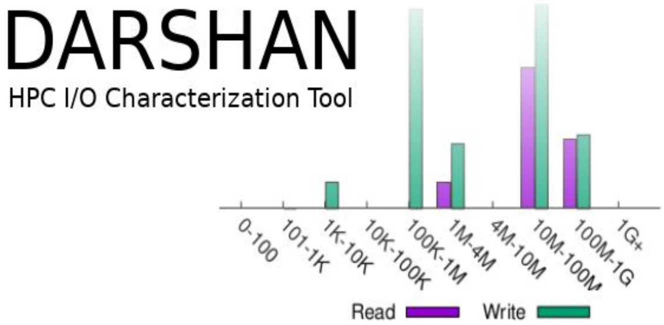
February 1, 2023

Enabling Insights Into HPC Application I/O Behavior With Darshan



Shane Snyder
ssnyder@mcs.anl.gov
Argonne National Laboratory

HSF Software Developer Tools and Packaging Working Group Meeting

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Understanding and improving HPC I/O

- The ability to characterize and understand application I/O workloads is critical to ensuring efficient use of an evolving and increasingly complex HPC I/O stack
  - Deep layers of coordinating I/O libraries and entirely new-to-HPC storage paradigms (e.g., object storage)
  - Emerging storage hardware (e.g., PMEM) and storage architectures (e.g., burst buffers)

- I/O analysis tools are invaluable in helping to navigate this complexity and to better understand I/O
  - Characterize I/O behavior of individual jobs to inform tuning decisions
  - Characterize job populations to better understand system-wide I/O stack usage and optimize deployments

Darshan: A tool for HPC I/O understanding

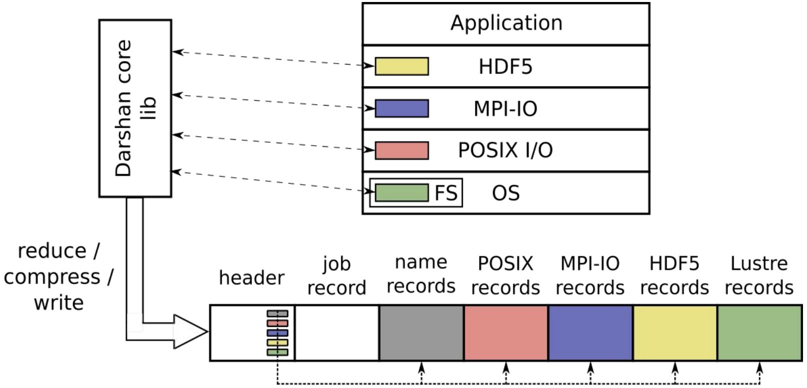
What is Darshan?

- Darshan is a lightweight I/O characterization tool that captures concise views of HPC application I/O behavior
  - Produces a summary of I/O activity for each instrumented job
    - Counters, histograms, timers, & statistics
    - If requested by user, full I/O traces

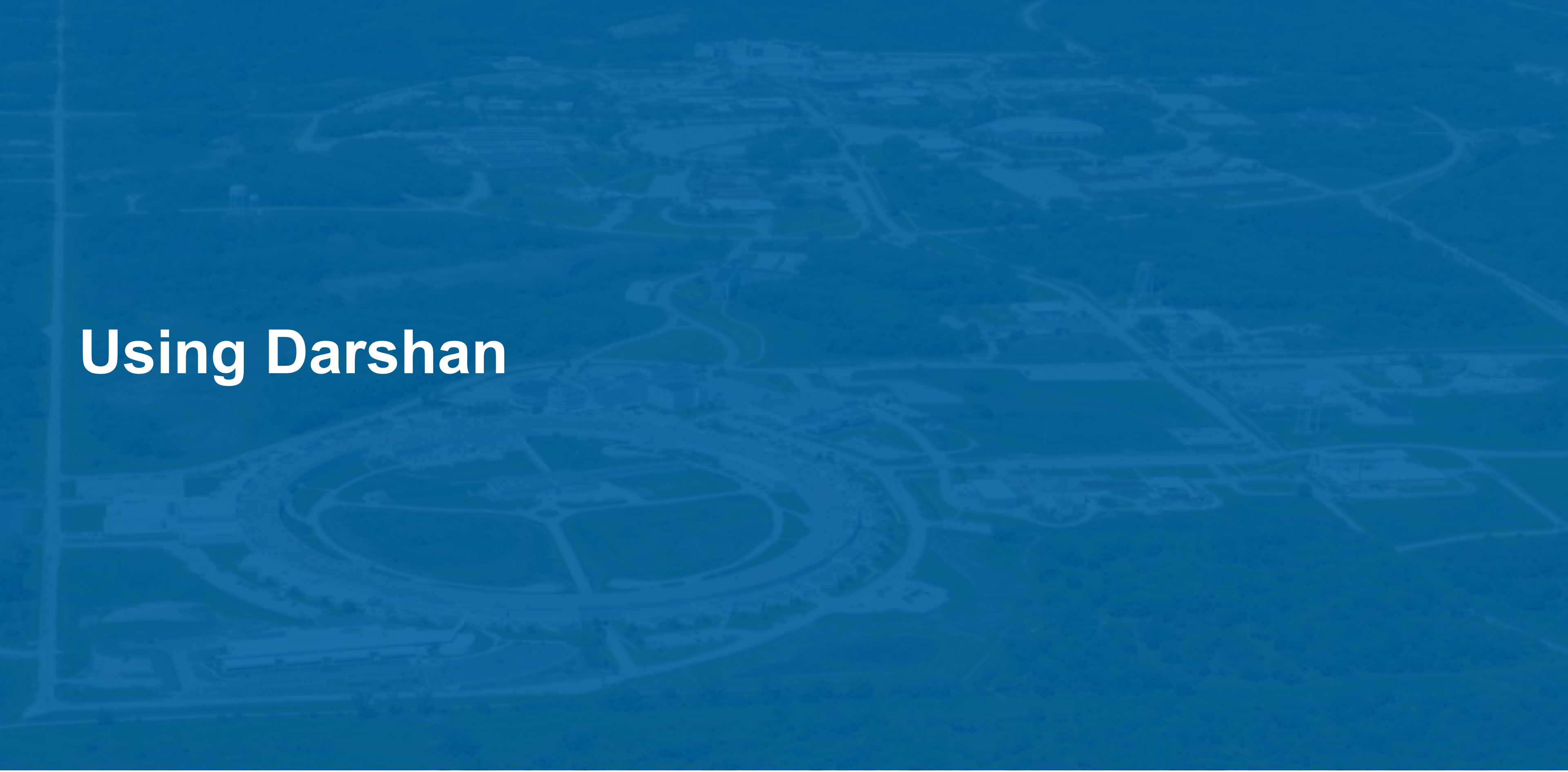
- Widely available
  - Deployed (and commonly enabled by default) at many HPC facilities around the world
- Easy to use
  - No code changes required to integrate Darshan instrumentation
  - Negligible performance impact; just “leave it on”
- Modular
  - Adding instrumentation for new I/O interfaces or storage components is straightforward

How does Darshan work?

- ❖ Darshan records file access statistics for each process as app executes
- ❖ At app shutdown, collect, aggregate, compress, and write log data
- ❖ After job completes, analyze Darshan log data
  - ➢ `darshan-job-summary` - provides a summary PDF characterizing application I/O behavior
  - ➢ `darshan-parser` - provides complete text-format dump of all counters in a log file
  - ➢ *`PyDarshan`* - Python analysis module for Darshan logs



- ❖ Originally designed for MPI applications, but in recent Darshan versions (3.2+) any dynamically-linked executable can be instrumented
  - ➢ In MPI mode, a log is generated for each *app*
  - ➢ In non-MPI mode, a log is generated for every *process*

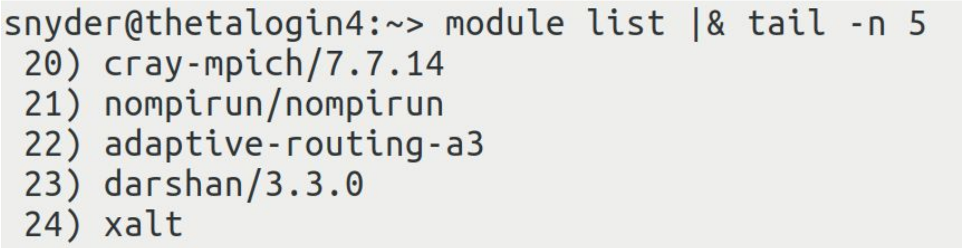


Using Darshan

Instrumenting apps with Darshan

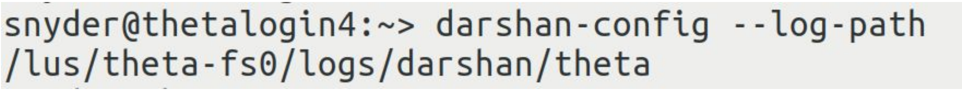
Traditional usage on HPC platforms

- On many HPC platforms (e.g., ALCF Theta, NERSC Cori & Perlmutter, OLCF Summit), Darshan is already installed and enabled by default
  - **Just compile and run your apps like normal**
  - Logs are written to a central repository for all users when the app terminates



```
snyder@thetalogin4:~> module list |& tail -n 5
 20) cray-mpich/7.7.14
 21) nompirun/nompirun
 22) adaptive-routing-a3
 23) darshan/3.3.0
 24) xalt
```

Darshan 3.3.0 is enabled by default on ALCF Theta



```
snyder@thetalogin4:~> darshan-config --log-path
/lus/theta-fs0/logs/darshan/theta
```

‘`darshan-config --log-path`’ command can be used to find output log directory. Directory is further organized into year/month/day subdirectories.

Log file name includes username, app name, and job ID for easy identification, e.g.: snyder_ior_id12345…

Instrumenting apps with Darshan

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Important caveats related to non-MPI usage:

- Requires dynamically-linked executables
- Non-MPI mode must be explicitly enabled via env variable
  - `export DARSHAN_ENABLE_NONMPI=1`
- Some systems may have dated Darshan versions that don't properly support non-MPI mode

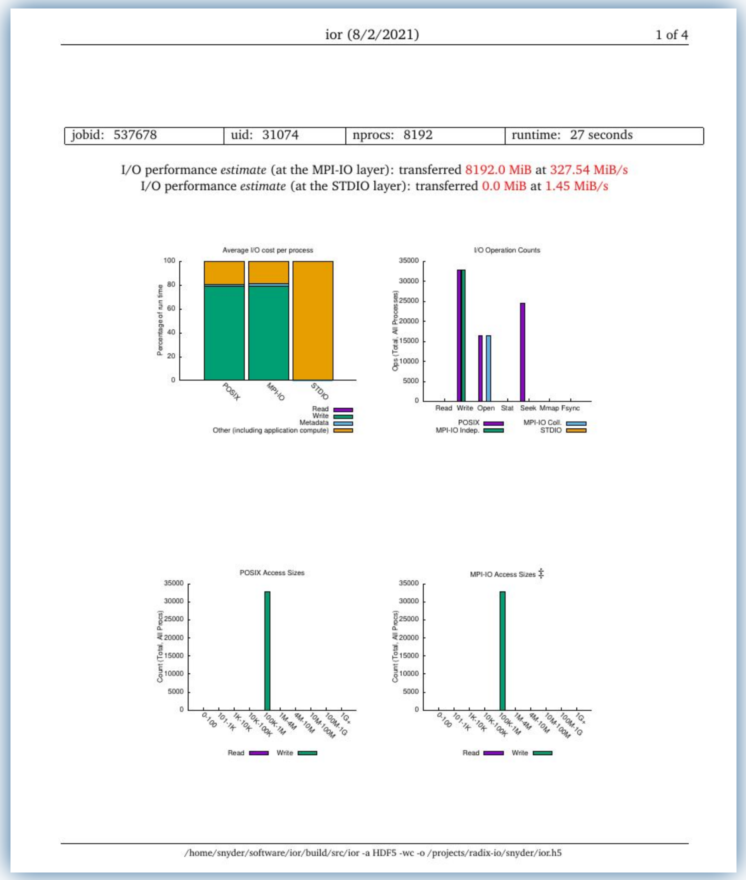
Instrumenting apps with Darshan

Installing and using your own Darshan tools

- In some circumstances, it may be necessary to roll your own install
  - Darshan not installed or lacking necessary features
  - Need to build Darshan in specific software environments (e.g., containers with old compilers)
- Beyond installing from source, Darshan is also available on Spack
  - *darshan-runtime*: runtime instrumentation library linked with application
  - *darshan-util*: log analysis utilities
  - E.g., “**`spack install darshan-runtime`**”
- Once installed, users can `LD_PRELOAD` the darshan-runtime library
  - Output logs are written to directory pointed to by `DARSHAN_LOG_DIR_PATH` environment variable (defaults to `$HOME`)

Analyzing Darshan logs

- ❖ After locating your log, the `darshan-job-summary` script is a useful starting point for visualizing application I/O behavior:
  - ➢ "**`darshan-job-summary.pl <input_log>`**" produces a PDF with same name as input log
  - ➢ Contains useful graphs, tables, and performance estimates describing application I/O behavior



ior (8/2/2021) 1 of 4

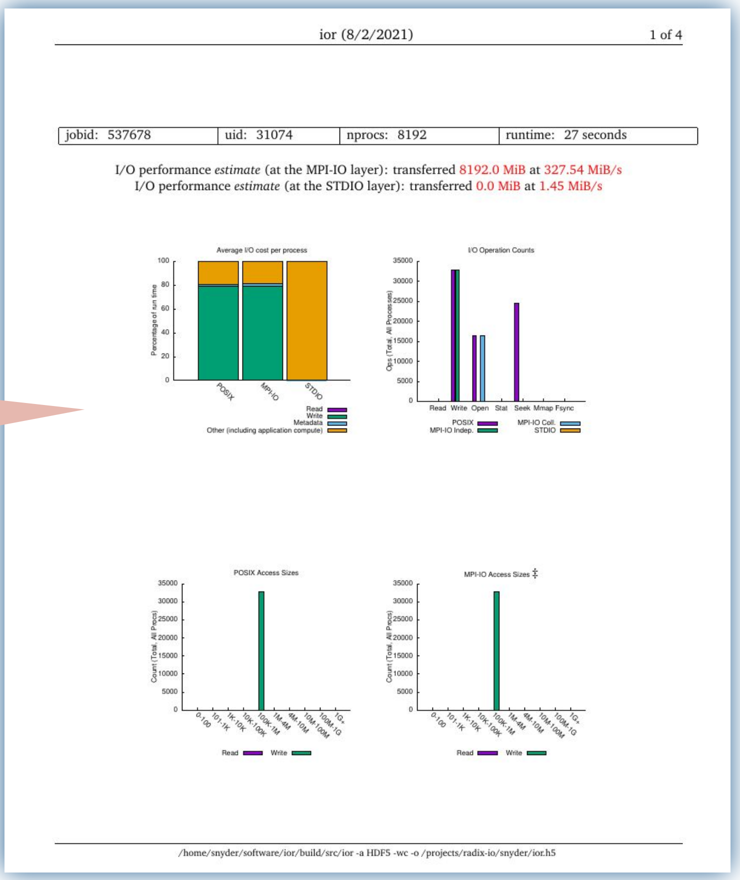
jobid: 537678	uid: 31074	nprocs: 8192	runtime: 27 seconds

I/O performance *estimate* (at the MPI-IO layer): transferred 8192.0 MiB at 327.54 MiB/s
I/O performance *estimate* (at the STDIO layer): transferred 0.0 MiB at 1.45 MiB/s

/home/snyder/software/ior/build/src/ior -a HDF5 -wc -o /projects/radix-io/snyder/ior.h5

Analyzing Darshan logs

Note: This `darshan-job-summary.pl` tool will soon be deprecated by a new, more comprehensive Python-based Darshan summary tool – more on this coming soon!



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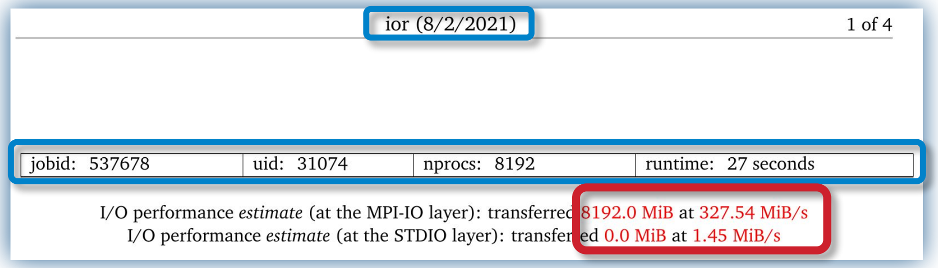

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Job metadata and performance estimates

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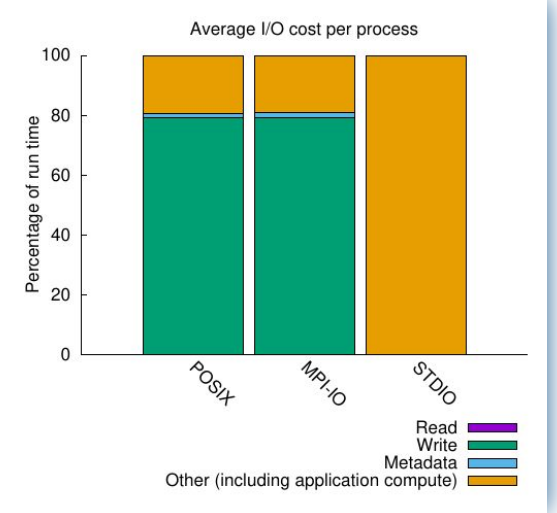

Across main I/O interfaces, how much time was spent reading, writing, doing metadata, or computing?

If mostly compute, limited opportunities for I/O tuning

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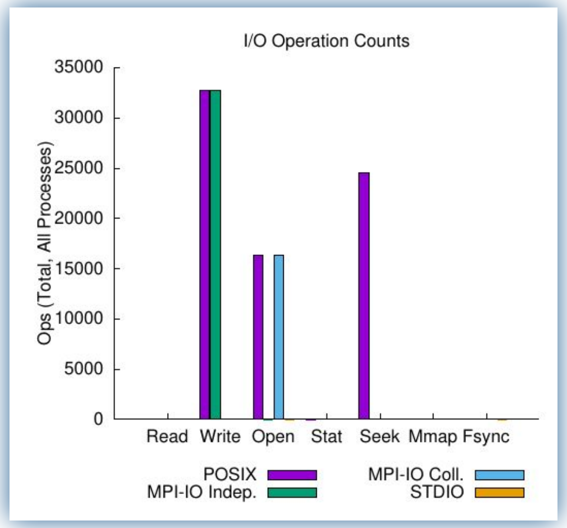

What were the relative totals of different I/O operations across key interfaces?

Lots of metadata operations (open, stat, seek, etc.) could be a sign of poorly performing I/O

Key Darshan instrumentation capabilities

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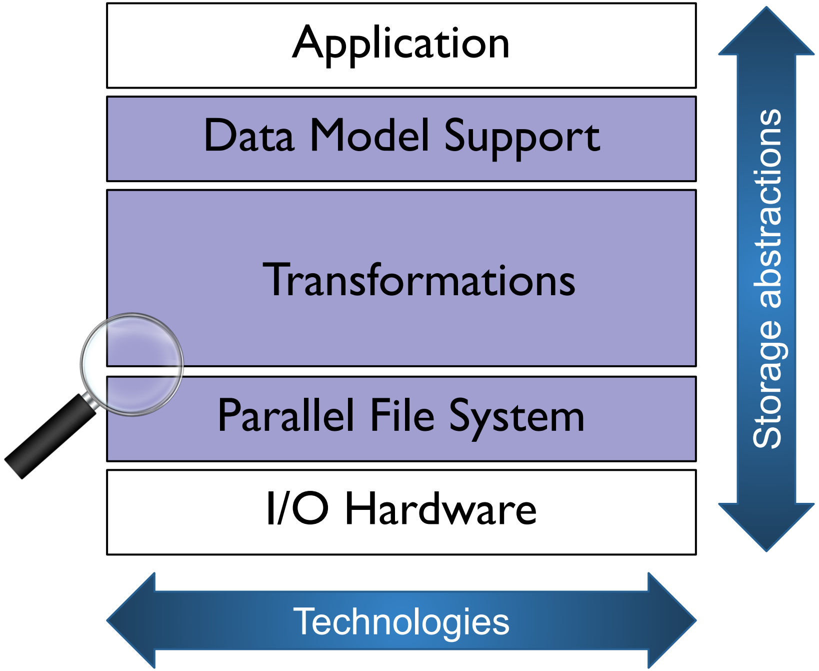
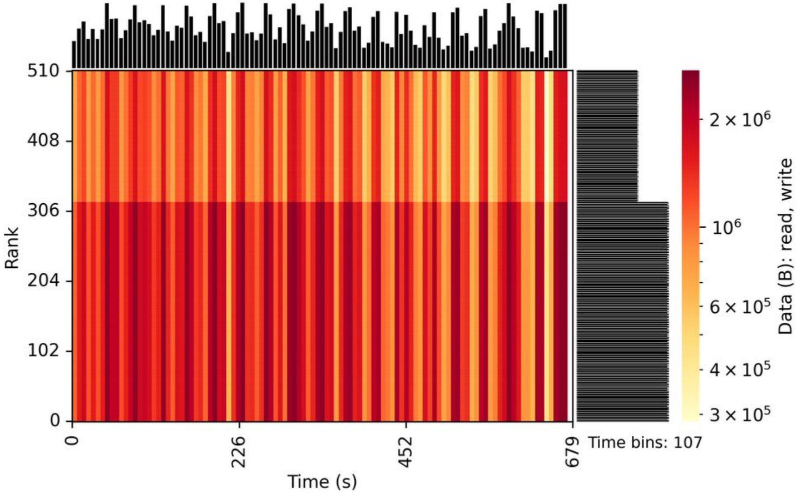
Low-level I/O instrumentation

- Darshan provides in-depth instrumentation of the lower layers of traditional HPC I/O stack:
  - **MPI-IO** parallel I/O interface
  - **POSIX** file system interface
  - **STDIO** buffered stream I/O interface
  - **Lustre** file system striping parameters
- Captures fixed set of statistics, properties, and timing info for each file accessed using these interfaces
- Informs on key I/O performance characteristics of foundational components of the HPC I/O stack



Low-level I/O instrumentation

- Beyond its traditional capture mode, Darshan offers features for obtaining finer-grained details of low-level I/O activity:
  - **Heatmap module**: captures histograms of I/O activity at each process using a fixed size histogram
    - Available for POSIX, MPI-IO, and STDIO interfaces by default in 3.4+ versions of Darshan
  - **DXT modules**: captures full I/O traces at each process using a configurable buffer size
    - Available for POSIX and MPI-IO modules
    - Enabled using `DXT_ENABLE_IO_TRACE` environment variable



Heatmaps showcase application I/O intensity across time, ranks, and interfaces – helpful for identifying hot spots, I/O and compute phases, etc.

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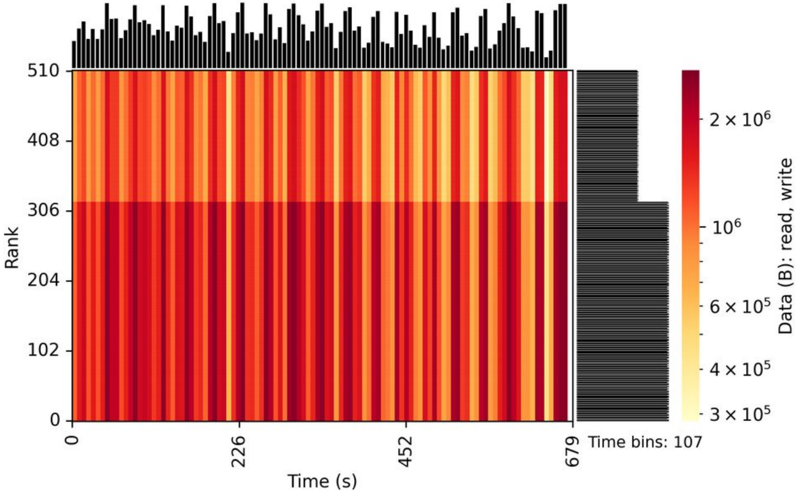
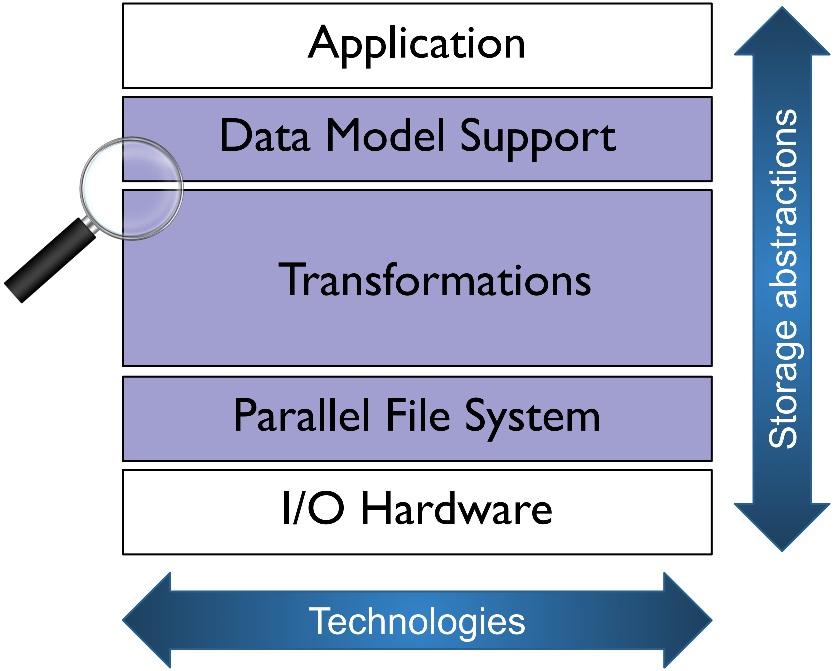


These heatmaps could similarly be used to show I/O intensity across a set of processes involved in an HEP workflow, rather than ranks in an MPI app

High-level I/O library instrumentation

- Darshan similarly provides in-depth instrumentation of HDF5 and Parallel netCDF, popular high-level I/O libraries for HPC
- HDF5 support is of particular interest, given its gaining traction in different HEP contexts
  - Darshan provides detailed instrumentation of accesses to HDF5 files and datasets in 3.2+ versions
- Full-stack characterization allows deeper understanding of app usage of I/O libraries, as well as underlying performance characteristics for these usage patterns



HDF5 application instrumentation example

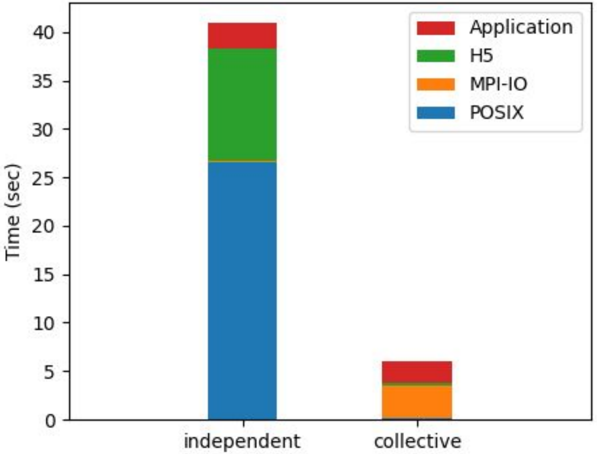
- The MACSio[1] benchmark evaluates behavior of multi-physics I/O workloads using different I/O backends, including HDF5
  - We instrumented using Darshan's HDF5 module to see what insights we could gain into performance characteristics of independent and collective I/O configurations

b/w: **~30 MB/sec**

POSIX I/O dominates, **H5** incurs non-negligible overhead forming this workload

Negligible time spent in **MPI-IO**

Average per-process time spent in I/O



b/w: **~290 MB/sec**

H5 and **POSIX** incur minimal overhead for this workload

MPI-IO collective I/O algorithm dominates

[1] https://github.com/LLNL/MACSio

New Darshan log analysis capabilities

PyDarshan log analysis framework

- ❖ Darshan has traditionally offered only the C-based darshan-util library and a handful of corresponding tools to users for log file analysis
  - ➢ Implementing customized analysis tasks can become extremely cumbersome
- ❖ PyDarshan developed to simplify the interfacing of analysis tools with log data
  - ➢ Use Python CFFI module to define Python bindings to the native darshan-utils C API
  - ➢ Expose Darshan log data as dictionaries, pandas dataframes, and NumPy arrays
- ❖ PyDarshan enables a richer ecosystem for development of Darshan log analysis tools, by the Darshan team and by end users

Available via PyPI or Spack:

- ★ “`pip install darshan`”
- ★ “`spack install py-darshan`”

PyDarshan development led by
Jakob Luttgau (UTK), Tyler Reddy
and Nik Awtrey (LANL)

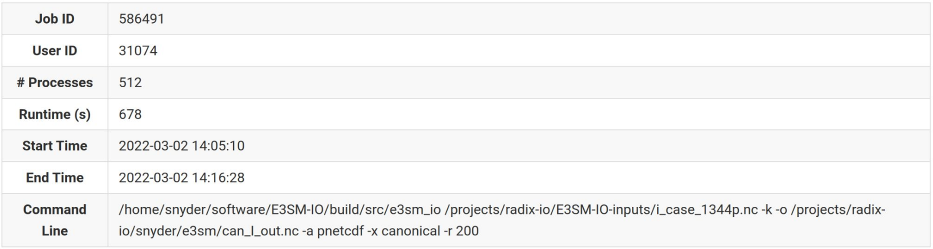
PyDarshan job summary tool

- PyDarshan includes a new job summary tool that will soon replace the `darshan-job-summary.pl` script
  - Generates detailed HTML reports summarizing application I/O behavior using different plots, graphs, and statistics
  - Builds off popular Python libraries like `matplotlib` (plotting), `seaborn` (plotting), and `mako` (HTML templating)
- Users can generate summary reports for a given Darshan log file using the following command:
  - ‘**`python -m darshan summary <path_to_log_file>`**’
  - Generates an output HTML report describing job’s I/O behavior

PyDarshan job summary tool

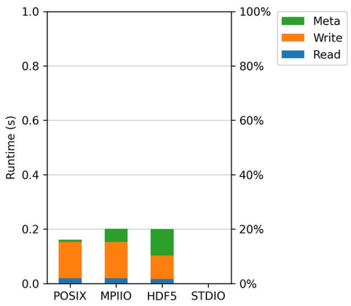
Detailed job metadata

Job Summary



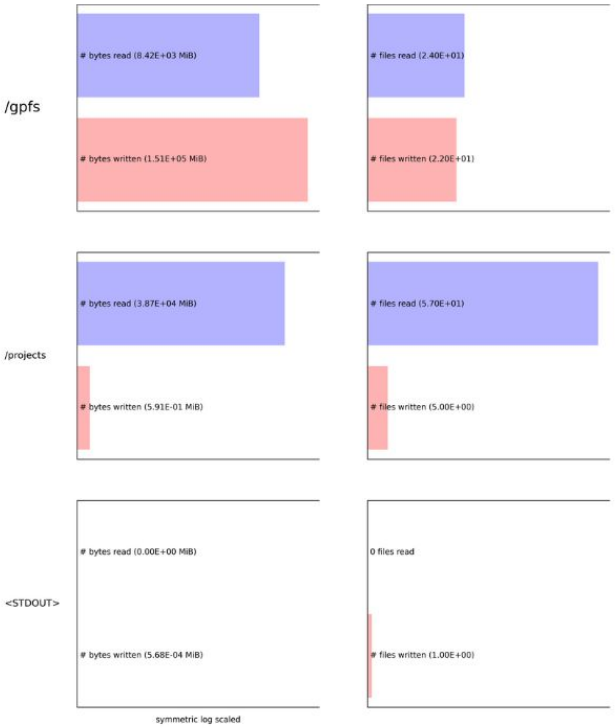
Job ID	586491
User ID	31074
# Processes	512
Runtime (s)	678
Start Time	2022-03-02 14:05:10
End Time	2022-03-02 14:16:28
Command Line	/home/snyder/software/E3SM-IO/build/src/e3sm_io /projects/radix-io/E3SM-IO-inputs/i_case_1344p.nc -k -o /projects/radix-io/snyder/e3sm/can_I_out.nc -a pnetcdf -x canonical -r 200

I/O Cost



I/O cost for all APIs

Data Access by Category



Total files and bytes read/written to different categories (mount points, standard streams, etc.)

Darshan analysis of HEP workflows

Thanks to Rui Wang (ANL) for
ATLAS Athena analysis!

Darshan usage in HEP contexts

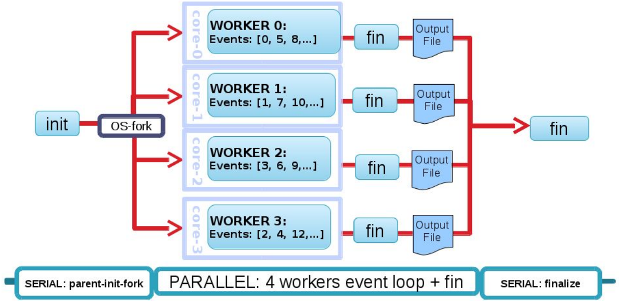
- *HEP-CCE IOS project*: Investigate how to utilize Darshan to understand and improve the I/O behavior of HEP workflows
  - What are the performance characteristics of different HEP I/O workloads?
  - How does HEP software interact with HPC I/O libraries and storage systems? Can these interactions be optimized?
- Our studies have motivated a couple of important improvements to Darshan
  - Proper instrumentation of forked processes
    - Darshan library now detects when a fork occurs and resets instrumentation state on all child processes to start from a clean slate
  - Runtime library configuration
    - Gives user fine-grained runtime control over instrumentation scope (i.e., what interfaces and what files to instrument) and library memory usage

ATLAS offline software – Athena

Various Athena Modes

- **AthenaMP (multi-Process)+standalone merging – Run2 original**
  - Independent parallel workers are forked from main process with shared memory allocation
  - Each worker produces its own outputs and merged later via a post-processing merge process
- **AthenaMP+SharedWriter (multi-Process) – Run2**
  - A shared writer process does all the output writes
  - Reduce time on single thread merging process
- **AthenaMP+SharedWriter (parallelCompression) – Run3**
  - Uses parallel compression to reduce the time increment when moving to higher No. of process
- **AthenaMT (multi-thread)**
  - Gaudi task scheduler maps tasks to kernel threads
  - Shared single pool of heap memory

Schematic View of ATLAS AthenaMP

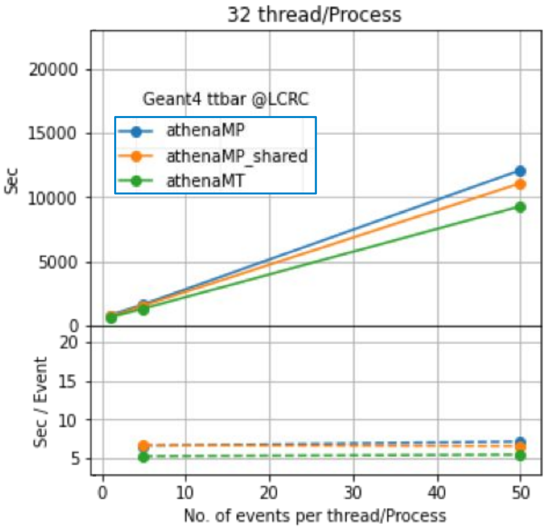


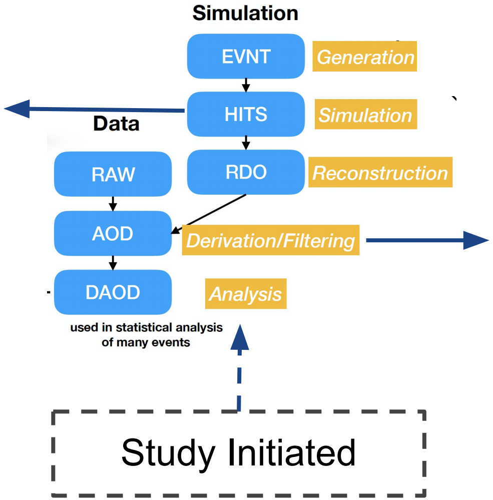
https://twiki.cern.ch/twiki/bin/view/AtlasPublic/ComputingandSoftwarePublicResults

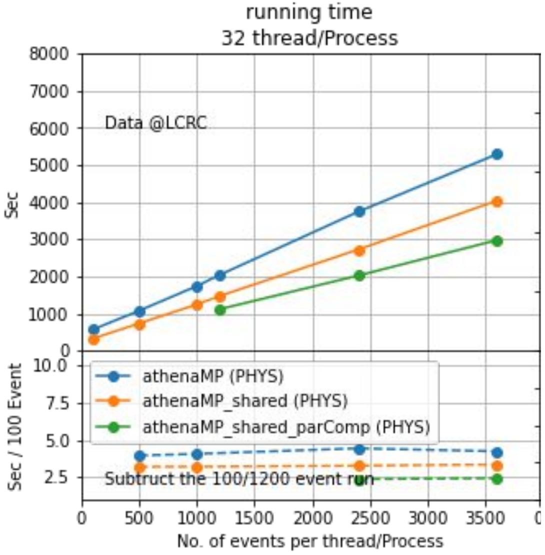
Athena I/O monitoring

- ❖ MC Simulation – CPU intensive
  - ➢ AthenaMP+Standalone merging
  - ➢ AthenaMP+SharedWriter
  - ➢ AthenaMT

- ❖ Derivation (DAOD) production – I/O intensive
  - ➢ AthenaMP+Standalone merging
  - ➢ AthenaMP+SharedWriter
  - ➢ AthenaMP+SharedWriter (parallel compression)







Running on 1 node with 36 cores

Athena I/O monitoring

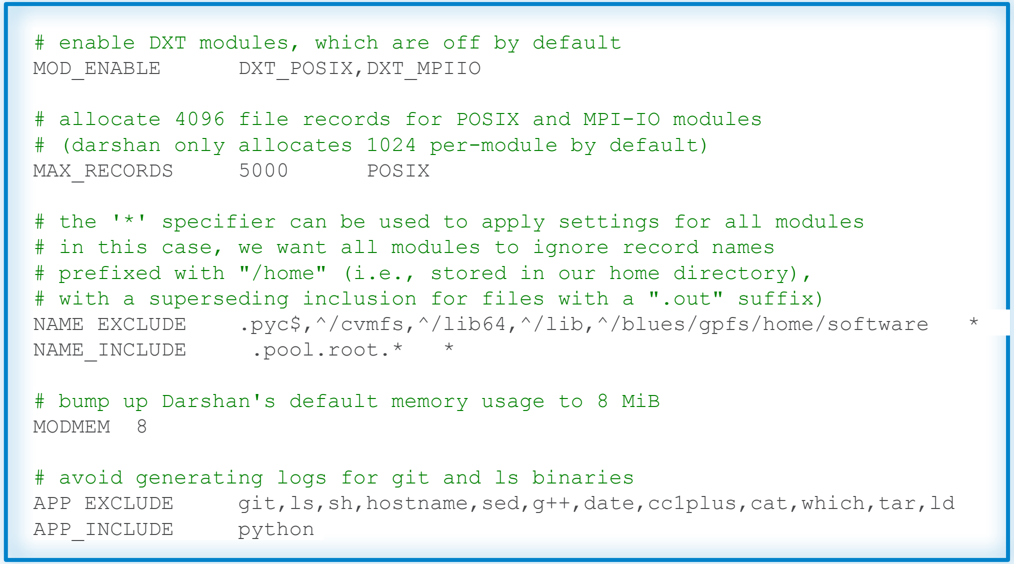
❖ Use Darshan as the I/O monitoring tool for Atlas HPC workflow to gain deeper insights into I/O patterns of Athena

Use `LD_PRELOAD` to interpose Darshan instrumentation in Athena

```
Derivation_tf.py …… --athenaopts='
--preloadlib=$DARSHAN_BASE_DIR/lib/
libdarshan.so'
```

```
> head log.EVNTtoHITS
11:00:45 Thu Oct  6 11:00:45 CDT 2022
11:00:45 Preloading
/lcrc/group/ATLAS/users/rwang/Argonne_computing/PPS-CCE/dar
shan/build_darshan/dev-fork-child-issue786/lib/libdarshan.so
11:00:45 ##############################
11:00:45 ##### DARSHAN CONFIG #####
11:00:45 ##############################
```

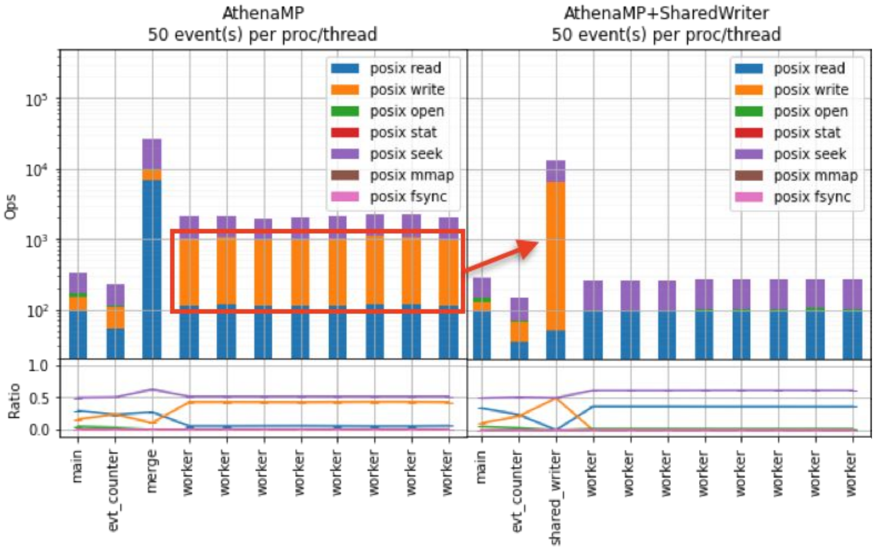
Use custom Darshan configuration to exclude `/cvmfs` activities in runtime environment



```
# enable DXT modules, which are off by default
MOD_ENABLE      DXT_POSIX,DXT_MPIIO

# allocate 4096 file records for POSIX and MPI-IO modules
# (darshan only allocates 1024 per-module by default)
MAX_RECORDS     5000      POSIX

# the '*' specifier can be used to apply settings for all modules
# in this case, we want all modules to ignore record names
# prefixed with "/home" (i.e., stored in our home directory),
# with a superseding inclusion for files with a ".out" suffix)
NAME_EXCLUDE    .pyc$,^/cvmfs,^/lib64,^/lib,^/blues/gpfs/home/software   *
NAME_INCLUDE     .pool.root.*   *

# bump up Darshan's default memory usage to 8 MiB
MODMEM  8

# avoid generating logs for git and ls binaries
APP_EXCLUDE     git,ls,sh,hostname,sed,g++,date,cc1plus,cat,which,tar,ld
APP_INCLUDE     python
```

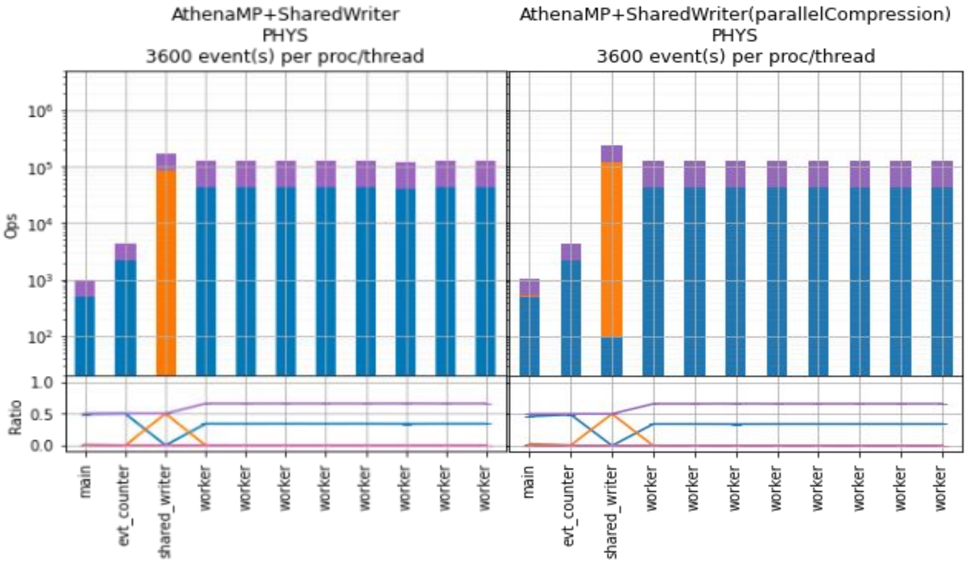
Darshan POSIX I/O analysis

Simulation



- In AthenaMP each worker writes, while a standalone merge process reads all output file of each worker then write to a single file
- In SharedWriter, a single process writes on behalf of workers

DAOD production



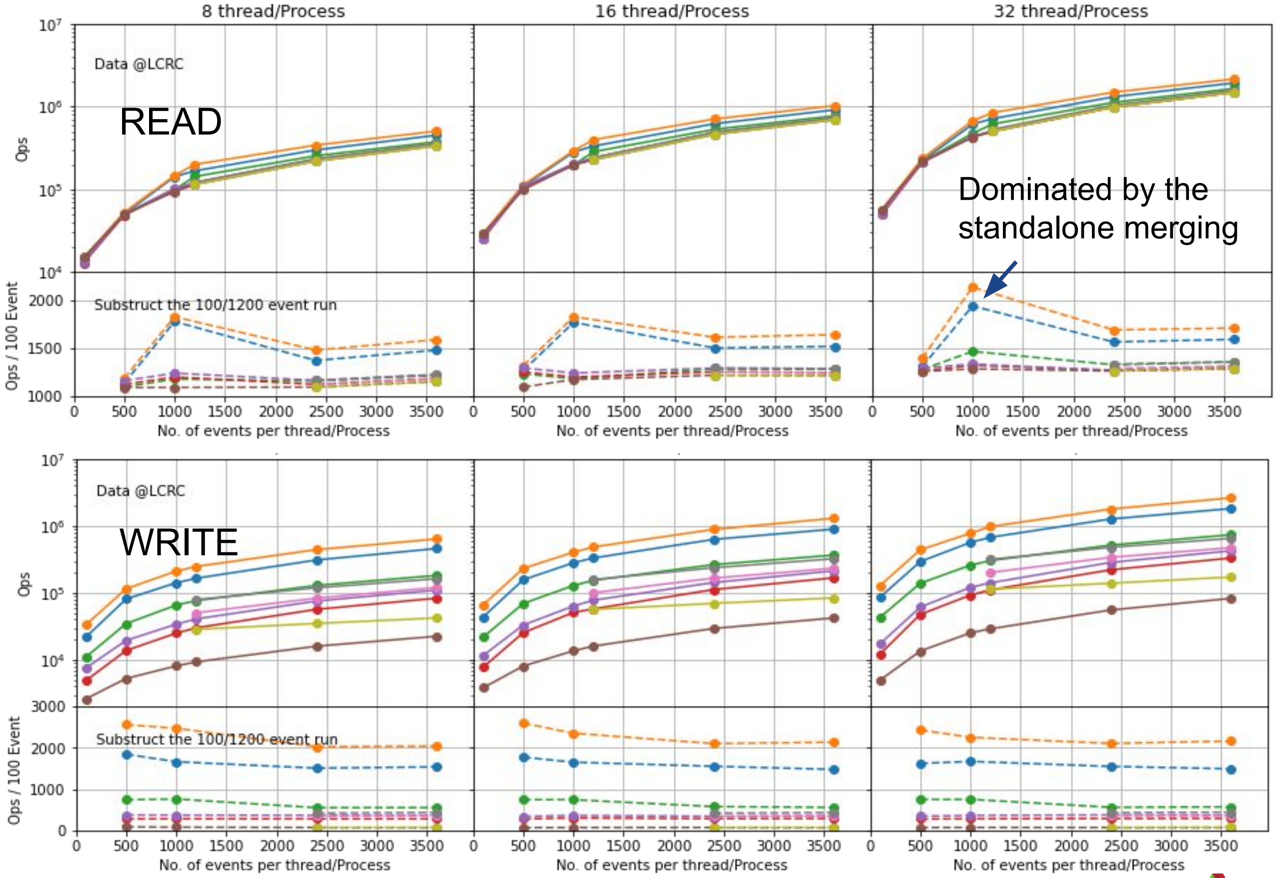
- Additional reads in the shared writer process when using parallel compression

Darshan POSIX I/O analysis

- *Parallel Compression is disabled for < 1K process*
- *Chunk size=100*

DAOD production

- **PHYS**: AOD data model with reduced trigger, MC truth and tracking info
- **PHYSLITE:** event with calibrated objects, further reduced list of variables from PHYS
- **PHYS-PHYSLITE:** producing PHYS then PHYSLITE in a train (default for ATLAS production)



READ

WRITE

Dominated by the standalone merging

What’s next for Darshan?

Ongoing Darshan development activities

- Instrumentation of DAOS libraries
  - ALCF Aurora will feature Intel's DAOS storage system, a first-of-a-kind object-based storage system for large-scale HPC platforms
  - Darshan will implement instrumentation for DAOS file and object interfaces to better understand how apps and I/O middleware make use of this new paradigm
- Continued development efforts on log analysis tools
  - Refining new PyDarshan log analysis framework
  - Recommendations, warnings, and other feedback based on observed I/O patterns
  - Analysis tools for workflows (i.e., multiple Darshan logs created by multiple job steps)

Wrapping up

- ❖ Darshan is an invaluable tool for HPC application scientists, facilities, and I/O researchers for better understanding application I/O behavior
  - ➢ Detailed instrumentation of application access to multiple layers of the HPC I/O stack
  - ➢ Helpful tools for extracting salient data from Darshan logs and summarizing for users
- ❖ Ongoing efforts from the Darshan team and the HEP community to leverage Darshan for better understanding/improving HEP I/O behavior on HPC systems!
- ❖ Please reach out with any questions, comments, or feedback!

- ❖ Darshan website, docs: https://www.mcs.anl.gov/research/projects/darshan/
- ❖ Source code, issue tracking: https://github.com/darshan-hpc/darshan
- ❖ Darshan-users mailing list: darshan-users@lists.mcs.anl.gov

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