Northwestern

A Case Study on Parallel HDF5 Dataset Concatenation for High-Energy Physics Data Analysis

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Introduction to A Case Study on HEP Data Aggregation

Metadata I/O

Raw data I/O

End-to-End Performance Evaluation

High-Energy Physics Workflow and Data Storage

- In High-Energy Physics (HEP), the quantities of experimental data generated from large-scale instruments are often immense
- Traditional HEP workflows are designed for grid-oriented environment: many independent processes produce ***a large number of files of moderate sizes***
- To better facilitate data management, transfer, and analysis on large-scale HPC platforms, it is advantageous to aggregate data into ***a smaller number of larger files***

A Case Study

- Considering the fast growth in size of HEP data, the data aggregation becomes the bottleneck of data analysis workflow

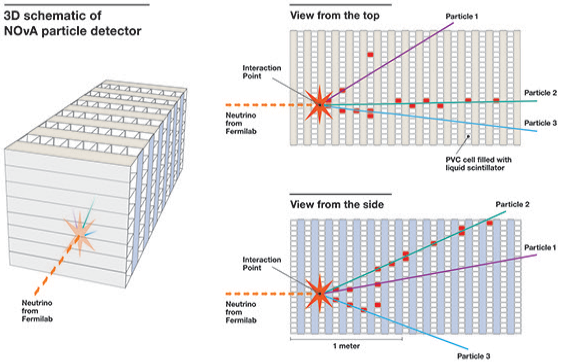
- In this work, we consider data aggregation of a large-scale HEP data
  - NOvA experiment data (hundreds to thousands HDF5 files)
  - Raw data: 1TB ~ 17TB
  - Compressed files: 35GB ~ 213 GB

- Explore a subset of HDF5 features used to implement NOvA data aggregation, and present our evaluation and analysis of their performance impacts

NOvA Experiment Data

- NuMI Off-axis ν_e Appearance (NOvA) experiment
  - Designed to study neutrino oscillations using the particle collision event data recorded by two detectors

- Near Detector (ND) data and Far Detector (FD) data
  - ND is at the Fermilab in Batavia, IL, and FD is in Ash River, MN
  - Both detectors observe neutrinos from a beam generated at Fermilab
  - NOvA produces many HDF5 files because of the grid-oriented processing environment



https://phys.org/news/2014-02-nova-long-distance-neutrinos.html

Tabular Structure of NOvA Experiment Data

- ***Run***: a period of data collection that represents a stable period of detector operation (a few hours ~ 24 hours)
- ***Subrun***: a subdivision of a run period that limits the output file size
- ***Spill (event)***: one 10 μs pulse of neutrinos generated at the Fermilab every 1.3 sec
- ***Slice*** (***subevent***): a fixed period of detector activity discovered within a spill
- Each file contains all spills in one ***subrun***

Table 1
NOvA data table organization with one entry per slice.

Run	Subrun	Event	Sub-event	distallpngtop	... 35 more ...
433	61	6124	35	nan	
433	61	6124	36	-0.7401	
433	61	6124	37	nan	
433	61	6125	1	nan	
433	61	6125	2	423.633	
433	61	6125	3	-2.8498	

NOvA Experiment Data Statistics

	ND files	FD files
Number of files	165	6,400
Number of groups per file	999	701
Number of 1-D datasets	15,965	12,925
Number of 2-D datasets	8	6
Number of empty datasets	13,396	9,374
Raw data size before compression	***1001.1 GB***	***17 TB***
Raw data size after compression	***23.5 GB***	***101.9 GB***
Metadata size	***11.7 GB***	***104.1GB***
Total file size	35.2 GB	212.5

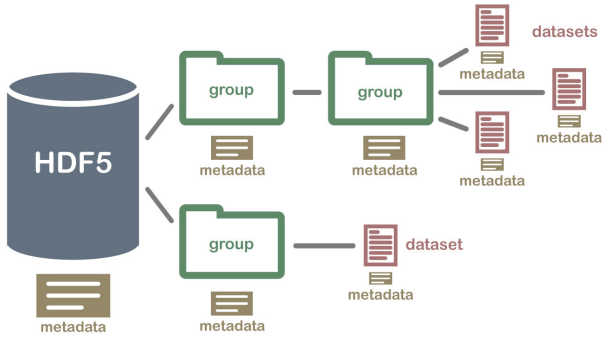
1. High compression ratio
2. A large amount of metadata

Hierarchical Data Format (HDF5)

- HDF5 is a popular I/O library in scientific communities, that enables users to store data in a portable, self-describing file format
  - Many open-source and commercial software packages for data visualization and analysis use HDF5
  - HDF5 supports parallel I/O for data compression (from 1.10.3)

- An HDF5 file consists of ‘group’s and ‘dataset’s
  - One file can have multiple groups
  - Each group can have multiple groups
  - Each group can have multiple datasets
  - Each HDF5 object has its own metadata

- We use HDF5 1.10.5 in this case study



Hierarchical Data Formats - What is HDF5? | NSF NEON | Open Data to Understand our Ecosystems (neonscience.org)

Parallel Data Aggregation

- Given F HDF5 files, all individual datasets are concatenated across the F files and stored into a single large output file
  - All files have the same groups and datasets of various sizes

- Parallel dataset concatenation workflow
  1. Evenly distribute F input files to P processes
  2. Collect and aggregate dimension sizes of D datasets from all input files
  3. Create a new shared output file
  4. Create D datasets of aggregated sizes in the output file
  5. For each dataset, read the dataset from all assigned input files to a memory buffer by appending one after another and then write the concatenated buffer to the output file

Experimental Settings

- All experiments are conducted on Cori XC40 supercomputer at NERSC
  - Used Haswell nodes to take advantage of the larger memory space and I/O speed than KNL nodes
  - Each node has 128 GiB DDR4 memory space, two sockets of Intel Xeon E5-2698v3 CPUs

- Parallel File System of Cori
  - Both the input files and the output file are stored on a disk-based Lustre parallel file system
  - File stripe size is 1MiB and the file stripe count is 128

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Reading Metadata From Input Files (1/2)

- To concatenate each dataset, the data type and array sizes should be read from all the input files

- Collecting the metadata from many NOvA files can be expensive
  - HDF5 allows metadata and raw data to be stored separately in almost any where in the file
  - Metadata collection: small and non-contiguous accesses to many files
  - Hundreds to thousands of files each of which has 13K~16K datasets

Reading Metadata From Input Files (2/2)

- Two possible options for metadata reading
  - On-the-fly I/O: many small and non-contiguous I/O
  - In-Memory I/O: read the entire files in a memory buffer at once (memory footprint ↑)

Metadata collection time for 165 ND files. Up to four processes run on each node.

# of processes	3	6	11	21	42	83	165
# of nodes	1	2	3	6	11	21	42
On-the-fly I/O	4099 sec	2188 sec	1122 sec	663 sec	304 sec	131 sec	64 sec
In-memory I/O	***61.9 sec***	***26.8 sec***	***16.3 sec***	***8.9 sec***	***4.9 sec***	***3.6 sec***	***1.5 sec***

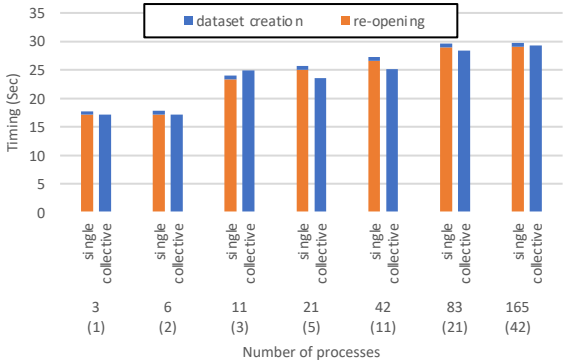
Metadata collection time for 6,400 FD files.

# of processes	100	200	400	800	1600
# of nodes	25	50	100	200	400
On-the-fly I/O	356 sec	180 sec	93 sec	55 sec	37 sec
In-memory I/O	***42.1 sec***	***21.3 sec***	***13.9 sec***	***8.7 sec***	***5.7 sec***

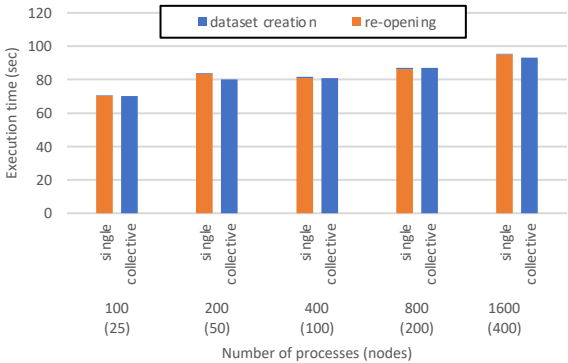
Writing Metadata To Output File (New Dataset Creation)

- Once the metadata is all collected, the same groups and datasets are created in the output file

- Two possible design options
  - One process opens the output file in POSIX mode and create all the datasets
  - All the processes open the output file in MPI I/O mode and collectively create all the datasets



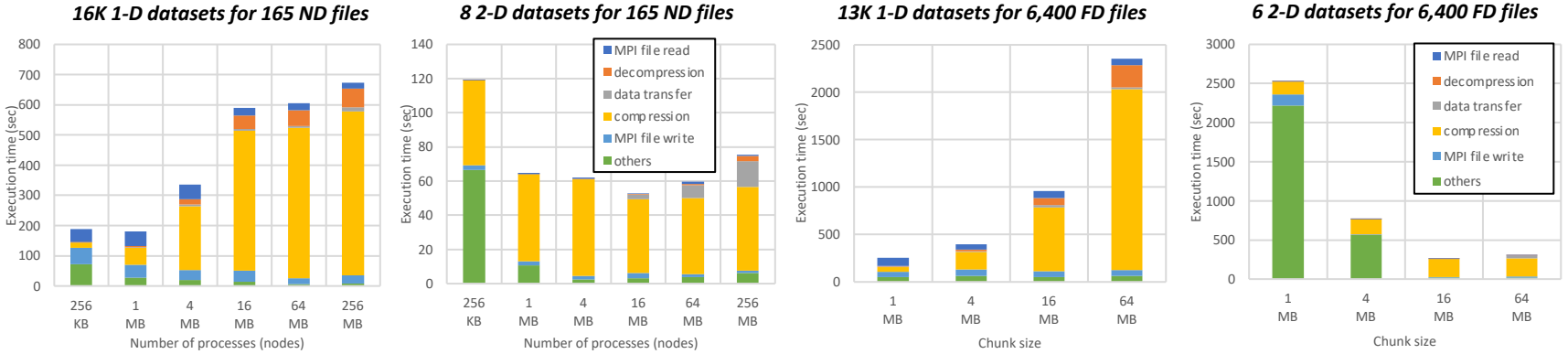
Timing breakdown for 165 ND files



Timing breakdown for 6,400 FD files

Chunking and Compression Strategy

- HDF5 requires users to use ‘chunked’ layout to enable data compression
- The chunk size affects not only I/O cost but also (de)compression and communication cost
  - Each chunk is owned by a unique process who has the largest portion of the chunk
  - When writing, all the processes collect their own chunks via inter-process communications, and then compress and write them into the output file



Metadata Caching

- Given 13K~16K datasets, caching metadata and later flushing in bigger and aggregated write requests appears to be a good strategy

- HDF5 allows users to adjust the metadata cache size (Default: 2MB and automatic increase based on hit-ratio)
  - Set the size to 128MB per process (maximum)
  - Turn off the automatic adjustment

Performance comparison (sec) between default setting and our setting for 165 ND files

Steps	Default	Our setting	Performance gain
Metadata collection	1.5	1.5	-
Dataset creation	30.7	29.3	4.5%
1-D dsets Read	15.5	15.9	-
1-D dsets Write	255.2	167.2	34.5%
2-D dsets Read	17.2	17.3	-
2-D dsets Write	54.1	48.2	10.9%
Overall	374.3	279.4	25.3%

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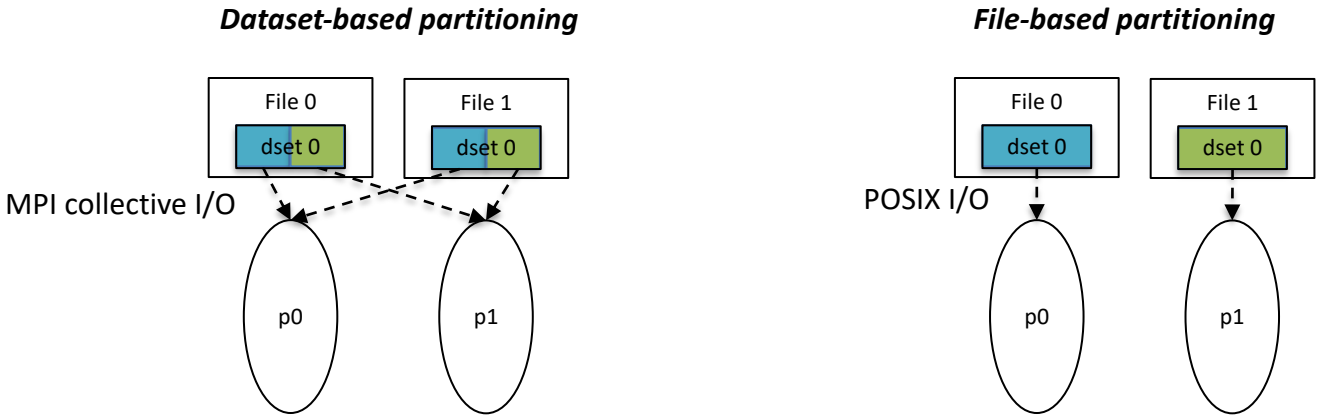
Parallel Read (1/2)

- Once all the datasets are created in the output file, each dataset is read from all the input files into a memory buffer
- Two design options for parallel read: ***dataset-based*** partitioning and ***file-based*** partitioning

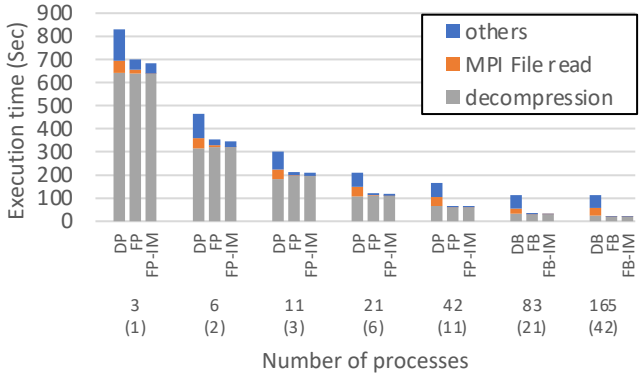


Parallel Read (2/2)

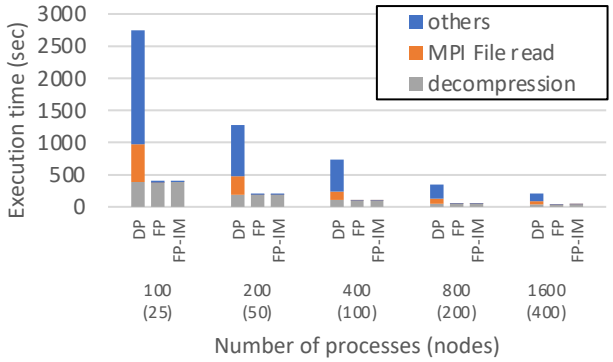
DP: Dataset-based Partitioning
FP: File-based Partitioning
FP-IM: File-based Partitioning with In-Memory I/O

- File-based partitioning better fits to NOvA experiment data
  - Enables each process to independently use POSIX I/O
  - The number of read operations is proportionally reduced as more processes run (Dataset-based partition always performs the same number of reads)

Timing breakdown of 2-D dataset read from 165 ND files



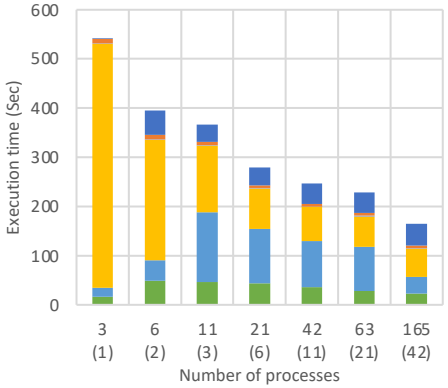
Timing breakdown of 2-D dataset read from 6,400 FD files



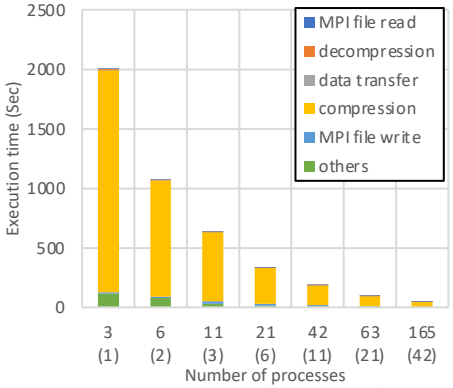
Parallel Write

- Finally, each concatenated dataset is written into a shared output file
- Regardless of the read strategy, parallel write is always MPI collective I/O (HDF5 allows only one dataset to be written at a time)

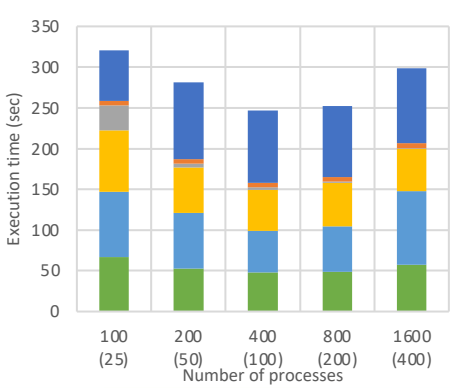
Timing breakdown of 1-D dataset write (165 ND files)



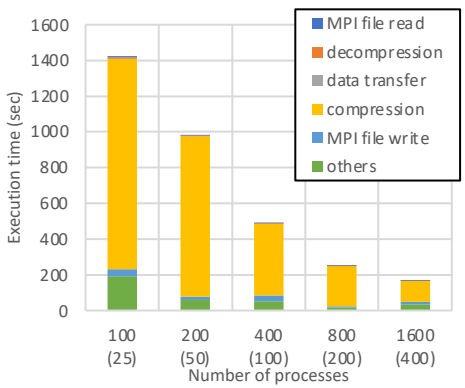
Timing breakdown of 2-D dataset write (165 ND files)



Timing breakdown of 1-D dataset write (6,400 FD files)



Timing breakdown of 2-D dataset write (6,400 FD files)



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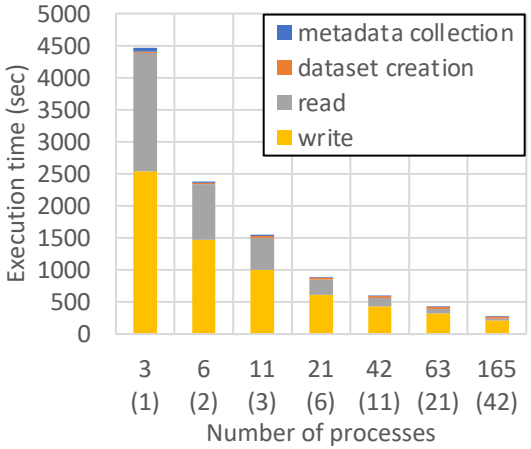
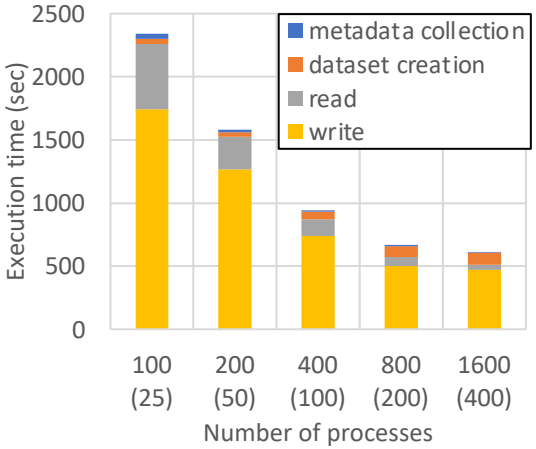
Concatenation time for 165 ND files



Concatenation time for 6,400 FD files



Data	ND files	FD files
# of processes (nodes)	165 (42)	1600 (400)
Timing (sec)	***279.4***	***611.8***
Data size before compression	1 TB	16.9 TB
Output file size	15.1 GB	77.9 GB
Metadata size	57.7 MB	93.8 MB
Raw data size	15.0 GB	77.4 GB

Summary

- Concatenating many small files into one large file is the first step of HEP analysis programs
- Our study explore a variety of HDF5 features and tune them to achieve scalable parallel I/O performance
- The lessons learned from our case study can provide guidance in selecting the appropriate HDF5 settings for scientific applications that exhibit similar I/O characteristics
- Currently under review (2nd round) by Elsevier Parallel Computing

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Q & A