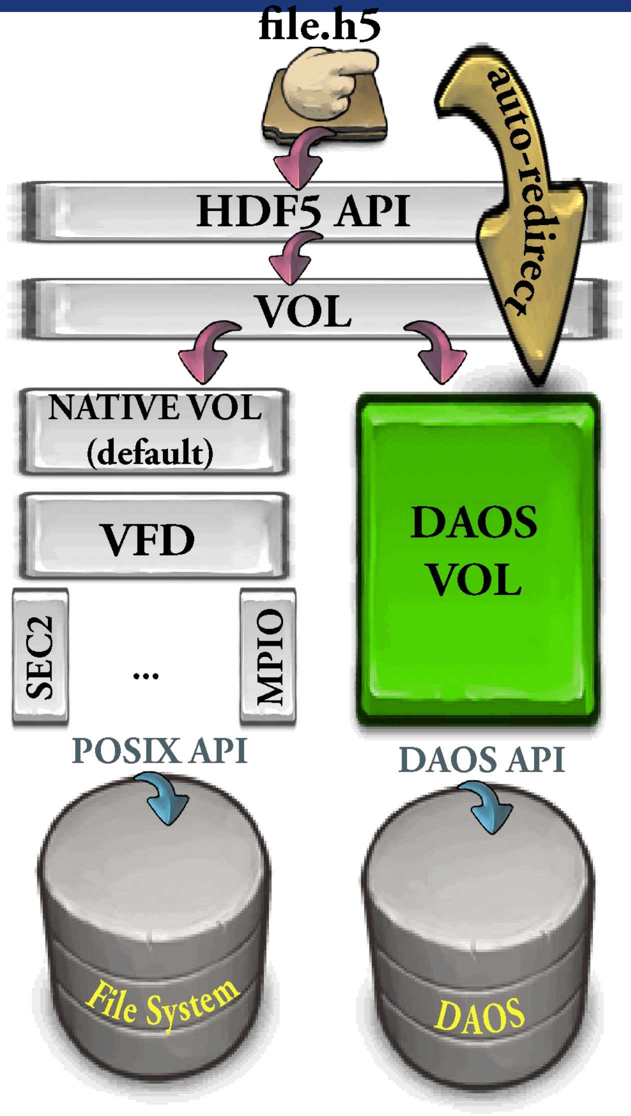
https://github.com/hpc-io/vol-async

On Summit



- More details in PDSW Paper:
  - https://sc19.supercomputing.org/proceedings/workshops/workshop_files/ws_pdsw109s2-file1.pdf

DAOS VOL Connector



HDF5 VOL connector for I/O to Distributed Asynchronous Object Storage (DAOS)

https://github.com/HDFGroup/vol-daos

Deployed at ANL.

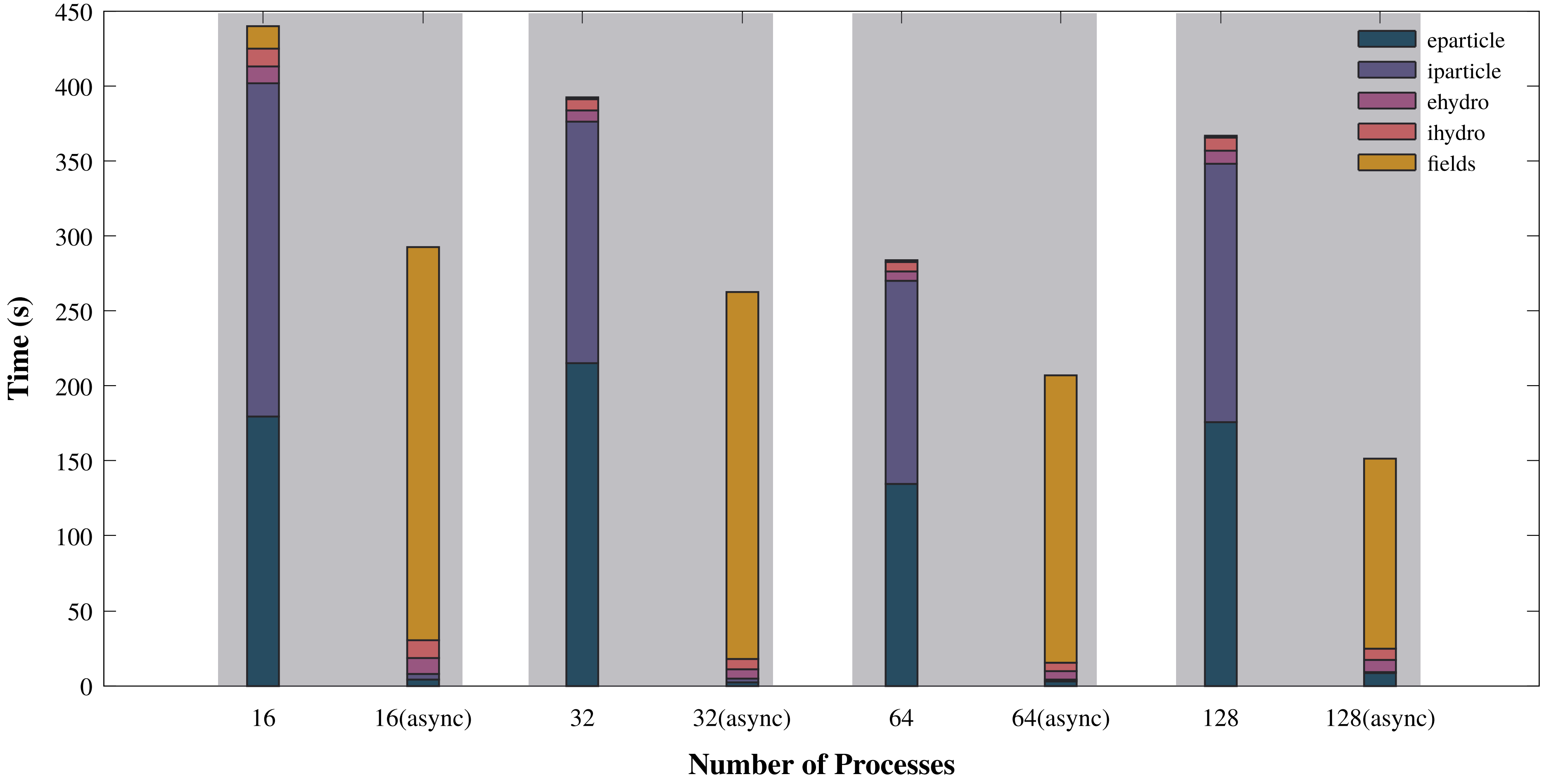
Minimal code changes needed to use, enable via environment variables or through HDF5 APIs.

HDF5 tools are supported

h5dump, h5ls, h5diff, h5repack, h5copy, etc.

Supports async I/O

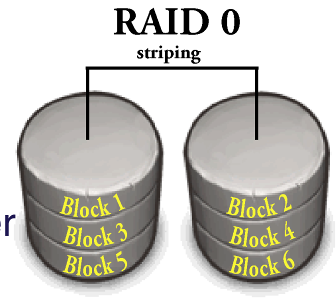
VPIC – explicit async (ANL testbed)



Subfiling

Subfiling is a compromise between file-per-process (*fpp*) and a single shared file (*ssf*)

- Use the Subfiling VFD, ***H5Pset_fapl_subfiling***(…);
- Multiple files organized as a Software RAID-0 Implementation
  i. Configurable "stripe-depth" and "stripe-set size"
  ii. A default "stripe-set" is created by using 1 file per node
  iii. A default "stripe-depth" is 32MB
  iv. The resulting collection can be read using subfiling, or fused together using the utility script *h5fuse.sh* into a single HDF5 file.

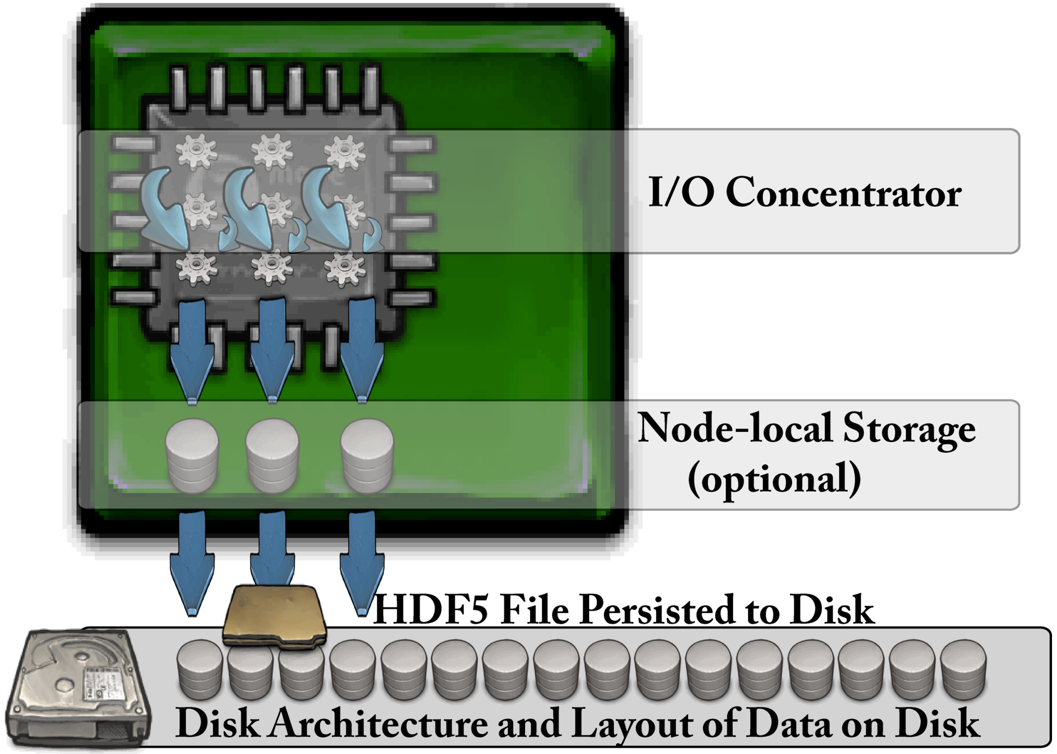


Use environment variables to control

- Number of I/O concentrators per node
- Number of I/O concentrator helper threads

- Benefits
  - Better use of parallel I/O subsystem (node-local storage)
  - Reduces the complexity of *fpp*
  - Reduced locking and contention issues to improve performance at larger processor counts over *ssf*
  - Available in *HDF5 1.14.0*

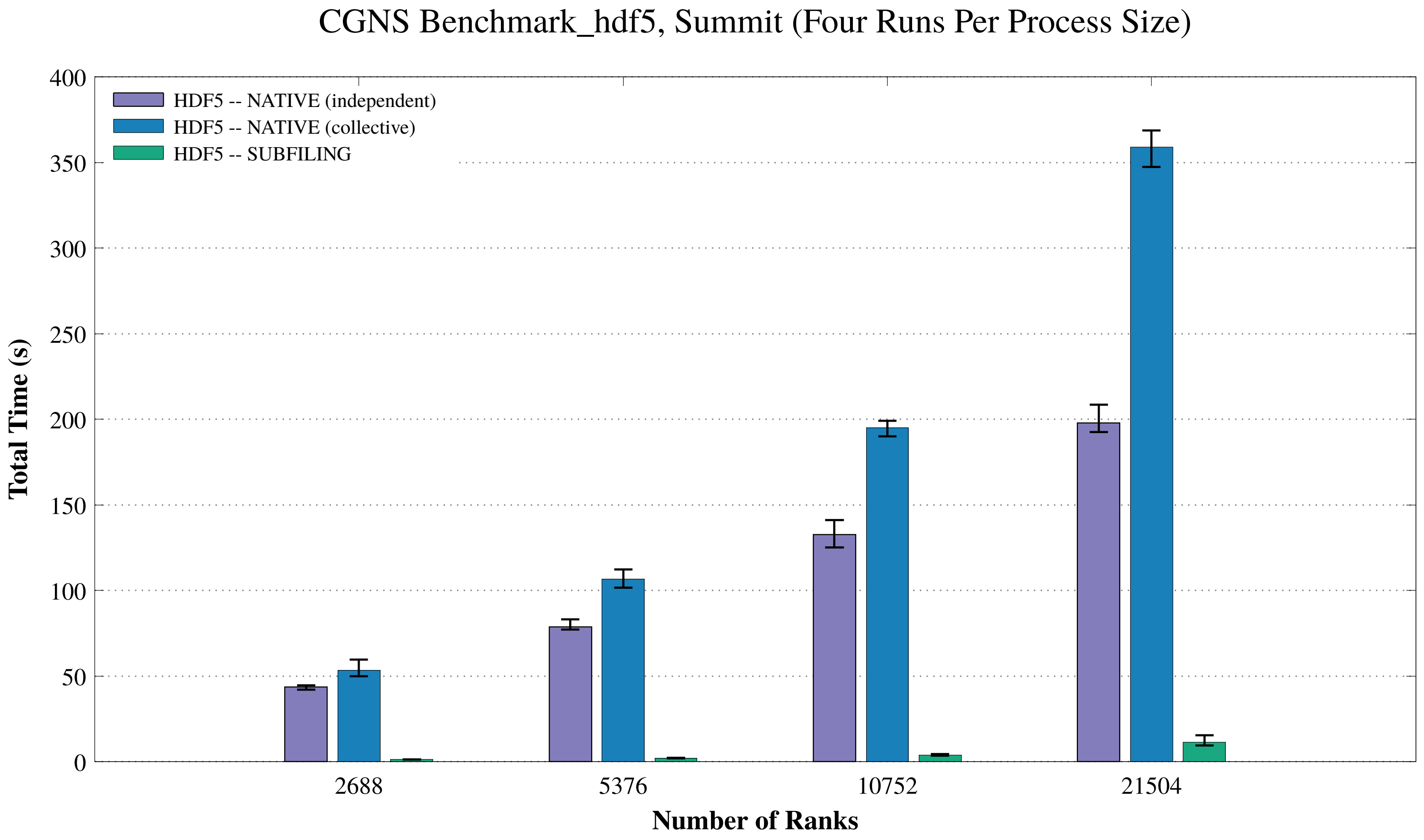
Subfiling



a. I/O Concentrators are implemented as independent threads attached to a normal HDF5 process.
b. MPI is utilized for communicating between HDF5 processes and the set of I/O Concentrators.
c. Because of (b), applications need to use *MPI_Init_thread* to initialize the MPI library.
d. Currently does not support collective I/O

Subfiling

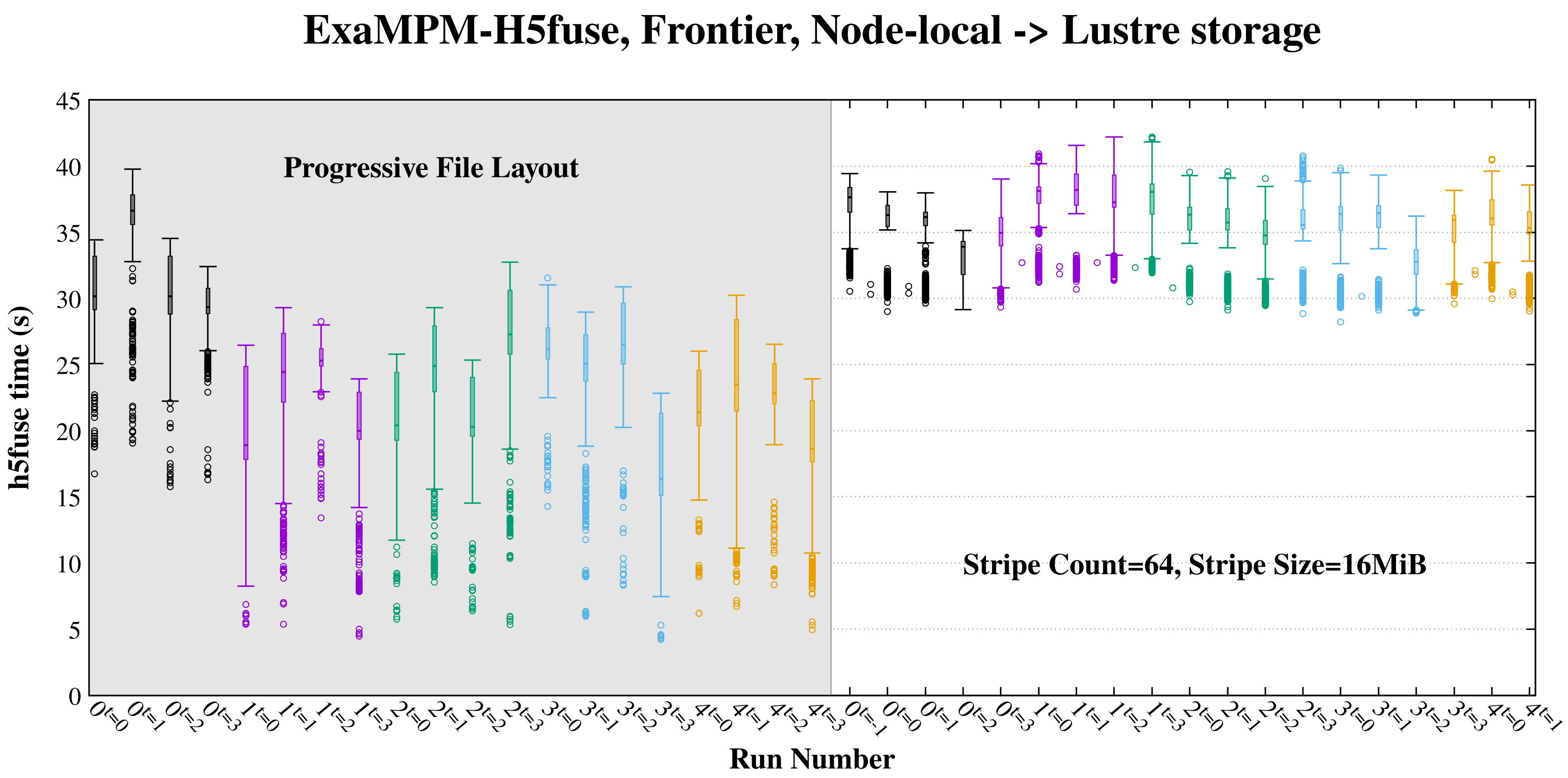
- (CGNS[1] **benchmark_hdf5**)
- The default settings for Subfiling were used, one subfile per node.



[1] CGNS = Computational Fluid Dynamics (CFD) General Notation System, cgns.org

Subfiling

- (Cabana/ExaMPM)



Need Help?

HDF-FORUM – https://forum.hdfgroup.org/

HDF Helpdesk – help@hdfgroup.org

Call the Doctor – Weekly HDF Clinic

https://zoom.us/meeting/register/tJwvf--gpjsqEtV0NSexRspn0NUjcNhZFmFb

THANK YOU!

Questions & Comments?