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
“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
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.*
Introduction to HDF5 with Python
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.
Core Topics Introduction
Data Model and Basic Usage
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

HDF5 Application

Compute node

Compute node

Compute node

HDF5 Library

MPI Library

HDF5 file on Parallel File System

Switch network + I/O servers

Disk architecture and layout of data on disk
Example of a PHDF5 C Program

A parallel HDF5 program has a few extra calls

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

fapl_id = H5Pcreate(H5P_FILE_ACCESS);
H5Pset_fapl_mpio(fapl_id, comm, info);

file_id = H5Fcreate(FNAME,..., fapl_id);
npace_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)

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

![Diagram showing Contiguous Storage]
Chunked Storage

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

![Diagram of Chunked Storage]

- **Metadata cache**
  - Dataset header
    - ....
    - Datatype
    - Dataspace
    - Attributes
    - ...
  - Chunk index
- **Dataset data**
  - A
  - B
  - C
  - D

- **Application memory**

- **File**
  - header
  - Chunk index
  - A
  - C
  - D
  - B
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
  • call A(); call B();
  • call A(); call B(); **right**
  • Process2
  • 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

- 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

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
Tools

DIAGNOSTICS AND INSTRUMENTATION
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 \(\rightarrow\) 4 columns
- Datatype is 8-byte floats (doubles)
- 4 processes \(\times\) 1000 rows \(\times\) 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 \(\rightarrow\) 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…
% 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=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.
Remedy:

- Collective I/O will combine many small independent calls into few but bigger calls.

- Chunks of columns speeds up too 230,000 rows.
Collective vs. independent write

The graph shows the relationship between the data size in MBs and the seconds to write, comparing independent and collective write operations. The y-axis represents the seconds to write, ranging from 0 to 1000 seconds, and the x-axis represents the data size in MBs, ranging from 0.25 to 2.75 MBs.

- **Independent write**: The blue line starts at approximately 20 seconds for 0.25 MBs and increases steeply to around 980 seconds for 2.75 MBs.
- **Collective write**: The red line remains consistently at zero seconds throughout the data size range, indicating negligible write time for collective operations.

This graph illustrates that collective write operations are significantly faster than independent write operations, especially as the data size increases.
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
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

![Graph showing performance metrics for POSIX and HDF5 in Write, Write Open-Close, Read, and Read Open-Close operations. The graph illustrates minimum, average, and maximum MB/s values for each operation.]
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
Blue Waters File System Performance Testing - Total = 1.18 TB/s

- Scratch: 980.7 GB/s
- Project: 100 GB/s
- Home: 104 GB/s
IOR on Blue Waters' /scratch

Performance (GB/s)

Number of Racks

WRITE
READ
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 size 1 MB
  • /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](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
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 \(\Rightarrow\) 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

- “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

Application
MPI Domains
20,000
6 threads per domain

MPI Aggregators

Lustre OSTs
Q: How long does it take to close/flush an HDF5 file?
A: A lot longer than you might expect!

Feature has not been released!
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.
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...*
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)

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

**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
• 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
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 …

- cg_open (CG_MODE_WRITE), IMPROVED
- cg_open (CG_MODE_WRITE), ORIGINAL

**Before Improvements**

**After Improvements**

**Impractical**
Metadata Read Storm Problem (I)

- All metadata “write” operations are required to be collective:

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

- Metadata read operations are not required to be collective

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

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

  ```c
  /* 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.

\[ \Rightarrow \text{READ STORM} \]
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 …

**CGNS Close**
**Hopper - Lustre**

<table>
<thead>
<tr>
<th>Number of Ranks</th>
<th>Seconds</th>
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</thead>
<tbody>
<tr>
<td>128</td>
<td>0</td>
</tr>
<tr>
<td>512</td>
<td></td>
</tr>
<tr>
<td>1024</td>
<td></td>
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<tr>
<td>2048</td>
<td></td>
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<tr>
<td>4096</td>
<td></td>
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<tr>
<td>8192</td>
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<tr>
<td>12284</td>
<td></td>
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<tr>
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</tbody>
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- **Patched**
- **Orig**

**CGNS Close**
**Cetus - GPFS**

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</table>

- **Patched**
- **Orig**
• **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
Resources

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