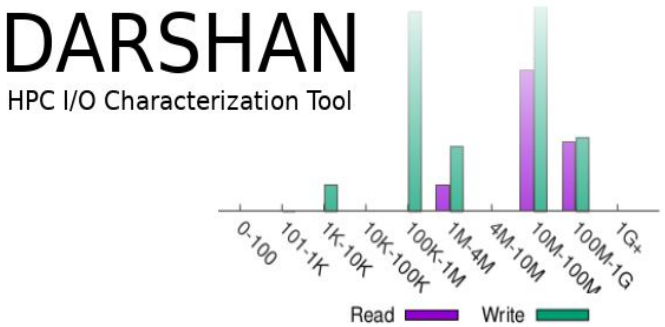
March 28, 2023

Argonne NATIONAL LABORATORY

Understanding and Improving the I/O Behavior of Scientific Computing Applications



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MCS CS Seminar Series

Understanding and improving HPC I/O

- Characterizing and understanding 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., CXL) 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

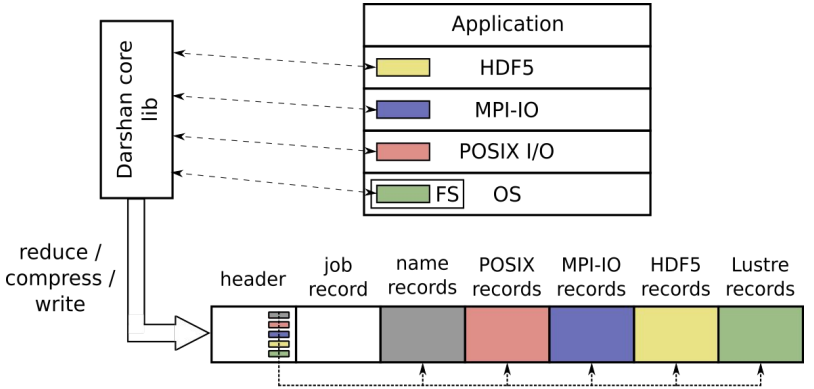
Darshan: An I/O characterization tool for HPC applications

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 independently on each process
- At app shutdown, collect, aggregate, compress, and write log data
- After job completes, analyze Darshan log data
  - `darshan-parser` - provides complete text-format dump of all counters in a log file
  - *PyDarshan* - Python analysis module for Darshan logs, including a summary tool for creating HTML reports



- 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 each *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 typically enabled by default

```
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

```
ssnyder@perlmutter:login37:~> module load darshan
ssnyder@perlmutter:login37:~> module -t list |& tail -n 5
Nsight-Systems/2022.2.1
cudatoolkit/11.7
craype-accel-nvidia80
gpu/1.0
darshan/3.4.0
```

Darshan module can typically be explicitly loaded if not available by default, e.g., Darshan 3.4.0 on NERSC Perlmutter

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 typically enabled by default
  - **Just compile and run your apps like normal**

```
ssnyder@perlmutter:login05: cc -o mpi-io-test mpi-io-test.c
ssnyder@perlmutter:login05: ldd mpi-io-test | grep darshan
        libdarshan.so.0 => /global/common/software/nersc/pm
```

```
ssnyder@perlmutter:nid004489: srun -n 32 ./mpi-io-test
# Using mpi-io calls.
nr_procs = 32, nr_iter = 1, blk_sz = 16777216, coll = 0
# total_size = 536870912
# Write: min_t = 0.416507, max_t = 0.456917, mean_t = 0.43
# Read:  min_t = 0.010588, max_t = 0.014461, mean_t = 0.01
Write bandwidth = 1174.985593 Mbytes/sec
Read bandwidth = 37124.695394 Mbytes/sec
```

E.g., compiling and running a simple example on NERSC Perlmutter

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 typically enabled by default
  - ➢ **Just compile and run your apps like normal**

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

Traditional usage on HPC platforms

- On many HPC platforms (e.g., ALCF Theta, NERSC Cori & Perlmutter, OLCF Summit), Darshan is already installed and typically 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**

```
ssnyder@perlmutter:login05: darshan-config --log-path
/pscratch/darshanlogs
ssnyder@perlmutter:login05: cd /pscratch/darshanlogs/2023/3/14
ssnyder@perlmutter:login05: ls | grep snyder
ssnyder_mpi-io-test_id6058027-191211_3-14-39483-261794756305089
8457_1.darshan
```

‘**`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.

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, users can utilize Darshan log analysis tools for gaining insights into application I/O behavior:

```
shane@shane-x1-carbon: darshan-parser ./log.darshan | grep POSIX_BYTES_WRITTEN | sort -nr -k 5
POSIX   387     6960057185861764086     POSIX_BYTES_WRITTEN     5413869452      /projects/radix
POSIX   452     6960057185861764086     POSIX_BYTES_WRITTEN     5413865644      /projects/radix
POSIX   197     6960057185861764086     POSIX_BYTES_WRITTEN     5413857652      /projects/radix
POSIX   5       6960057185861764086     POSIX_BYTES_WRITTEN     5413852168      /projects/radix
POSIX   451     6960057185861764086     POSIX_BYTES_WRITTEN     5413844532      /projects/radix
POSIX   64      6960057185861764086     POSIX_BYTES_WRITTEN     5413823236      /projects/radix
POSIX   68      6960057185861764086     POSIX_BYTES_WRITTEN     5413788992      /projects/radix
POSIX   195     6960057185861764086     POSIX_BYTES_WRITTEN     5413663132      /projects/radix
POSIX   323     6960057185861764086     POSIX_BYTES_WRITTEN     5413658668      /projects/radix
POSIX   132     6960057185861764086     POSIX_BYTES_WRITTEN     5413648628      /projects/radix
```

If you know what you're looking for, `darshan-parser` can be a quick way to extract important I/O details from a log, e.g., the 10 most heavily written files

Analyzing Darshan logs

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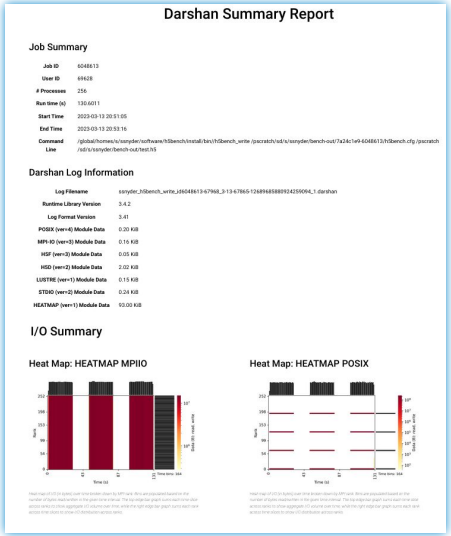

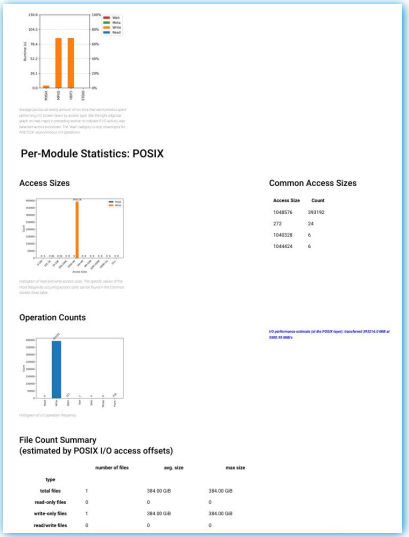

A more user-friendly starting point is the Darshan job summary tool. It can generate a summary report for a log containing useful graphs, tables, and performance estimates describing application I/O behavior

Analyzing Darshan logs

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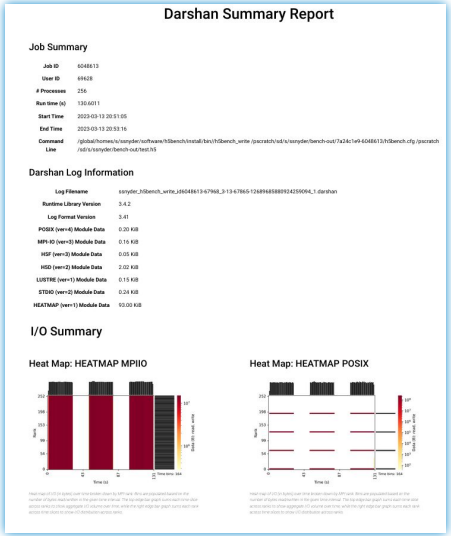
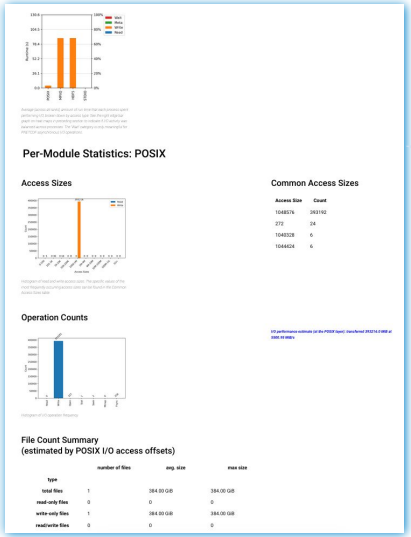


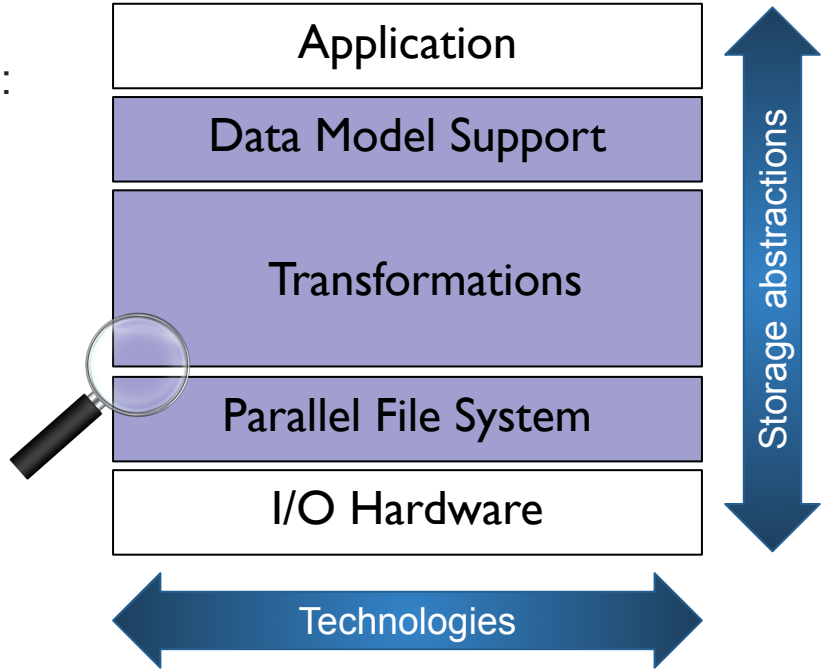


More details on the Darshan job summary tool coming shortly!

Key Darshan instrumentation capabilities

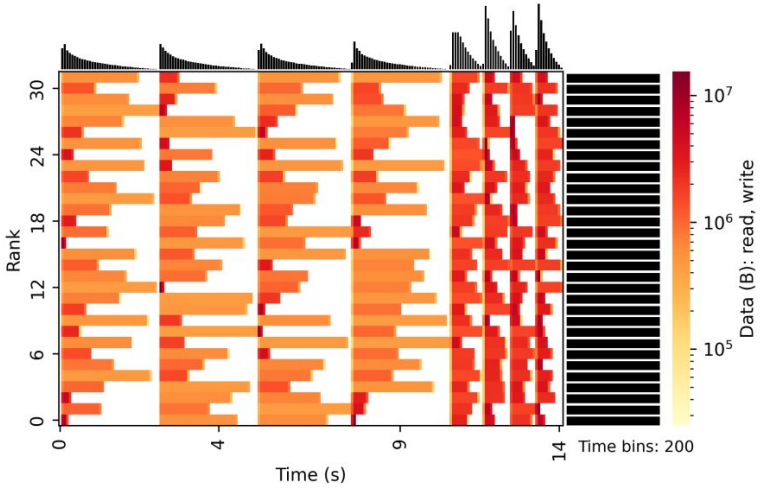
Low-level I/O instrumentation

- Darshan provides in-depth instrumentation of the lower layers of the traditional HPC I/O stack:
  - **MPI-IO** parallel I/O interface
  - **POSIX** file system interface
  - **STDIO** buffered stream I/O interface
  - **Lustre** 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

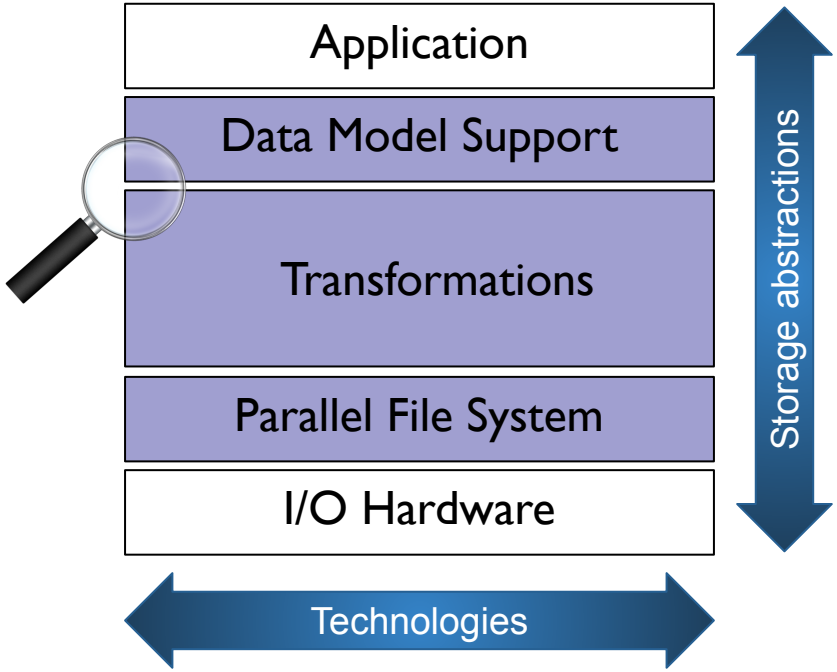
- Beyond its traditional capture mode, Darshan offers key features for obtaining finer-grained details of low-level I/O activity:
  - **Heatmap module**: captures histograms of I/O activity at each process using a fixed size histogram
    - Available for POSIX, MPI-IO, and STDIO interfaces by default 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.

High-level I/O library instrumentation

- Darshan similarly provides in-depth instrumentation of popular high-level I/O libraries for HPC
  - **HDF5**: detailed instrumentation of accesses to HDF5 files and datasets available starting in 3.2+ versions
  - **PnetCDF**: detailed instrumentation of accesses to PnetCDF files and variables available starting in 3.4.1+ versions
- Full-stack characterization allows deeper understanding of app usage of I/O libraries, as well as underlying performance characteristics for these usage patterns



High-level I/O library instrumentation

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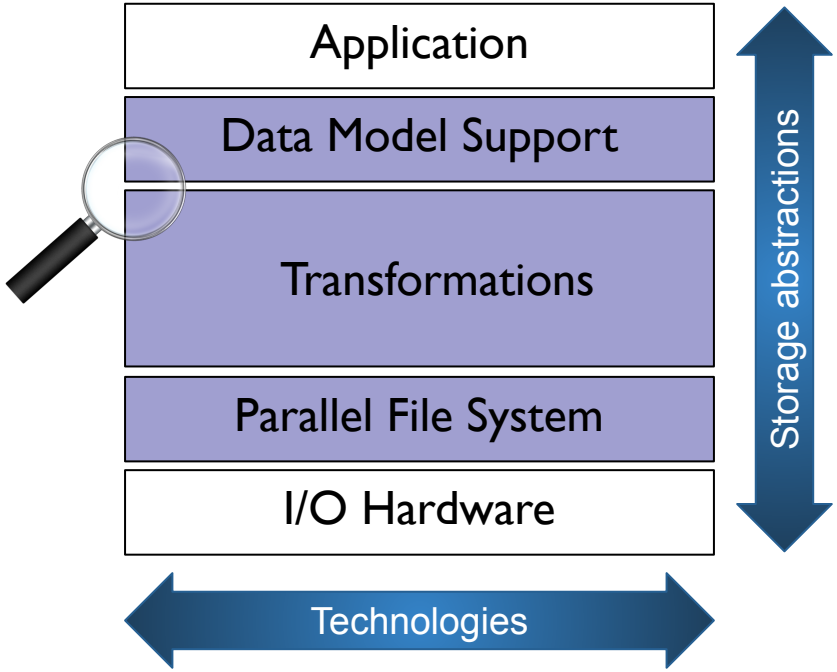
PnetCDF module contributed by
Wei-Keng Liao (NWU)



PyDarshan log analysis framework

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
  - Complicates development of custom Darshan analysis tools
- PyDarshan developed to simplify the interfacing of analysis tools with log data
  - Use Python CFFI module to define bindings to the native darshan-utils C API
  - Expose Darshan log data as dictionaries, pandas dataframes, and NumPy arrays
- PyDarshan should provide a richer ecosystem for development of Darshan log analysis tools, either by users or by the Darshan team

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 is replacing the original `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 output HTML report matching input log file name

PyDarshan job summary tool

Detailed job metadata

Job Summary

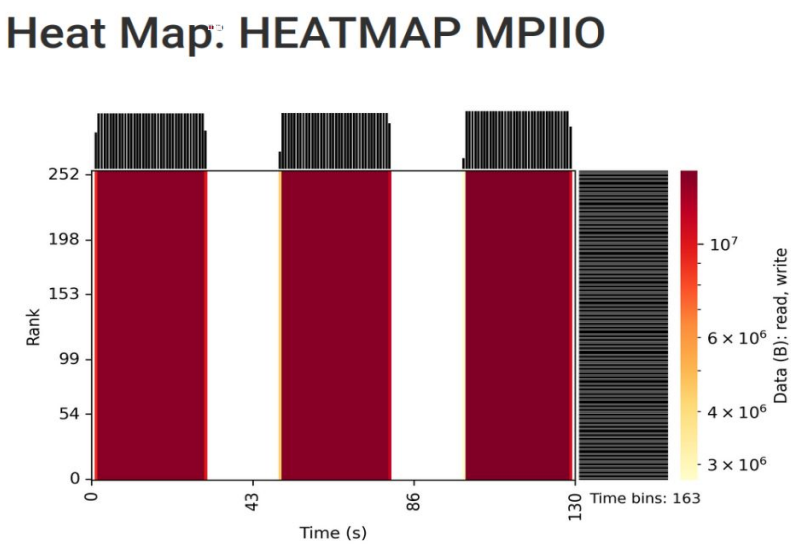
Job ID	6553753
User ID	69628
# Processes	256
Run time (s)	96.3942
Start Time	2023-03-27 11:15:18
End Time	2023-03-27 11:16:55
Command Line	/global/homes/s/ssnyder/software/h5bench/install/bin//h5bench_write /pscratch/sd/s/ssnyder/bench-out2/c1802902-6553753 /h5bench.cfg /pscratch/sd/s/ssnyder/bench-out2/test.h5

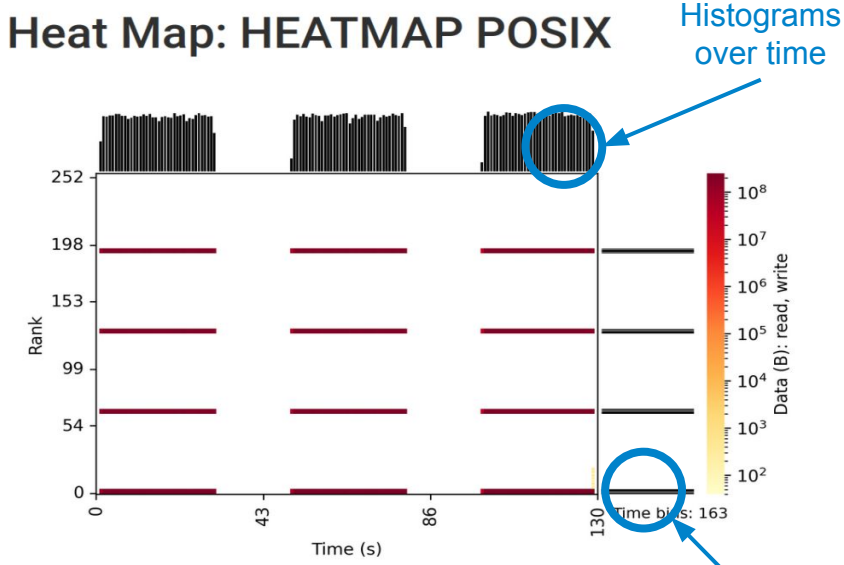
256 process (4 node) h5bench[1] runs on NERSC Perlmutter. h5bench contains lots of parameters (e.g., contiguous vs interleaved accesses, independent vs collective I/O, synchronous vs asynchronous I/O, etc.) for controlling characteristics of generated HDF5 workloads.

1. https://github.com/hpc-io/h5bench

PyDarshan job summary tool

Heatmaps for visualizing I/O activity

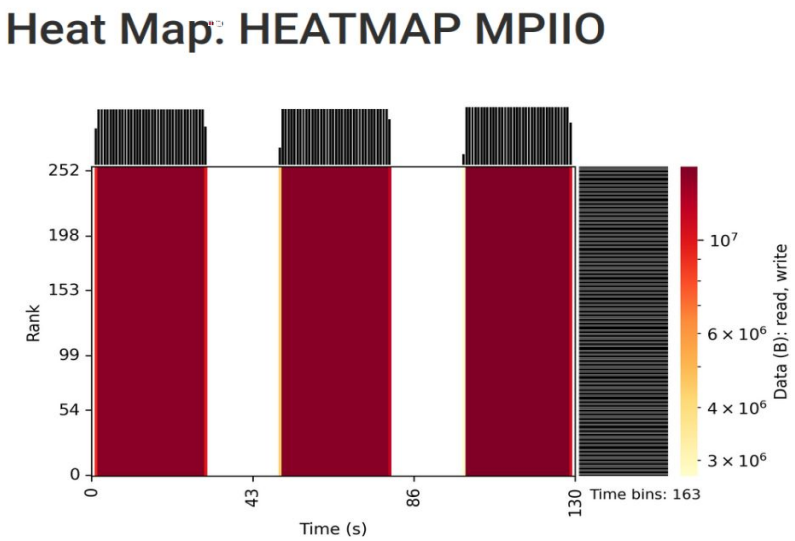


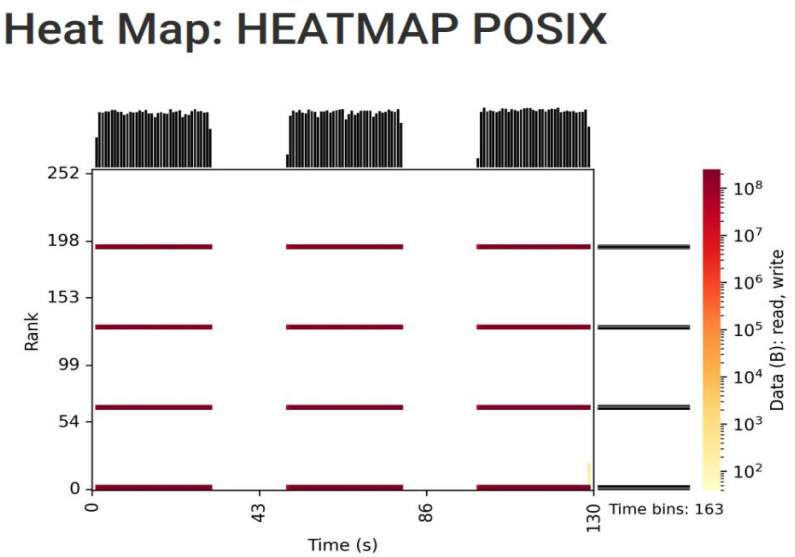


Analyzing I/O behavior over time, ranks, and interfaces can offer key insights into application I/O behavior.

PyDarshan job summary tool

Heatmaps for visualizing I/O activity

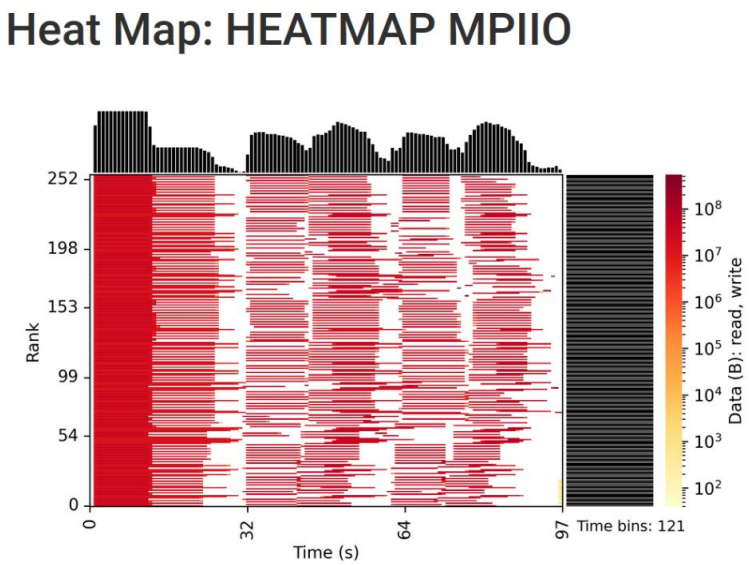


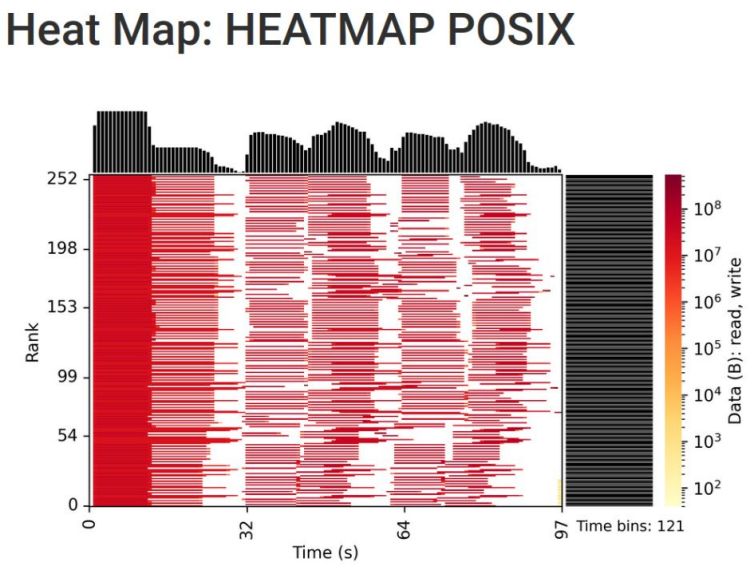


This example heatmap illustrates a typical MPI-IO collective I/O pattern. All MPI ranks perform MPI-IO operations (left), but only a subset of "aggregators" access the file via POSIX operations (right).

PyDarshan job summary tool

Heatmaps for visualizing I/O activity



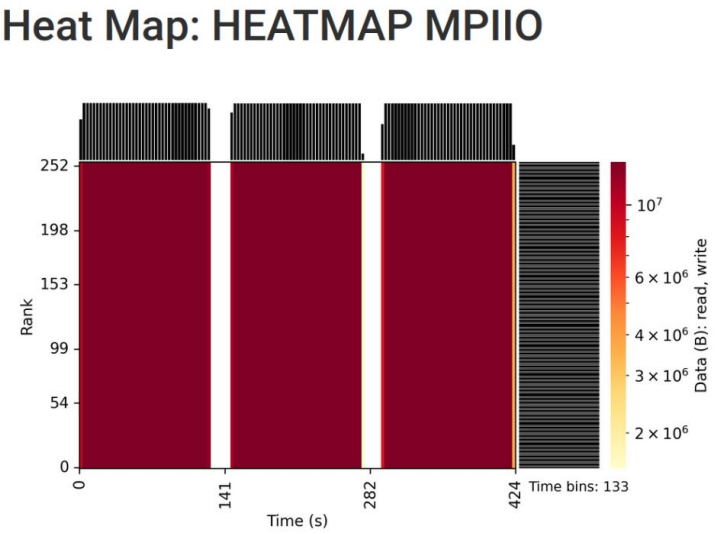


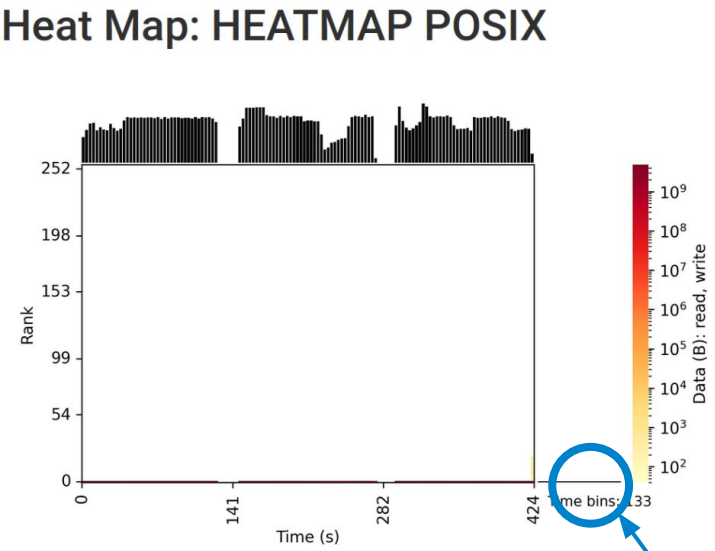
Heatmaps can help quickly detect common I/O pitfalls.

I could have sworn I enabled collective I/O in HDF5.

PyDarshan job summary tool

Heatmaps for visualizing I/O activity





Heatmaps can help quickly detect common I/O pitfalls.

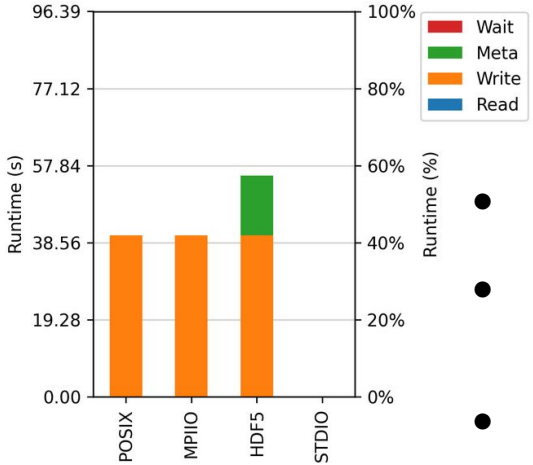
Oops, I enabled collective I/O, but forgot to tell Lustre to use more than one stripe.

All I/O funneled through rank 0

PyDarshan job summary tool

Average I/O cost across APIs

independent

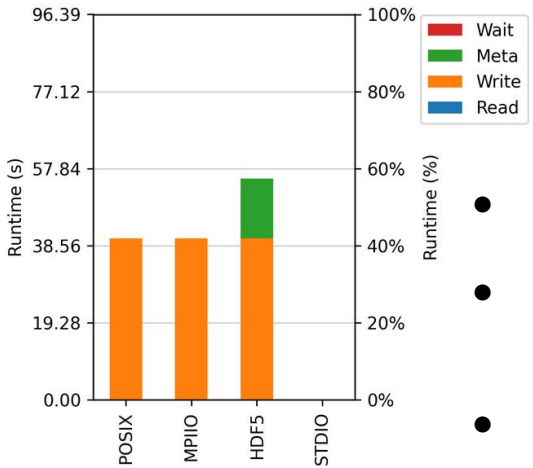


- POSIX write dominates
- MPI-IO/HDF5 negligible write overheads
- HDF5 incurs additional metadata overhead (flushes?)

PyDarshan job summary tool

Average I/O cost across APIs

independent



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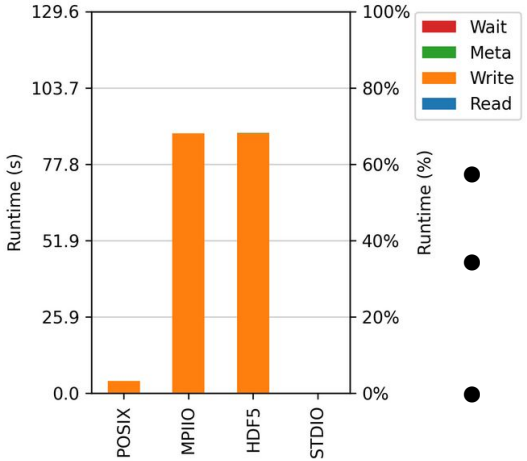
collective

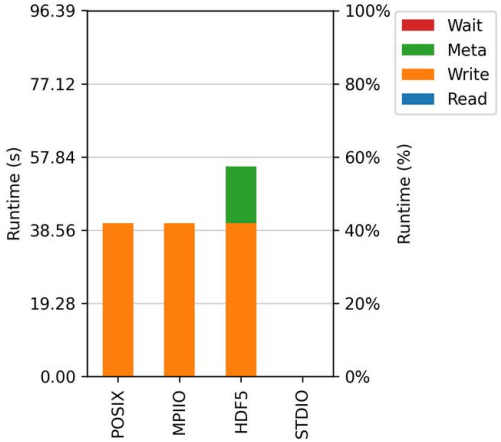


- POSIX write nearly negligible
- MPI-IO collective algorithm cost dominates
- No comparable HDF5 metadata overhead

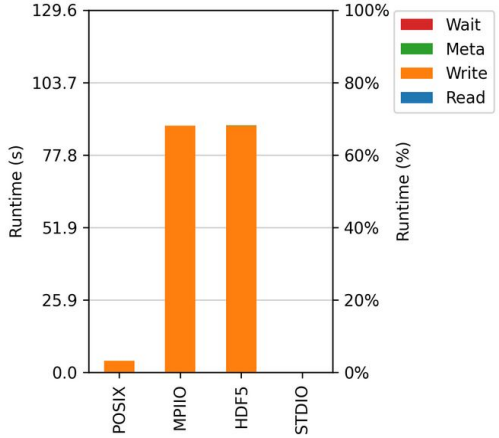
PyDarshan job summary tool

Average I/O cost across APIs

independent



collective



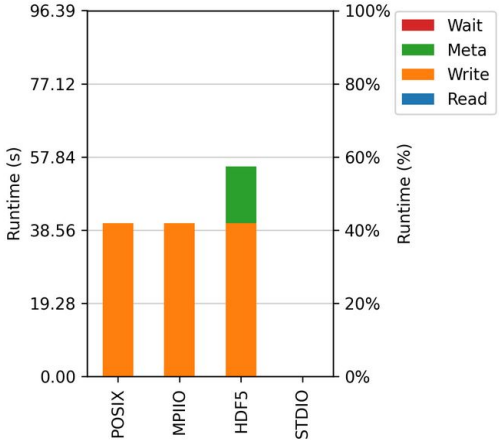
In this head-to-head comparison, independent mode (~55 seconds avg. I/O time) actually performs better than collective (~85 seconds avg. I/O time).

Collective I/O behavior affected by many factors (access patterns, FS parameters, job scale, MPI-IO parameters, dynamic system state, etc.).

PyDarshan job summary tool

I/O performance estimates

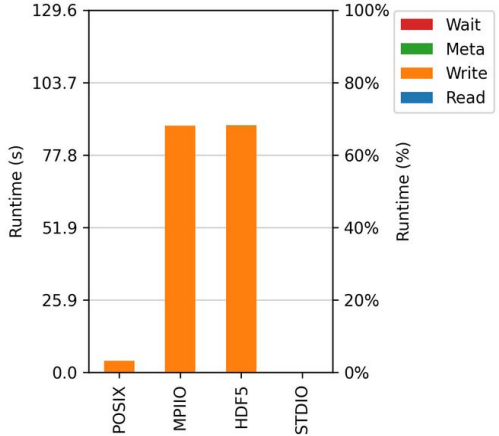
independent



I/O performance estimate (at the MPI-IO layer): transferred 393216.0 MiB at 7108.62 MiB/s

I/O performance estimate (at the POSIX layer): transferred 393216.0 MiB at 7112.29 MiB/s

collective



I/O performance estimate (at the MPI-IO layer): transferred 393216.0 MiB at 4451.17 MiB/s

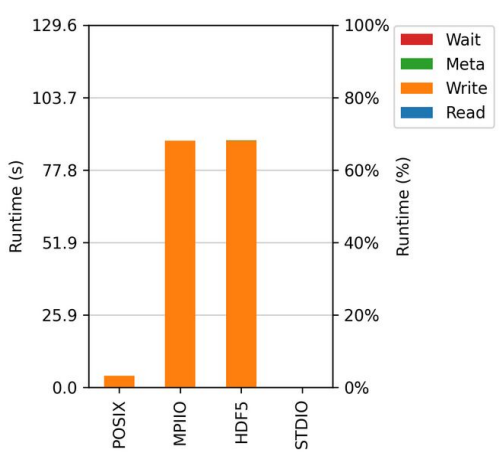
I/O performance estimate (at the POSIX layer): transferred 393216.0 MiB at 5571.27 MiB/s

PyDarshan job summary tool

I/O performance estimates

While I/O cost plots are based on averages across all processes, performance estimates are based on the slowest observed process.

Average cost metrics aren't the greatest at quantifying collective I/O – we are working to integrate more effective metrics into Darshan (e.g. cost by slowest process).



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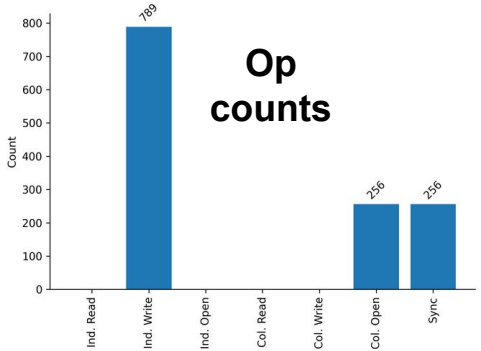
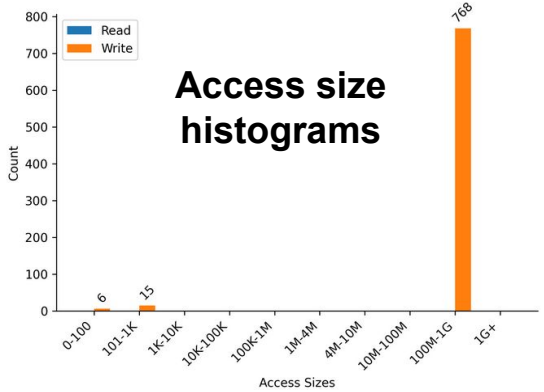
PyDarshan job summary tool

More per-API I/O stats

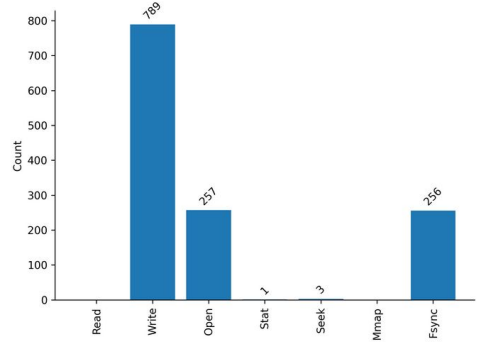
independent mode

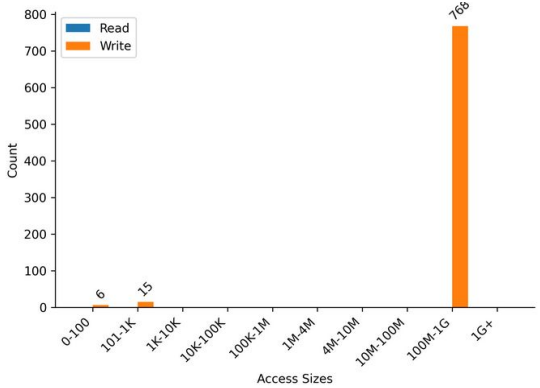
MPI-IO





POSIX





MPI-IO independent operations mostly map 1-to-1 with POSIX file operations.

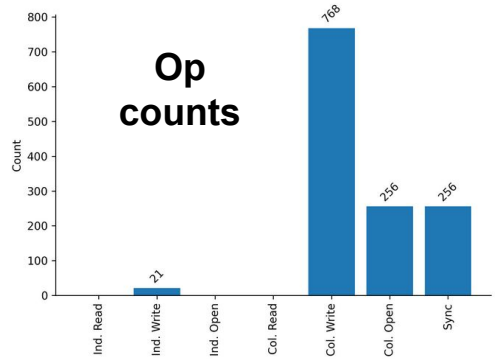
Access sizes mirror the 512 MiB accesses being made at the HDF5 layer.

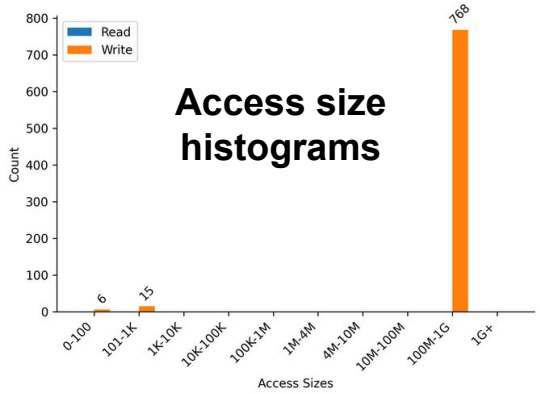
PyDarshan job summary tool

More per-API I/O stats

collective mode

MPI-IO





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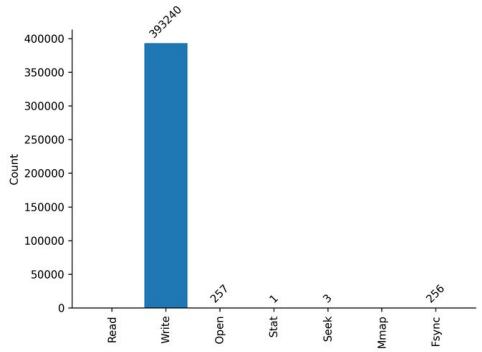
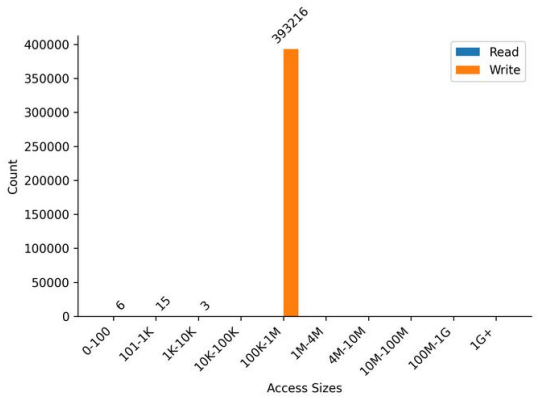




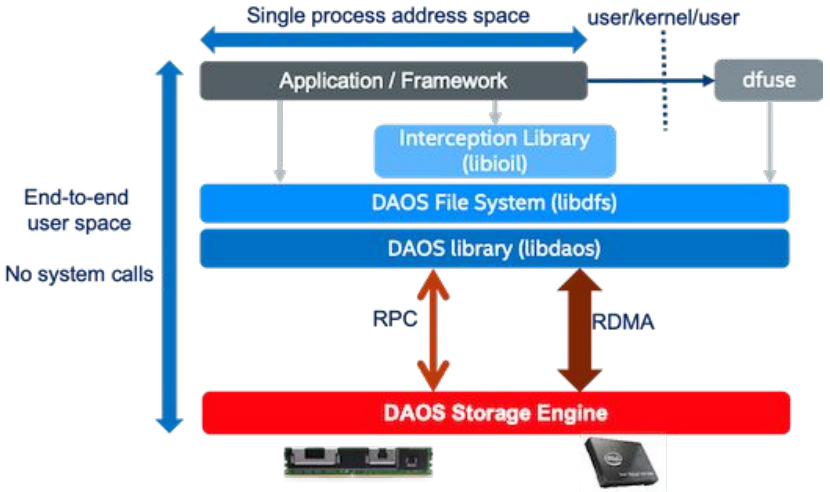
768 MPI-IO collective operations transform into nearly 400K POSIX file operations.

POSIX access sizes now match the collective I/O algorithm buffer size (which equals the Lustre stripe width, 1 MiB).

What’s next for Darshan?

DAOS instrumentation

- ALCF Aurora will feature Intel's DAOS storage system, a first-of-a-kind object-based storage system for large-scale HPC platforms
  - ➢ Leverages both SCM and SSDs for storage
- Darshan instrumentation will provide valuable insights into various ways apps and I/O middleware can utilize DAOS



Various access methods for DAOS users.

Figure courtesy of Intel

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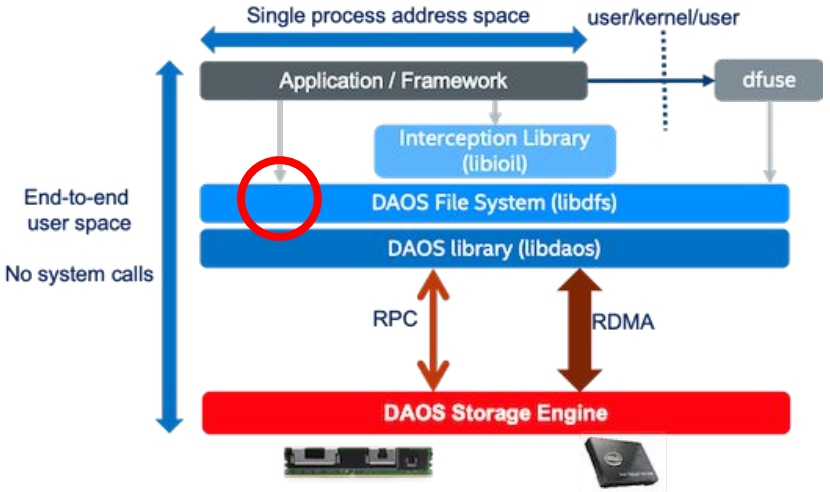
  - **Direct usage of POSIX-like DAOS file system (libdfs) interface**



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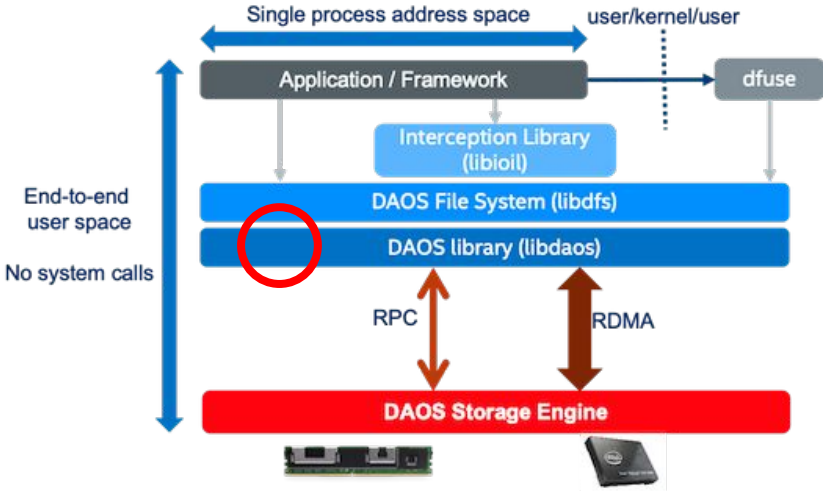

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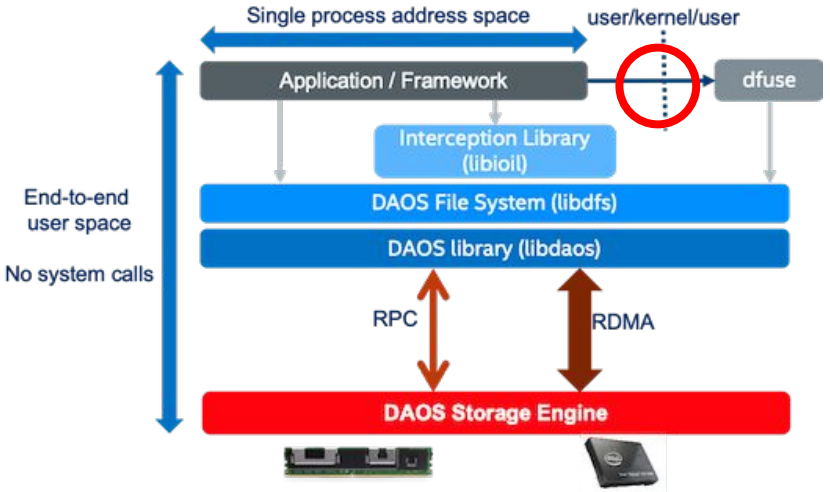
  - **Legacy POSIX support using FUSE**



Various access methods for DAOS users.

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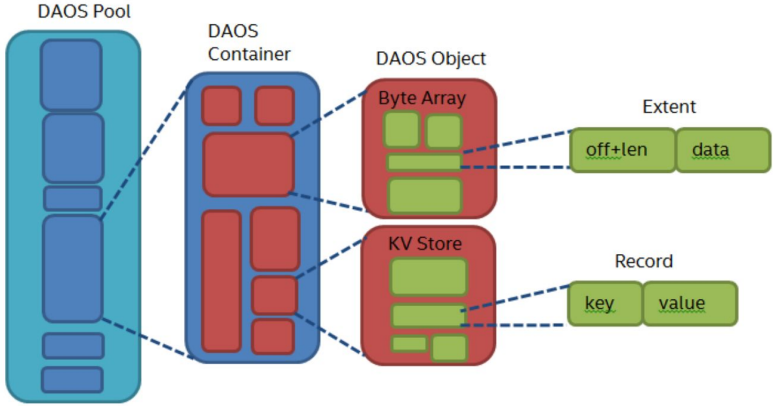
DAOS instrumentation

- The libdfs file interface is a natural fit for Darshan's traditional "record per-file" instrumentation strategy
- But, instrumenting the native libdaos object interface is a bit more complicated, as DAOS objects can take multiple forms
  - Array objects
    - Extent-based access, similar to files
  - Key-val objects
    - Data accessed using arbitrary keys



DAOS storage model. DAOS objects can be accessed using either key-val or array interfaces.

Figure courtesy of Intel

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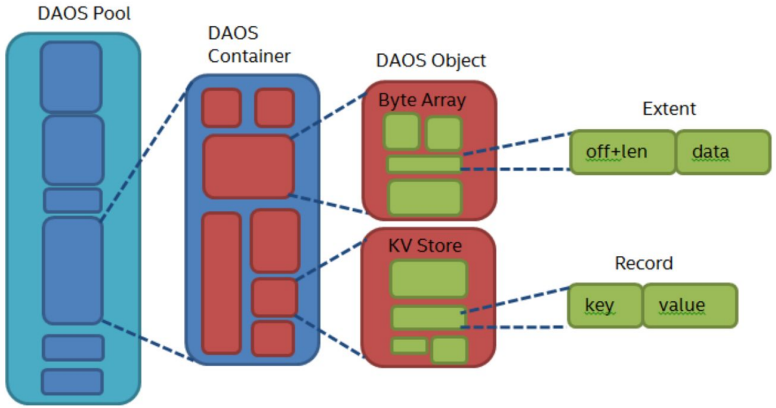
What helpful information could Darshan provide regarding key access distributions of DAOS key-val objects?



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PyDarshan analysis enhancements

Enabling multi-log analysis

- Darshan analysis tools have traditionally operated on a single input log, but analysis across multiple logs is useful in different contexts
  - Analysis of workflows
  - Analysis of arbitrary log collections
- We would like to support new PyDarshan analysis capabilities enabling reporting on I/O behavior beyond the context of a single “job”

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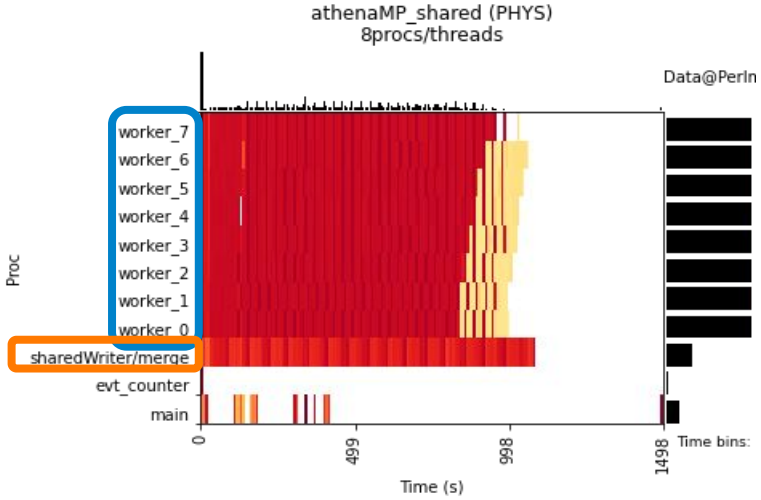

Heatmap visualization of an HEP multiprocess analysis workflow (AthenaMP). 8 **workers** read input data, while a **shared writer** process writes all worker output data from shared memory.

Athena analysis contributed by Rui Wang (ANL).

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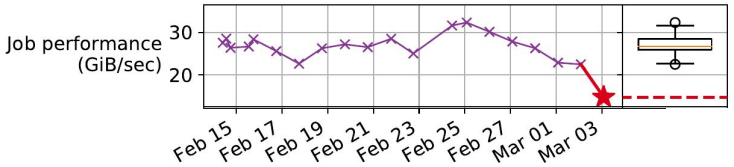

Visualizing overall app I/O performance over time to determine changes in I/O behavior. Borrowed from an I/O analysis tool from the TOKIO project that predated PyDarshan.

https://www.anl.gov/mcs/tokio-total-knowledge-of-io

G.K. Lockwood et al. "UMAMI: a recipe for generating meaningful metrics through holistic I/O performance analysis." PDSW’17.

PyDarshan analysis enhancements

From write-optimized to analysis-friendly formats

- Darshan's native log format is optimized for efficient writing by apps
  - Minimizes instrumentation overheads, but *creates problems for log analysis tools*
- We want to explore popular industry solutions like Apache Parquet/Arrow to help transform Darshan data into more analysis-friendly formats
  - Columnar format can save storage/memory and speed up analysis tasks, particularly when analyzing lots of Darshan data (e.g., all logs collected at a facility)
  - Integrations with popular data analysis frameworks like pandas and Dask

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
    - High-level I/O library usage
    - MPI-IO transformations
    - File system access (i.e., POSIX)
  - Helpful tools for extracting salient data from Darshan logs and summarizing for users

- 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

Acknowledgement

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