Tuning HDF5 Subfiling Performance on Parallel File Systems

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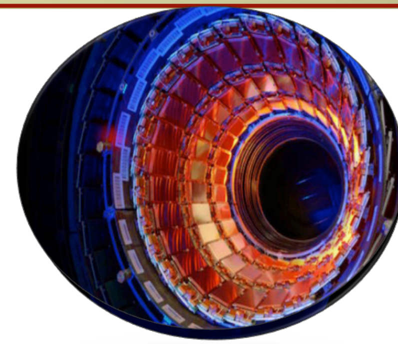
U.S. DEPARTMENT OF ENERGY | Office of Science

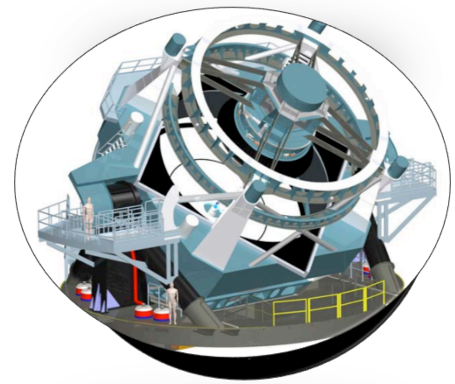
Outline of the talk

- Background to parallel I/O
- HDF5 basics
- HDF5 subfiling implementation
- Evaluation of HDF5 subfiling:
  - Edison to /scratch3 file system
  - Edison to cscratch file system on Cori
  - Cori Haswell to cscratch file system on Cori
  - Cori Haswell to DataWarp Burst Buffer on Cori

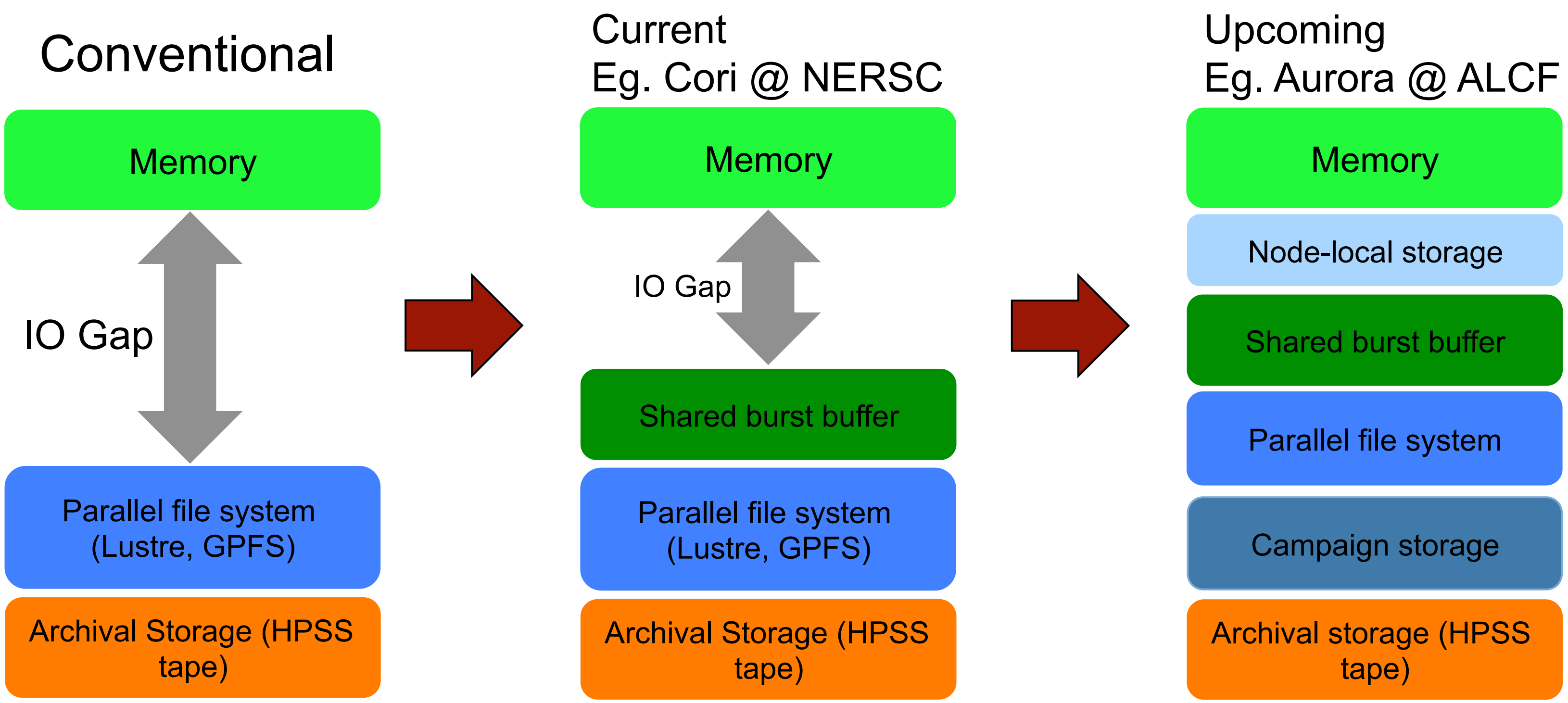
Scientific applications and massive data

- Simulations
  - Multi-physics (FLASH) – 10 PB
  - Cosmology (NyX) – 10 PB
  - Plasma physics (VPIC) – 1 PB
- Experimental and Observational data
  - High energy physics (LHC) – 100 PB
  - Cosmology (LSST) – 60 PB
  - Genomics – 100 TB to 1 PB
- Scientific applications rely on efficient access to data
  - Storage and I/O are critical requirements of HPC



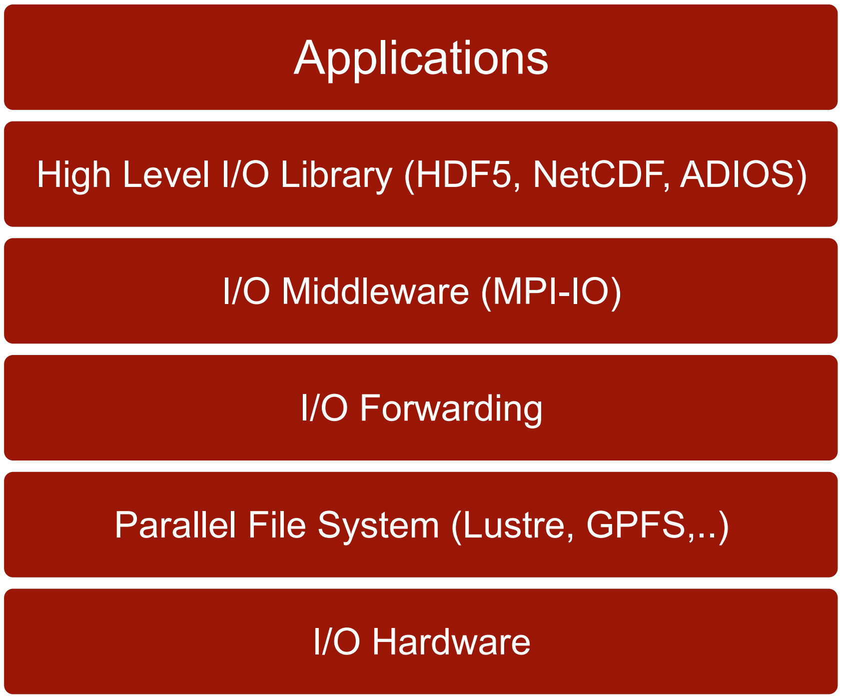


Trends – Storage system transformation



- IO performance gap in HPC storage is a significant bottleneck because of slow disk-based storage
- SSD and new memory technologies are trying to fill the gap, but increase the depth of storage hierarchy

Parallel I/O stack

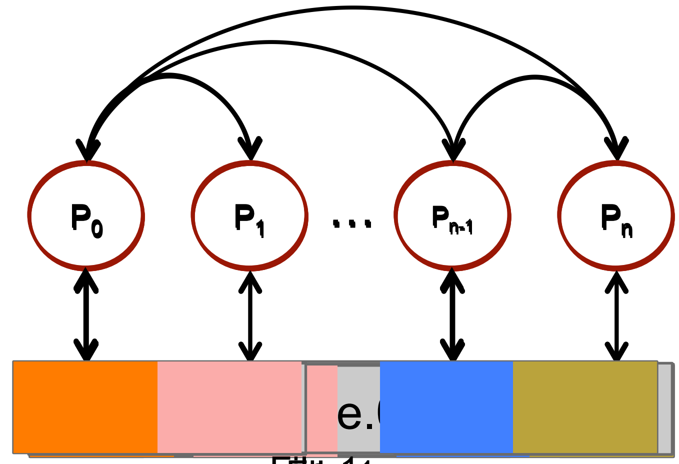


- I/O Libraries
  - **HDF5,** ADIOS, PnetCDF, NetCDF-4
- Middleware
  - POSIX-IO, MPI-IO
  - I/O Forwarding
- File systems:
  - Lustre
  - GPFS
  - Cray DataWarp (for burst buffers)
- I/O Hardware
  - disk-based
  - SSD-based

Parallel I/O – Application view

Types of parallel I/O

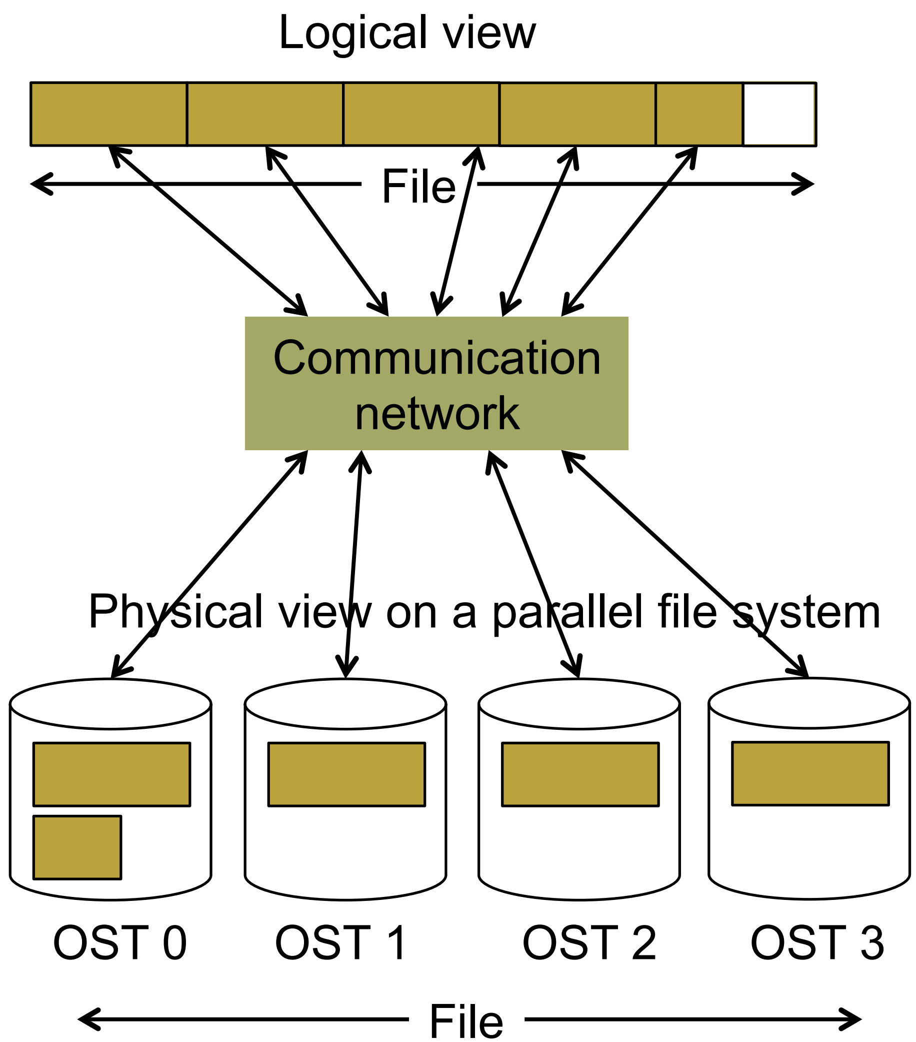
- 1 writer/reader, 1 file
- N writers/readers, N files (File-per-process)
- N writers/readers, 1 file
- M writers/readers, 1 file
  - Aggregators
  - Two-phase I/O
- M aggregators, M files (file-per-aggregator)
  - Variations of this mode



Source: http://www.erdc.hpc.mil/docs/Tips/garnet-lustre-adios.pdf

Parallel I/O – System view

- Parallel file systems
  - Lustre and GPFS
- Typical building blocks of parallel file systems
  - Storage hardware – HDD or SSD RAID
  - Storage servers
  - Metadata servers
  - Client-side processes and interfaces
- Management
  - Stripe files for parallelism
  - Tolerate failures



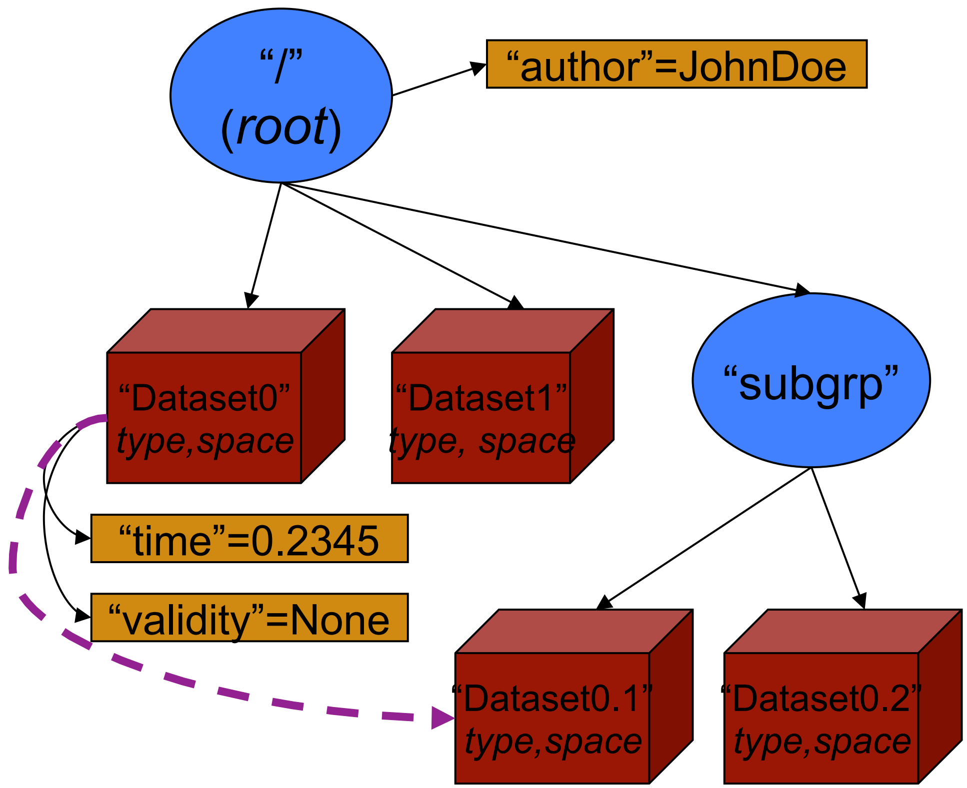
Source: https://www.nersc.gov/users/data-and-file-systems/i-o-resources-for-scientific-applications/
https://fs.hlrs.de/projects/craydoc/docs/books/S-2490-40/html-S-2490-40/chapter-4m6xftd3-oswald-basicsoflustreparallelio.htm

Hierarchical Data Format v5 (HDF5)

HDF5 is a data model, file format, and I/O library

- Groups
  - Arranged in directory hierarchy
  - root group is always '/'
- Datasets
  - Dataspace
  - Datatype
- Attributes
  - Bind to Group & Dataset
- References

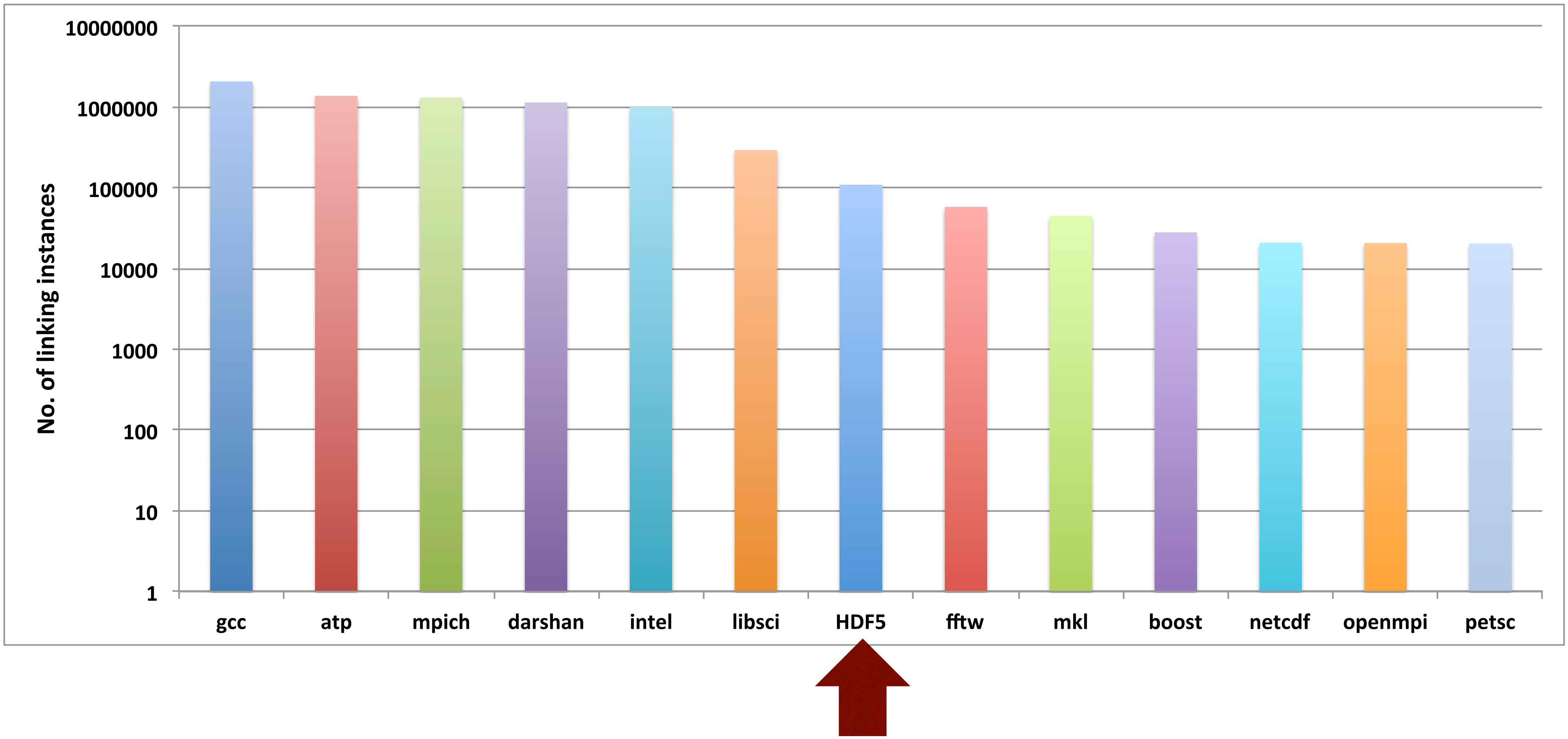
- Flexibility to design and implement data models



Slide courtesy of John Shalf

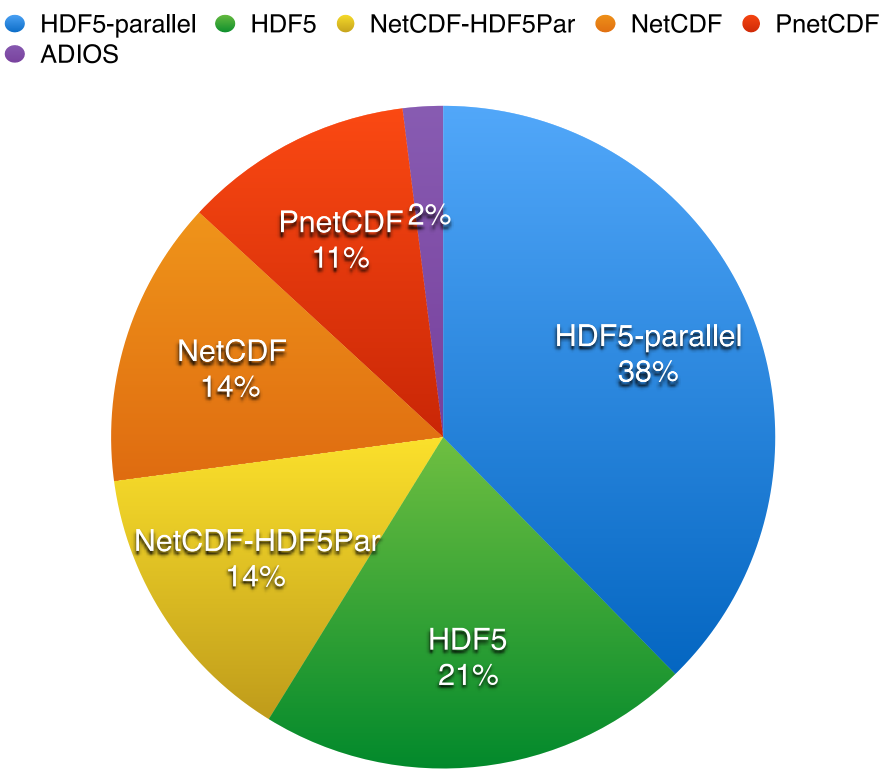
Heavily used at supercomputing centers

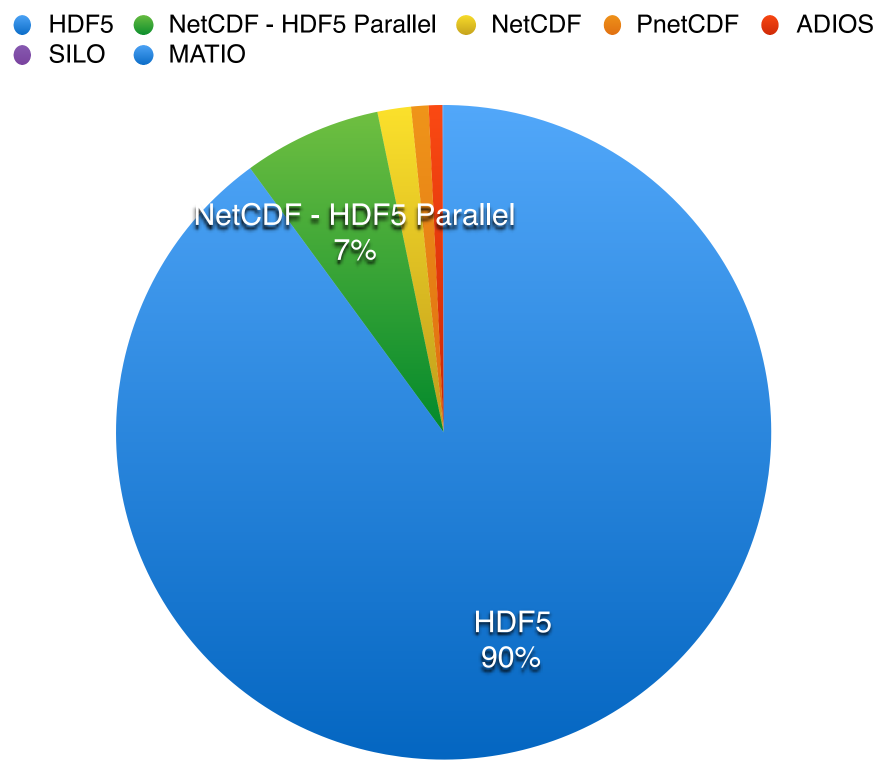
Library usage on Edison, Allocation Year 2015



Collected by Zhengji Zhao, NERSC

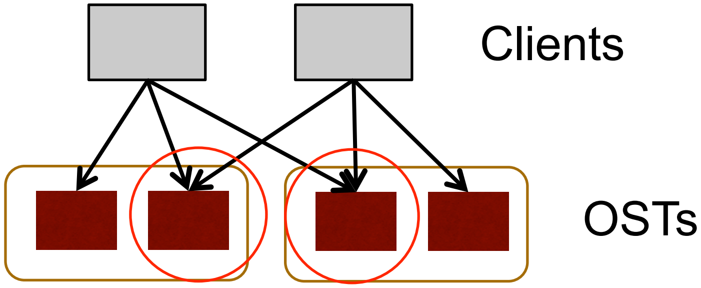
Top self-describing I/O library





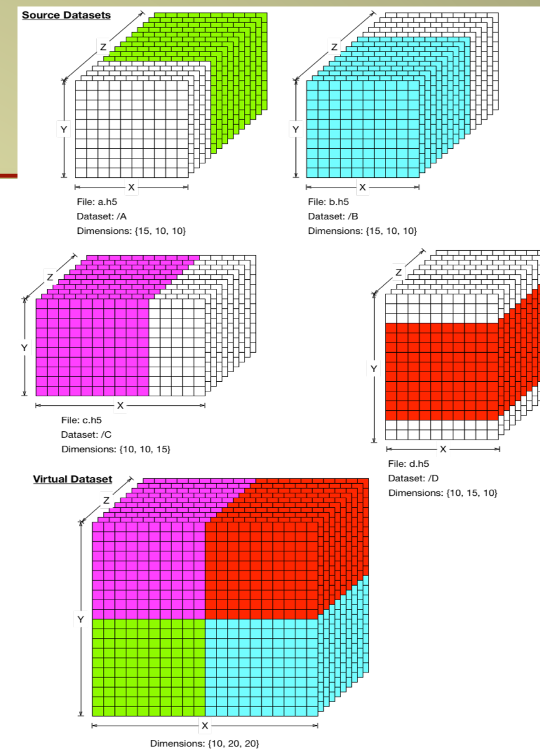
Subfiling

- Writing to single shared file may be slow due to:
  - Locking contention
  - Complications in moving large files
- A solution: Subfiling
  - Multiple small files
  - A metadata file stitching the small files together



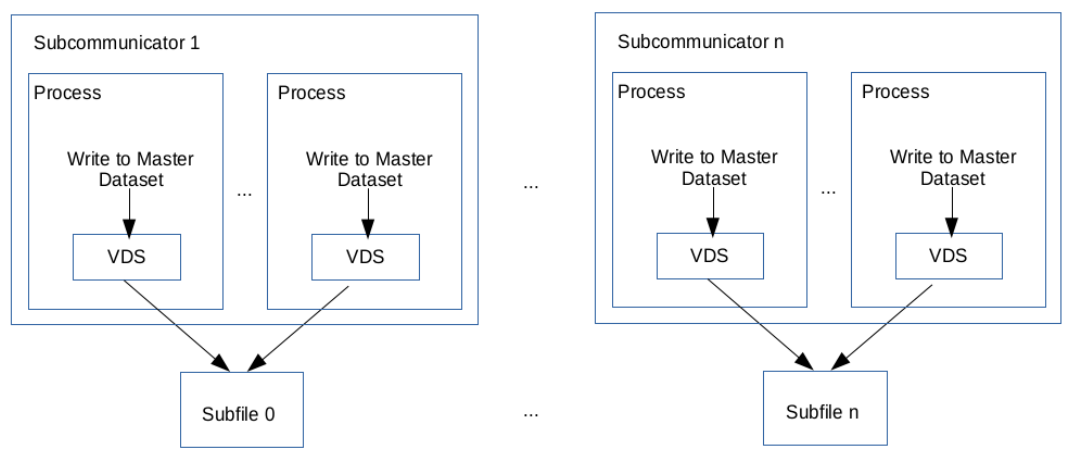
- Benefits
  - Better use of parallel I/O subsystem
  - Reduced locking and contention issues improve performance
- Related work
  - File system: PLFS
  - I/O middleware: PnetCDF, ADIOS
  - Application libraries: BoxLib

Subfiling in HDF5



- Virtual Datasets
  - Introduced in HDF5 1.10.0
  - Allows for pieces of a dataset to be stored in separate files, but would be viewed as a single dataset from a master file

- Creating subfiles
  - Split the MPI_COMM_WORLD communicator into multiple subcommunicators
  - One subfile per subcommunicator



Using HDF5 subfiling

- Split the MPI_COMM_WORLD communicator into multiple subcommunicators

```
int color = mpi_rank % subfile;
if (n_nodes > subfile)
color = (mpi_rank % n_nodes) % subfile;
MPI_Comm_split (..., &subfile_comm);
```

- Writing subfiles

```
sprintf (subfile_name, "Subfile_%d.h5", mpi_rank);
H5Pset_subfiling_access (fapl_id, subfile_name, MPI_COMM_SELF, MPI_INFO_NULL);
fid = H5Fcreate (filename, ..., fapl_id);
H5Sselect_hyperslab (sid, H5S_SELECT_SET, start, stride, count, block);
dapl_id = H5Pcreate (H5P_DATASET_ACCESS);
H5Pset_subfiling_selection(dapl_id, sid);
did = H5Dcreate (fid, DATASET, ..., sid, ..., dapl_id);
H5Dwrite (did, H5T_NATIVE_INT, mem_sid, sid, H5P_DEFAULT, wbuf);
```

Using HDF5 subfiling

- Split the MPI_COMM_WORLD communicator into multiple subcommunicators

```
int color = mpi_rank % subfile;
if (n_nodes > subfile)
color = (mpi_rank % n_nodes) % subfile;
MPI_Comm_split (..., &subfile_comm);
```

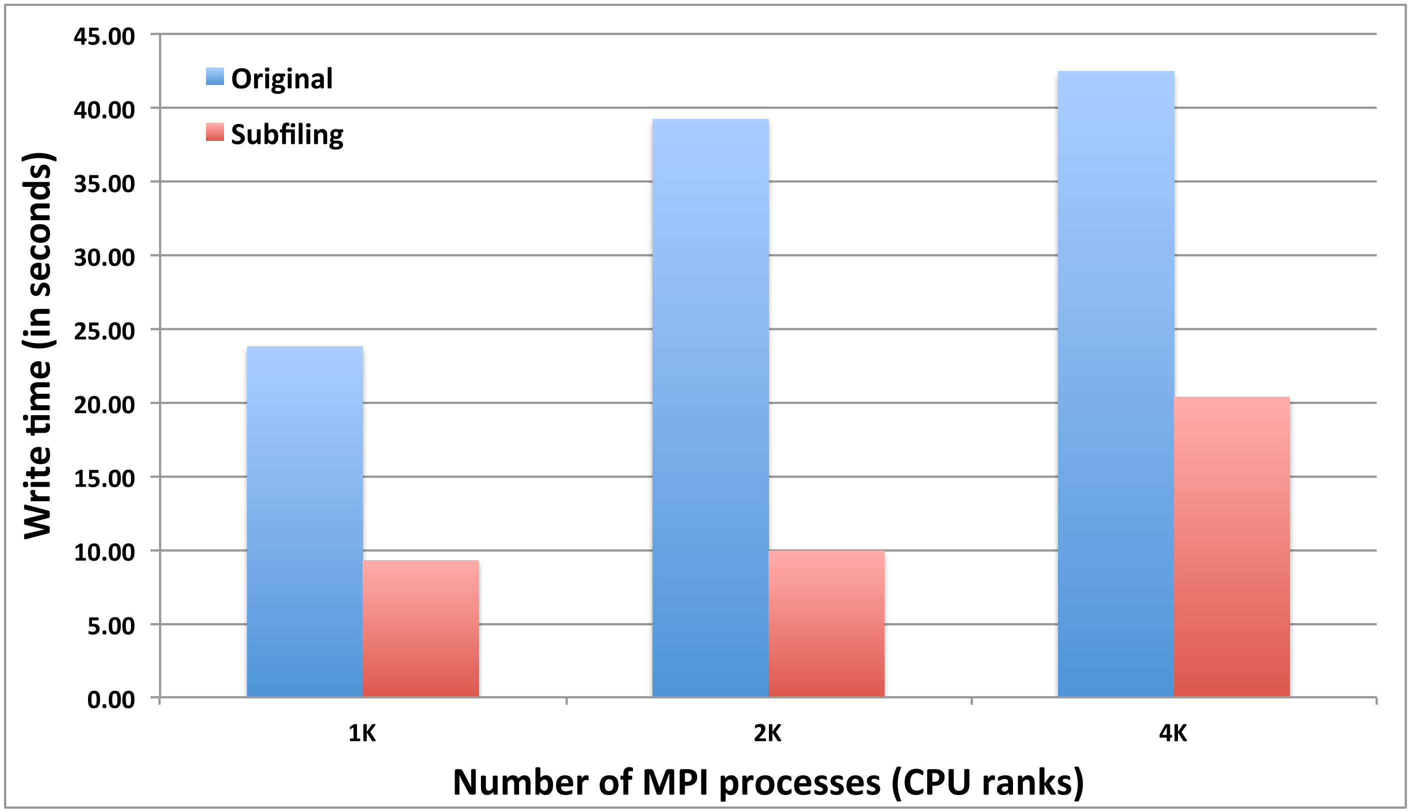
- Reading subfiles

```
sprintf (subfile_name, "Subfile_%d.h5", mpi_rank);
H5Pset_subfiling_access (fapl_id, subfile_name, MPI_COMM_SELF,
MPI_INFO_NULL);
H5Sselect_hyperslab (sid, H5S_SELECT_SET, start, stride, count, block);
H5Dread (did, H5T_NATIVE_INT, mem_sid, sid, H5P_DEFAULT, rbuf);
```

Experimental setup

- Systems
  - Cori
    - Haswell partition → 2388 nodes, 32-core Intel Xeon E5-2698 CPUs
    - File systems: cscratch (Lustre, 248 OSS, 248 OSTs), SSD-based burst buffer
  - Edison
    - 5586 compute nodes, 24-core Ivy Bridge processors
    - File system: scratch3 (Lustre, 36 OSTs), cscratch (Lustre, 248 OSS, 248 OSTs)
- Benchmarks
  - VPIC-IO
    - I/O kernel from a plasma physics simulation
    - 8 million particles per MPI process, 8 variables per particle
  - BD-CATS-IO
    - I/O kernel from Big Data Clustering application to run DBSCAN
    - Reads VPIC-IO data
- IO Measurements
  - IO time and IO rate
  - Each job was run at least three times

Scalability tests – Edison scratch3 – IO time

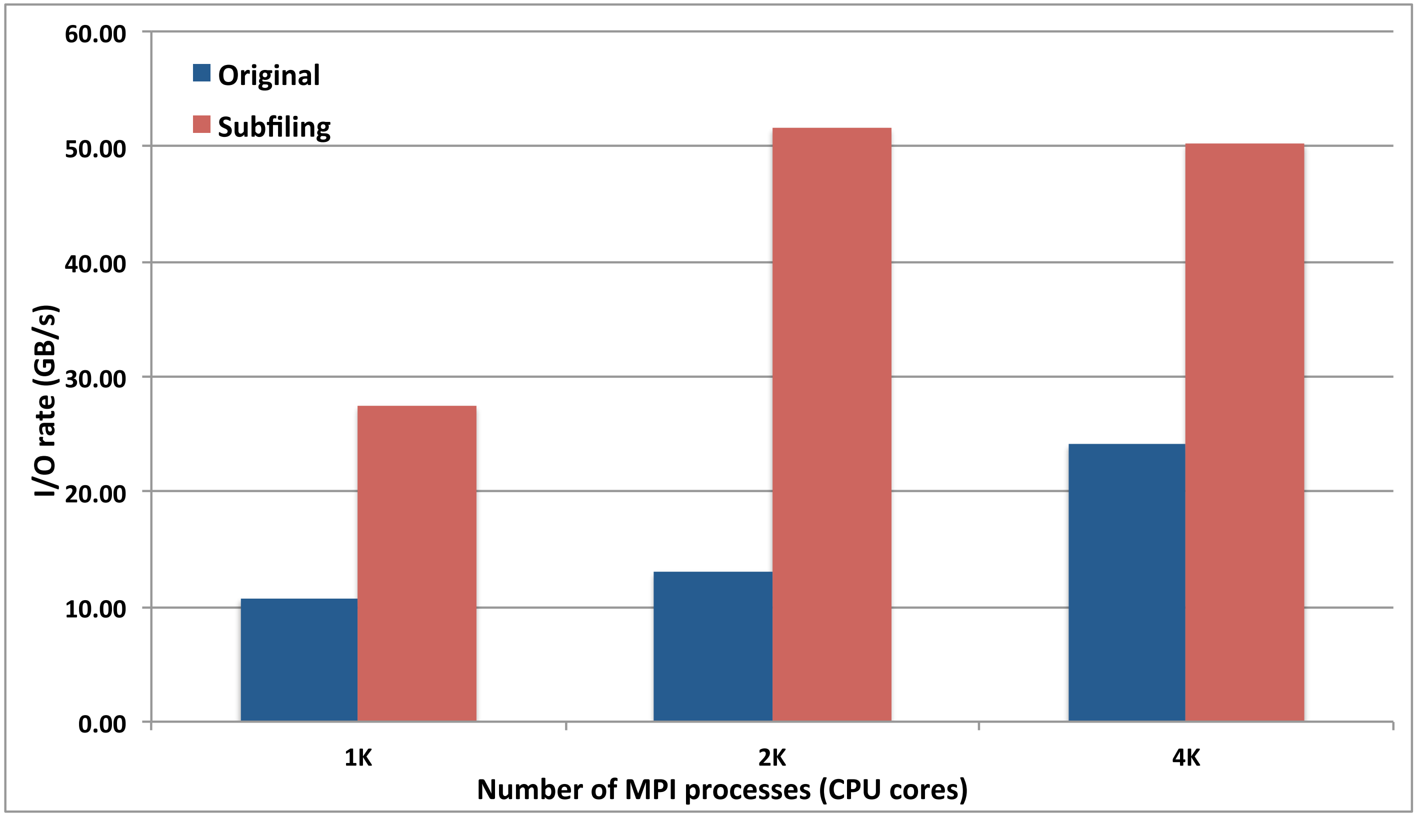


Configuration

- /scratch3 Lustre file system on Edison
- 36 OST, 32MB stripe size
- 72 GB/s peak BW
- Subfiling factor: 32
- # of subfiles:
  - 1K → 32
  - 2K → 64
  - 4K → 128

- Subfiling is 4X better at 2K and 2X better at 4K

Scalability tests – Edison scratch3 – IO rate



Configuration

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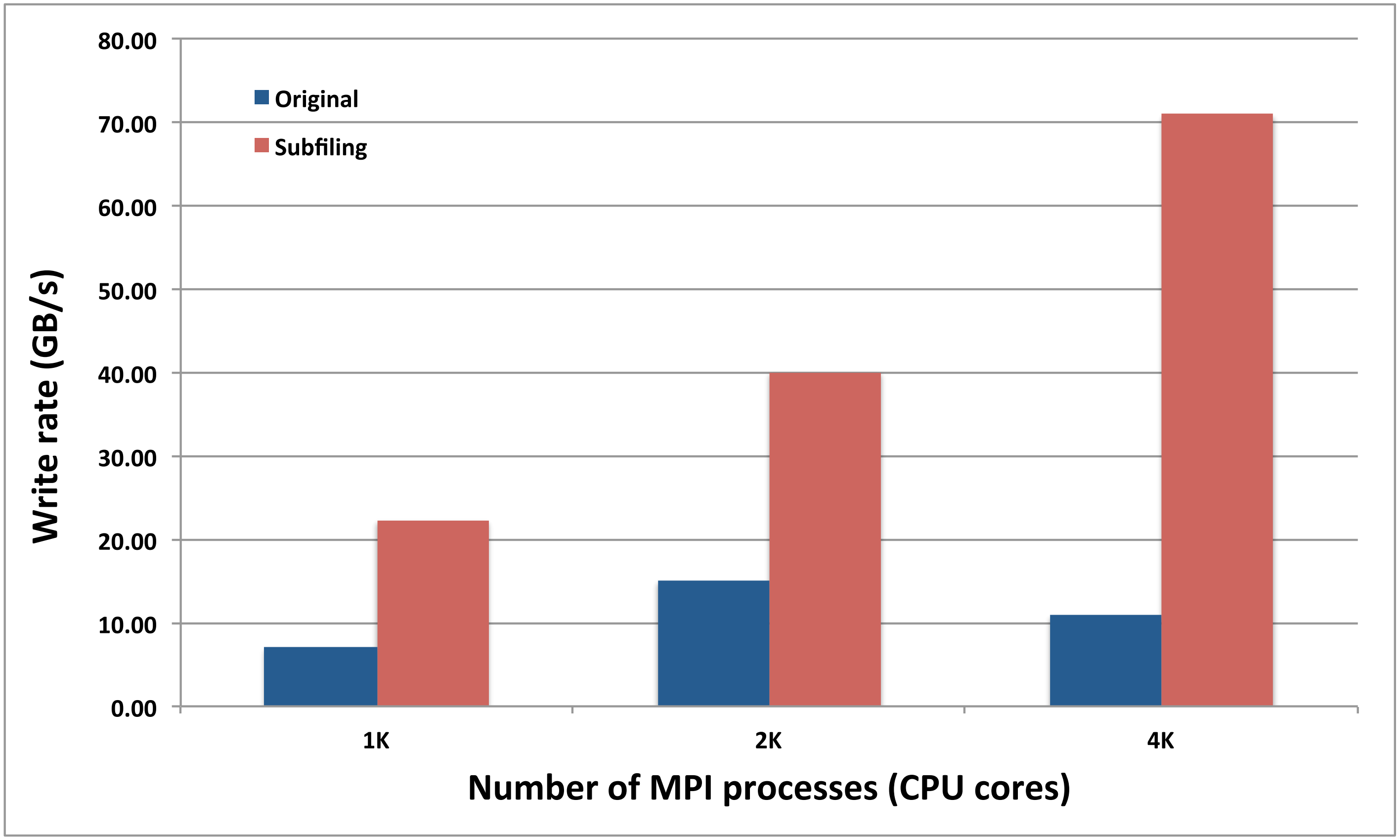
- 36 OST, 32MB stripe size
- 72 GB/s peak BW
- Subfiling factor: 32
- # of subfiles:
  - 1K → 32
  - 2K → 64
  - 4K → 128

- 67% of the peak bandwidth with subfiling

Scalability tests – cscratch from Edison

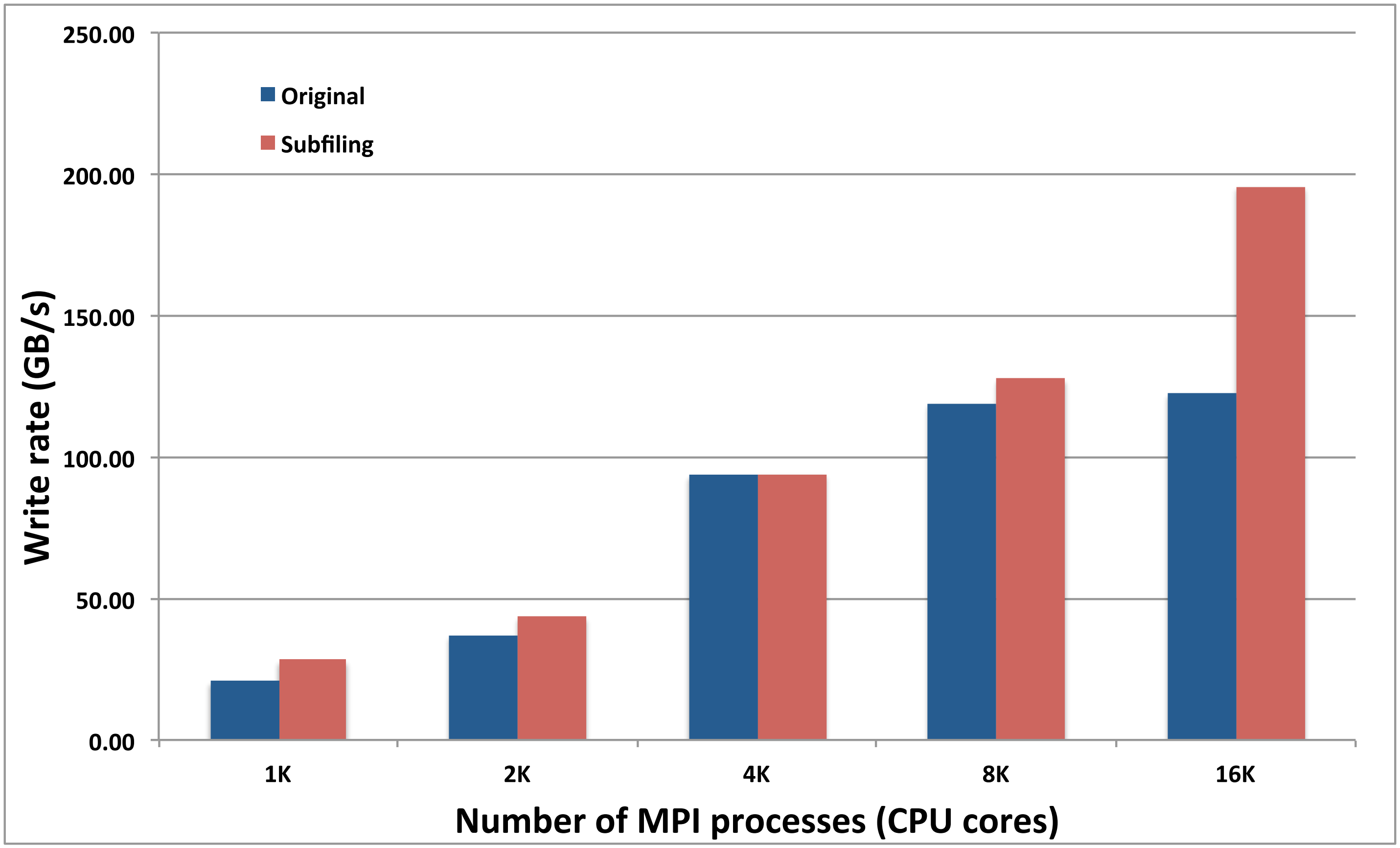


Configuration

- cscratch Lustre file system on Cori
- 128 OSTs out of 248, 32MB stripe size
- >700 GB/s peak BW
- Subfiling factor: 32
- # of subfiles:
  - 1K → 32
  - 2K → 64
  - 4K → 128

- Up to 6.5X better performance @ 4K cores

Scalability tests – cscratch from Cori

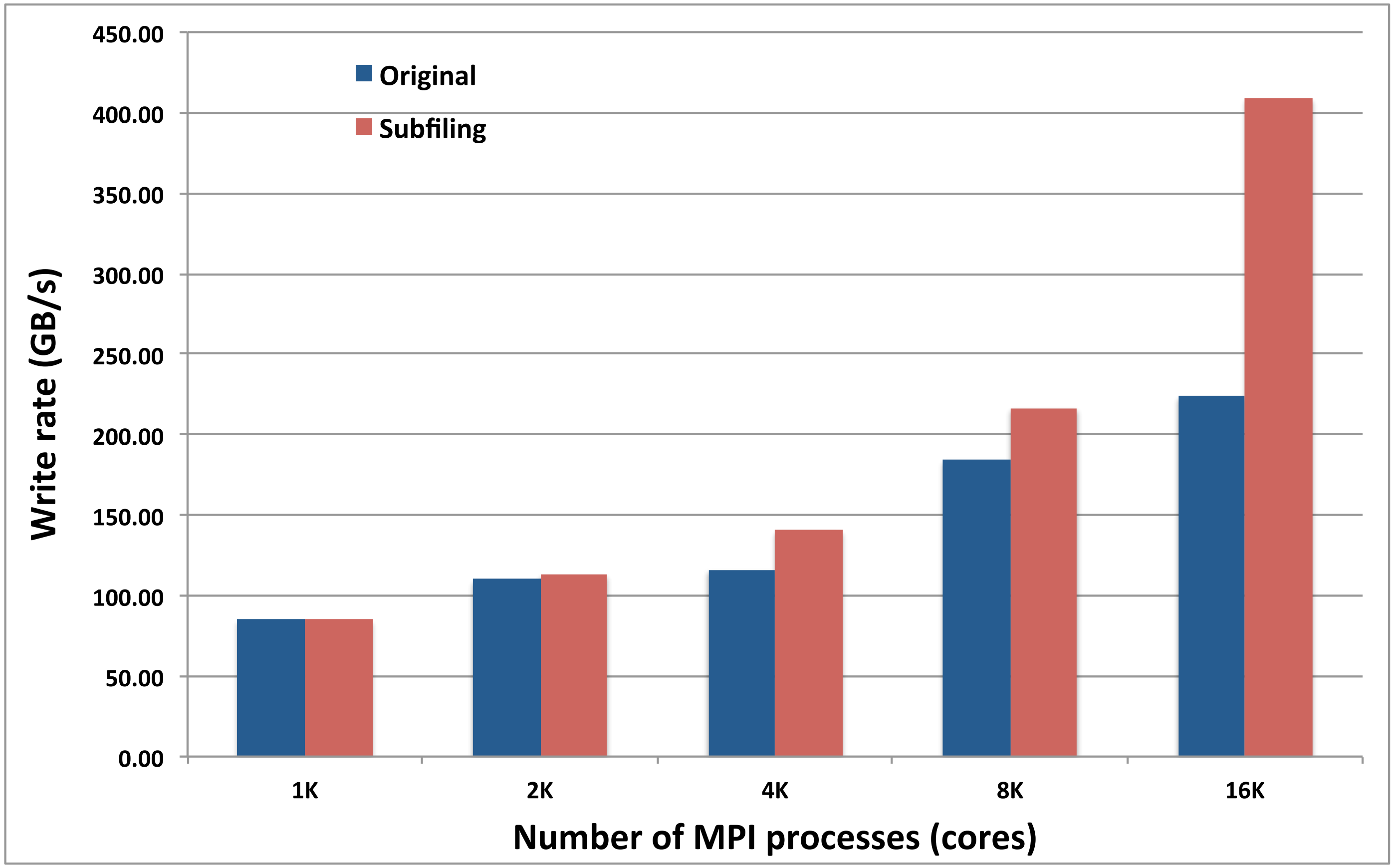


Configuration

- cscratch Lustre file system on Cori
- 128 OSTs out of 248, 32MB stripe size
- >700 GB/s peak BW
- Subfiling factor: 32
- # of subfiles:
  - 1K → 32
  - 2K → 64
  - 4K → 128
  - 8K → 256
  - 16K → 256 (subfiling factor 64)

- Up to 60% better performance @ 16K cores
- 195 GB/s IO rate at 16K processes

Scalability tests – Burst buffer from Cori

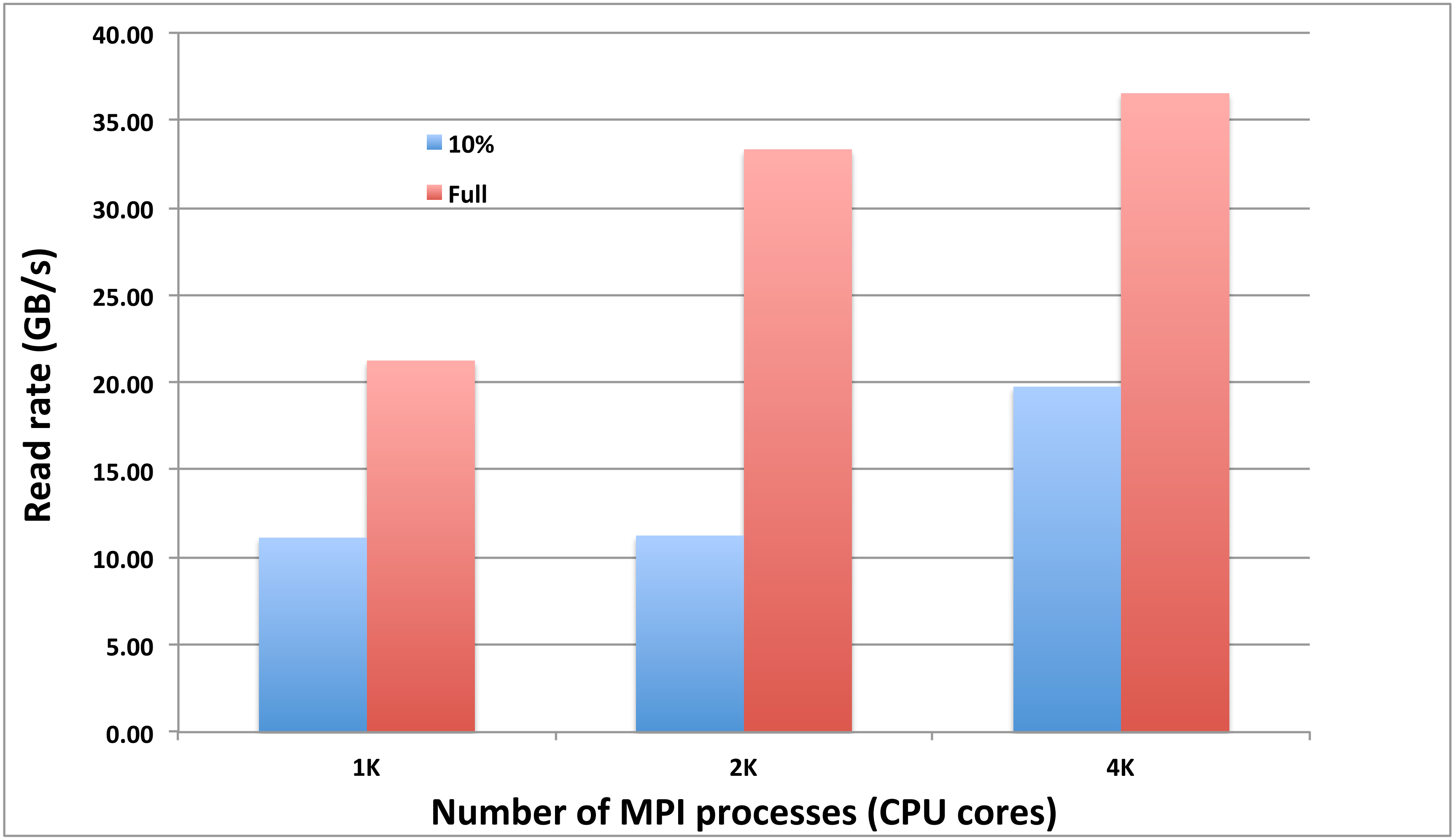


Configuration

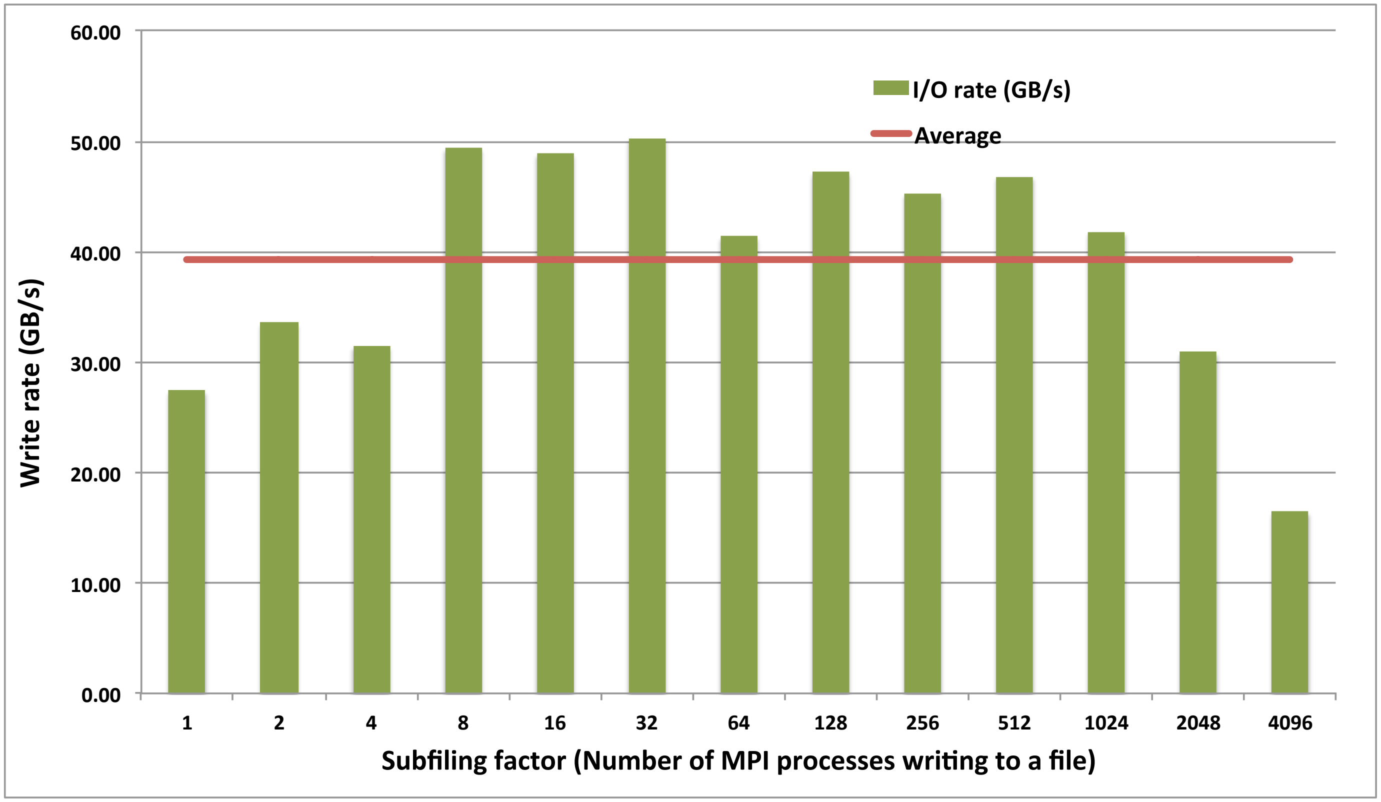
- Burst Buffer on Cori
- 1.8 TB/s peak BW
- Subfiling factor: 32
- # of subfiles:
  - 1K → 32
  - 2K → 64
  - 4K → 128
  - 8K → 256
  - 16K → 256 (subfiling factor 64)

- Up to 80% better performance @ 16K cores
- 410 GB/s IO rate at 16K processes

Reading HDF5 subfile data – cscratch from Edison



Tuning subfiling factor – Edison scratch3

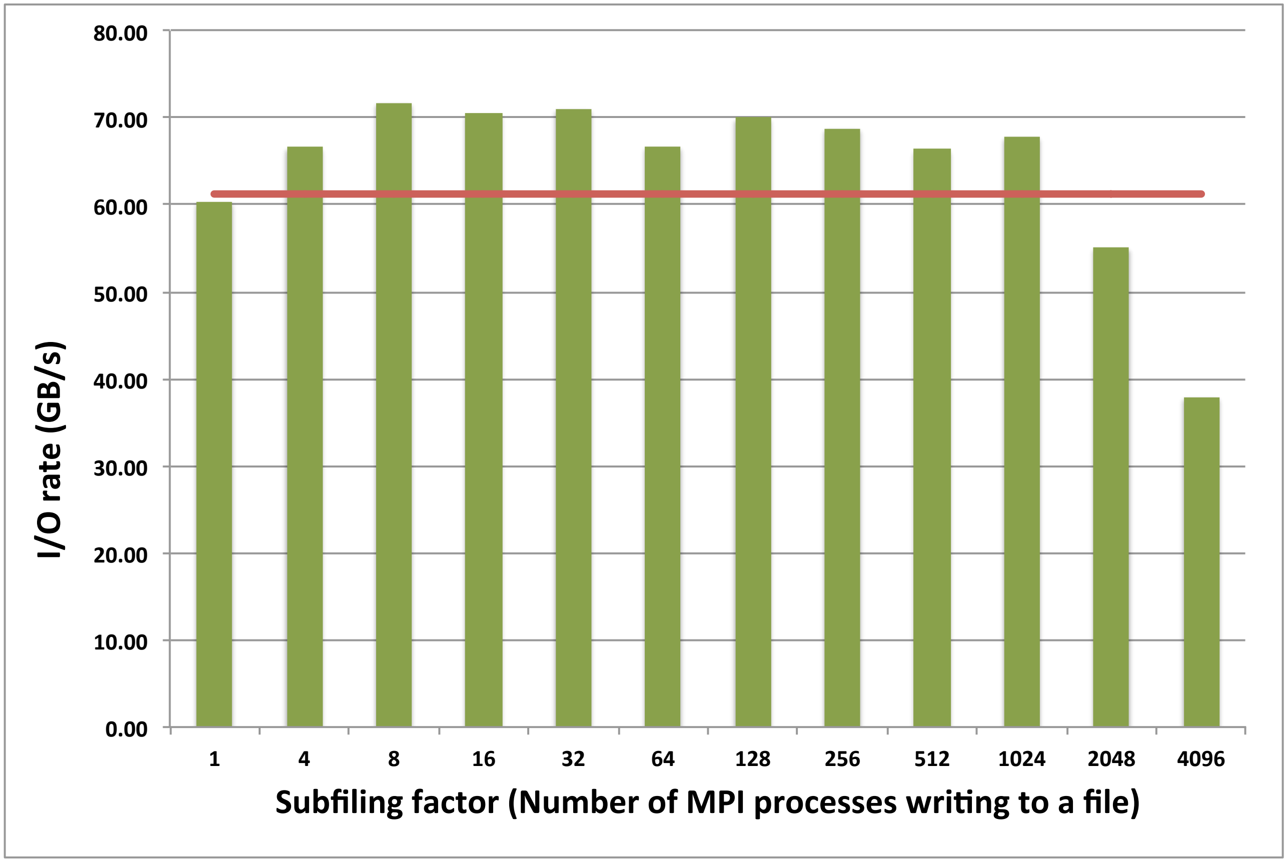


Configuration

- /scratch3 Lustre file system on Edison
- 36 OSTs, 32MB stripe size
- 72 GB/s peak BW
- 4K cores
- 1TB data
- Varied the number of subfiles

- Subfiling factors of 8 to 32 resulted in good performance
- Subfiling factor of 64 resulted in poor performance consistently; but 128 to 1024 was above average

Tuning subfiling factor – cscratch from Edison



Configuration

- cscratch Lustre file system on Cori
- 128 OSTs, 32MB stripe size
- >700 GB/s peak BW
- 4K cores
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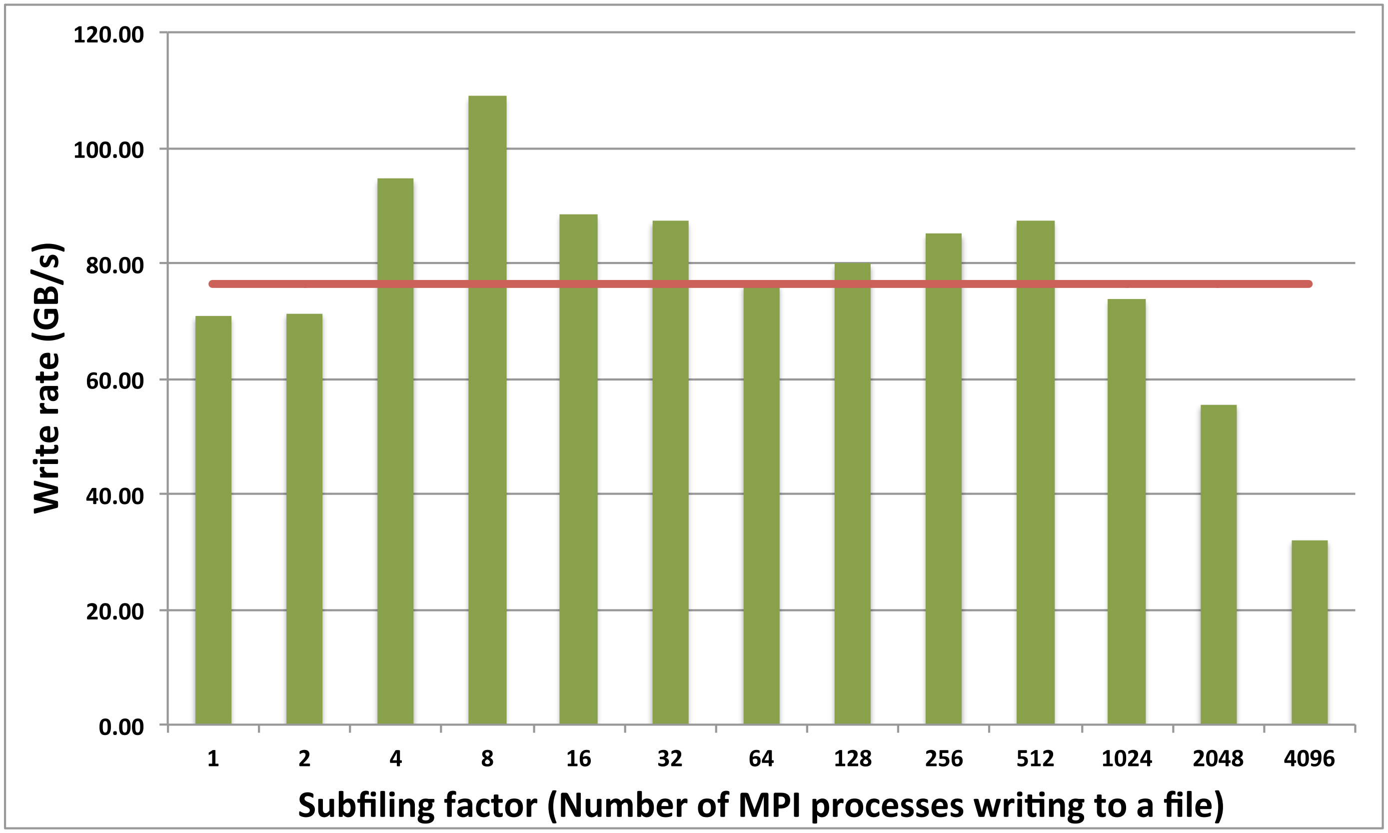
Tuning subfiling factor – cscratch from Cori

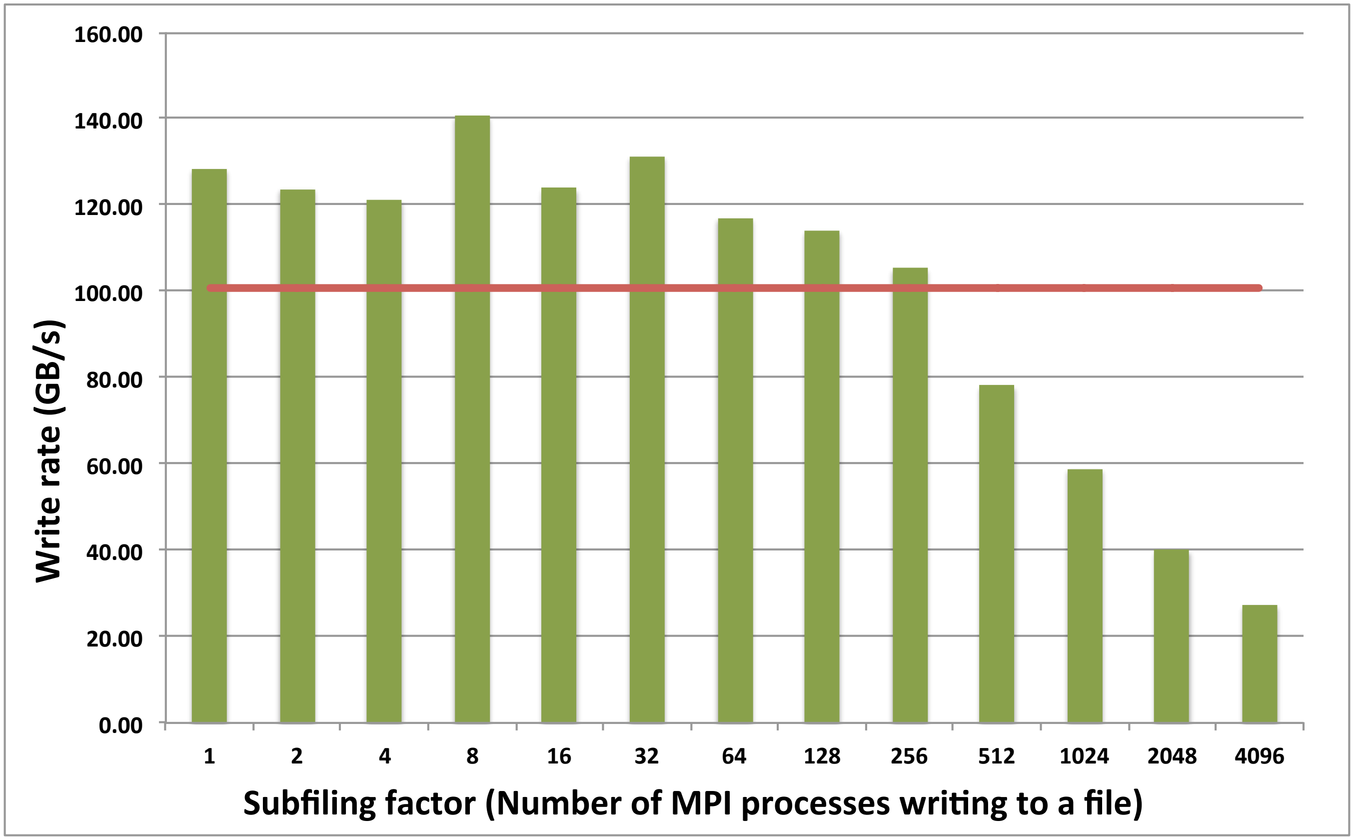


Configuration

- cscratch Lustre file system on Cori
- 128 OSTs, 32MB stripe size
- >700 GB/s peak BW
- 4K cores
- 1TB data
- Varied the number of subfiles

- Subfiling factors of 4 and 8 resulted in good performance
- Subfiling factors between 16 to 512 showed above average I/O rates

Tuning subfiling factor – Burst buffer on Cori

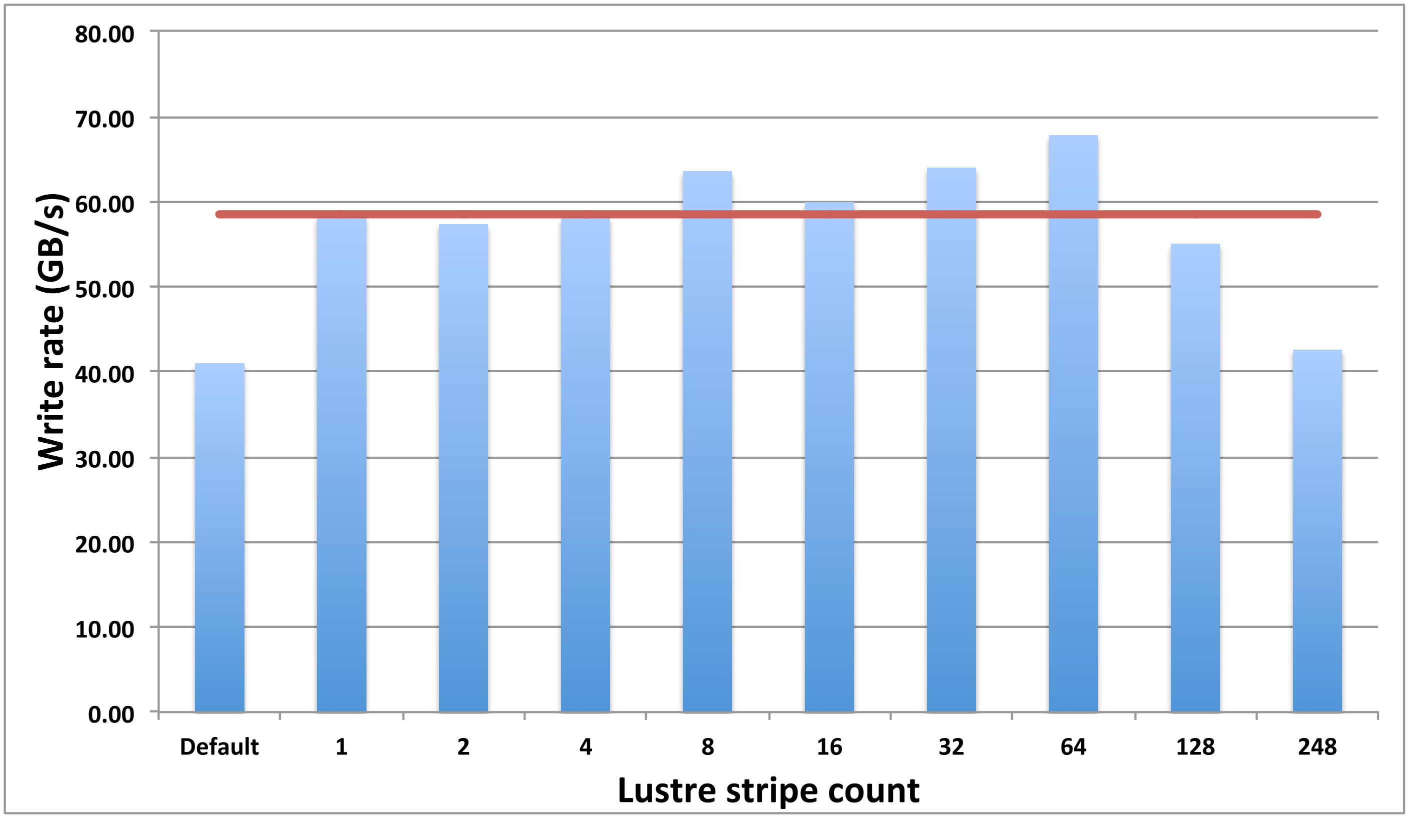


Configuration

- Burst buffer on Cori
- 1.8 TB/s peak BW
- 4K cores
- 1TB data
- Varied the number of subfiles

- Subfiling factors of 1 to 32 resulted in good performance
- Performance degraded with subfiling factors beyond 32 and beyond

Tuning Lustre striping – cscratch from Edison

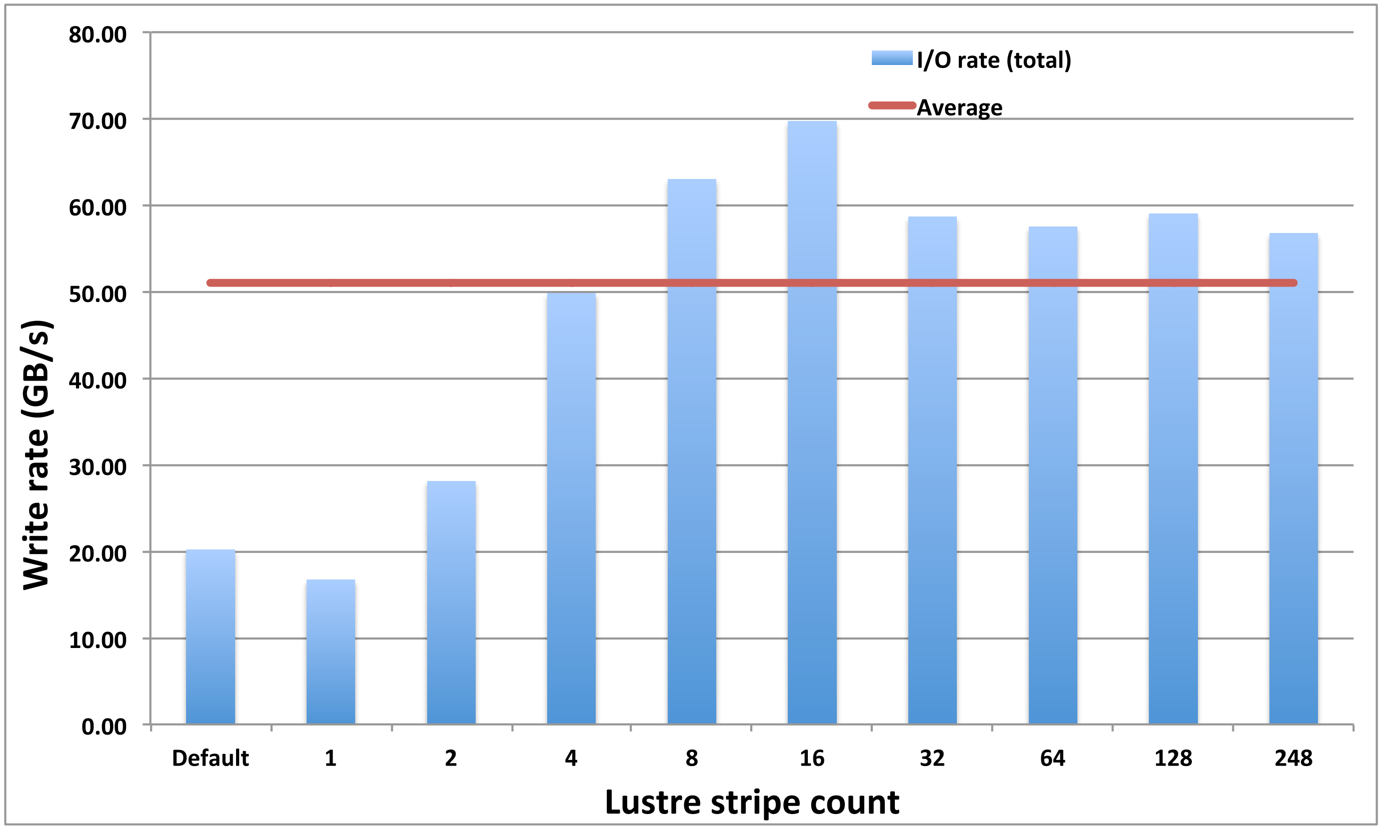


Configuration

- cscratch Lustre file system on Cori
- >700 GB/s peak BW
- 4K cores
- 1TB data
- Subfiling factor of 128
- Varied the number of OSTs
- Stripe size: 32MB
- Default: 1 OST, 1 MB stripe size

- Using 8 to 64 stripes resulted in more than average performance
- 70% better performance than default stripe settings

Tuning Lustre striping – cscratch from Cori – 4K

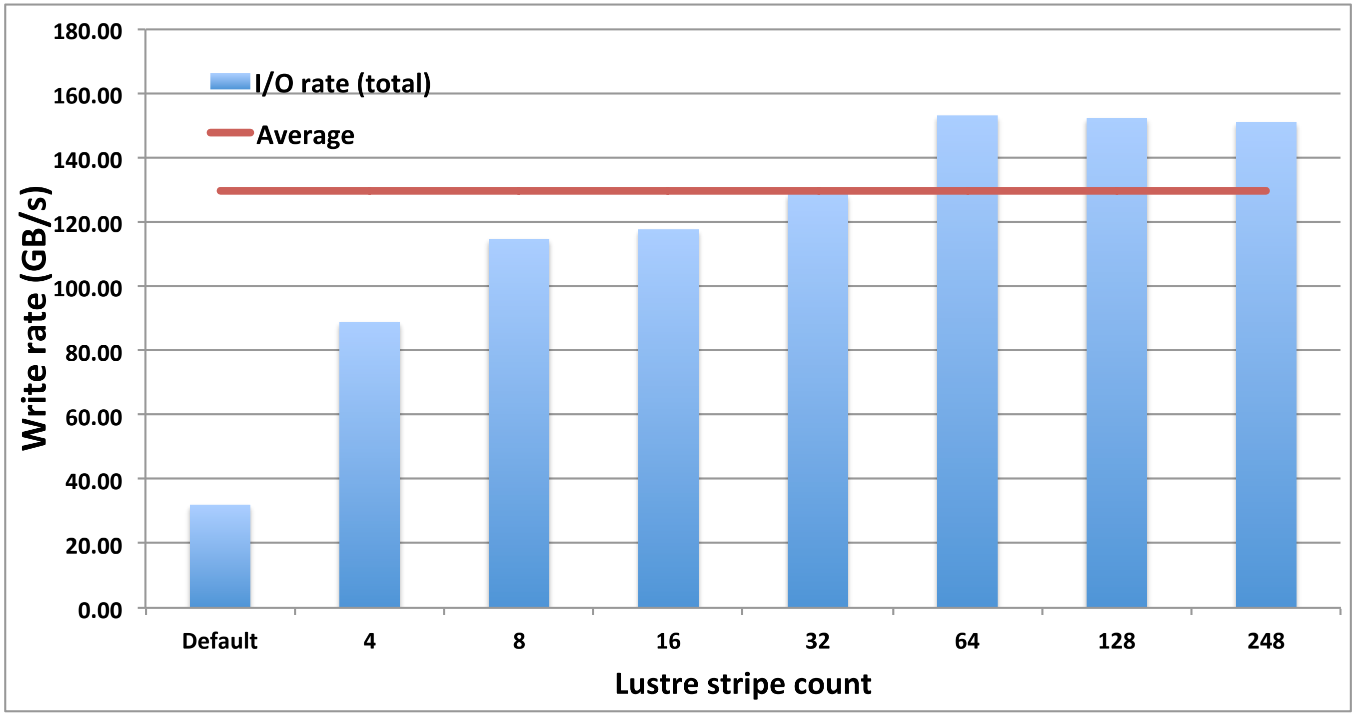


Configuration

- cscratch Lustre file system on Cori
- >700 GB/s peak BW
- 4K cores
- 1TB data
- Subfiling factor of 128
- Varied the number of OSTs
- Stripe size: 32MB
- Default: 1 OST, 1 MB stripe size

- Using 8 to 248 stripes resulted in good I/O performance
- 3.5X faster performance than default stripe settings @ 16 OSTs

Tuning Lustre striping – cscratch from Cori – 16K



Configuration

- cscratch Lustre file system on Cori
- >700 GB/s peak BW
- 16K cores
- 1TB data
- Subfiling factor of 64
- Varied the number of OSTs
- Stripe size: 32MB
- Default: 1 OST, 1 MB stripe size

- Using 64 stripes resulted in the best performance
- 4.8X faster performance than default stripe settings @ 64 OSTs

Conclusions

- Recommendations for obtaining good I/O rate
  - Subfiling factor of 8 to 64 is reasonable
  - Striping 16 at smaller scales, and 64 at larger scales
- Limitations
  - Using subfiling at 32K MPI processes failed
  - Failure observed for region sizes > 2GB (probably an MPI limitation)
  - Number of readers have to be equal to the number of writers
- Subfiling is showing better performance than writing to a single shared file
  - Up to 6.5X performance advantage
- Reading with an arbitrary number of MPI processes, without matching the number of readers will be useful

Thanks!

Advanced Scientific Computing Research (ASCR) for funding the ExaHDF5 project
Program Manager: Dr. Lucy Nowell