How to Understand and Tune HPC I/O Performance

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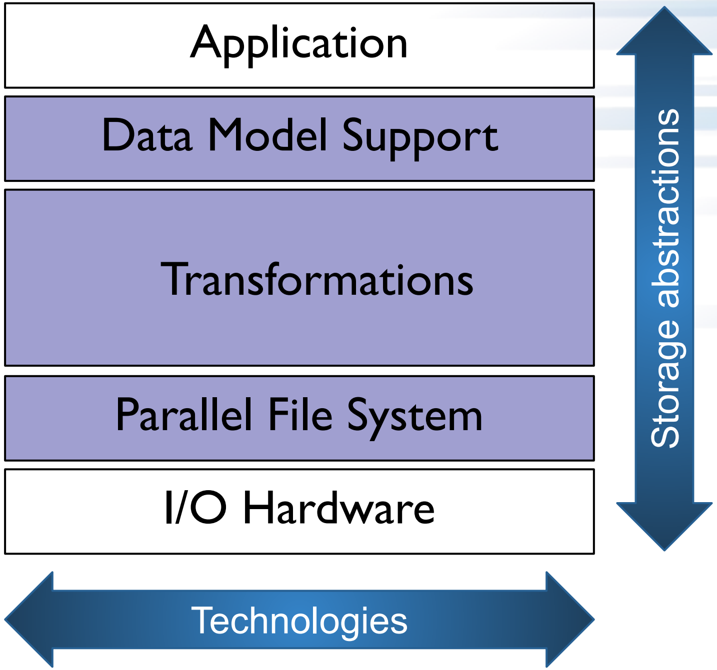
Surveying the HPC I/O landscape

A complex data management ecosystem

As evidenced by today's presentations, the HPC I/O landscape is deep and vast

- High-level data abstractions: HDF5, PnetCDF
- Parallel file systems: Lustre, GPFS
- Storage hardware: HDDs, SSDs, NVM

Understanding I/O behavior in this environment is difficult, much less turning observations into actionable I/O tuning decisions

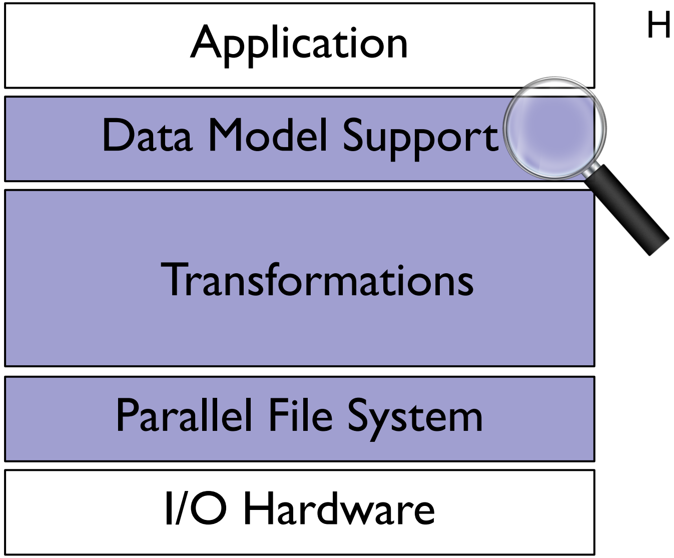


Characterizing HPC I/O workloads with Darshan

A look under the hood of an HPC application

You have already heard some basics about Darshan, a powerful tool for users to better understand and tune their I/O workloads

Darshan provides many helpful stats across multiple layers of the I/O stack that are critical to understanding application I/O behavior



HDF5 stats*:

- Accessed files/datasets
- Operation counts
- Total read/write volumes
- Common access info (including details of hyperslab accesses)
- Chunking parameters
- Dataset dimensionality and size
- MPI-IO usage
- I/O timing

*Note: Detailed HDF5 instrumentation can be optionally enabled only for Darshan versions 3.2.0+

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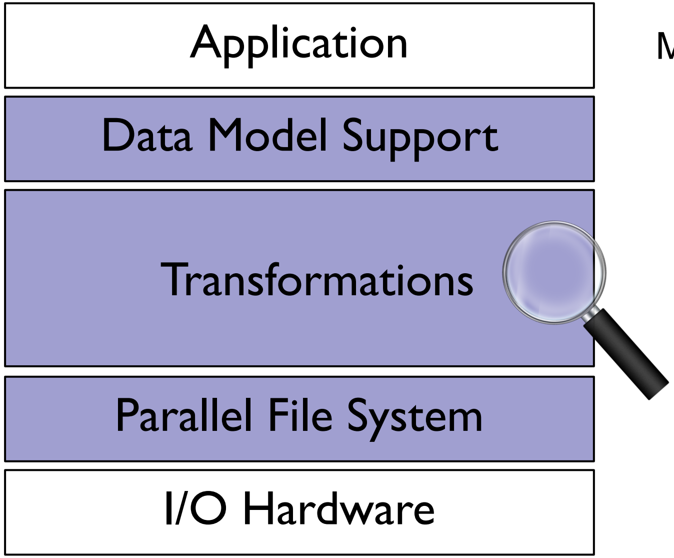

MPI-IO stats:

- Operation counts (open, read, write, sync)
- Collective and independent I/O usage
- Total read/write volumes
- Access size info
  - Common values
  - Histograms
- I/O timing

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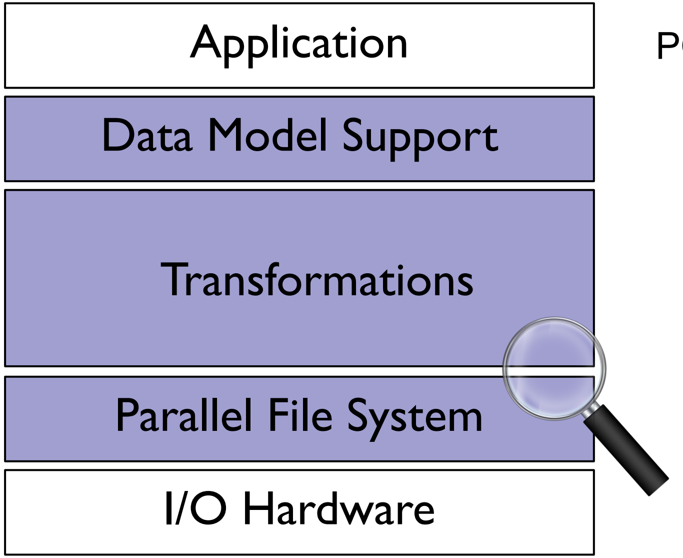

POSIX stats:

- Operation counts (open, read, write, seek, stat)
- Total read/write volumes
- File alignment
- Access size/stride info
  - Common values
  - Histograms
- I/O timing

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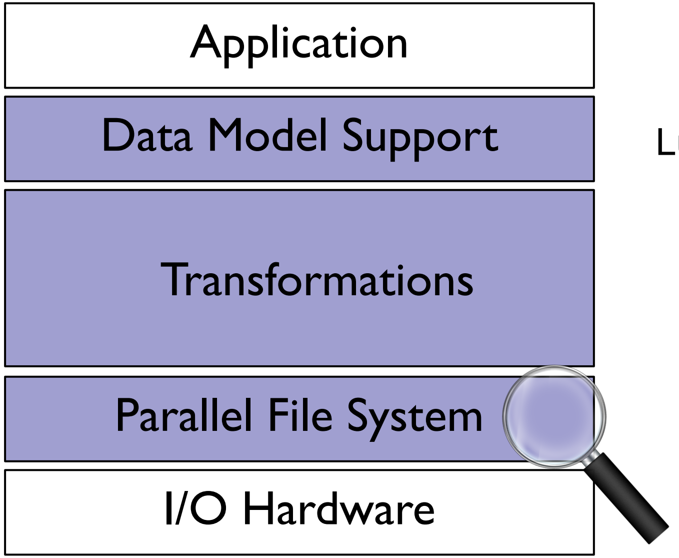

Lustre stats:

- Data server (OST) and metadata server (MDT) counts
- Stripe size/width
- OST list serving a file

Characterizing HPC I/O workloads with Darshan

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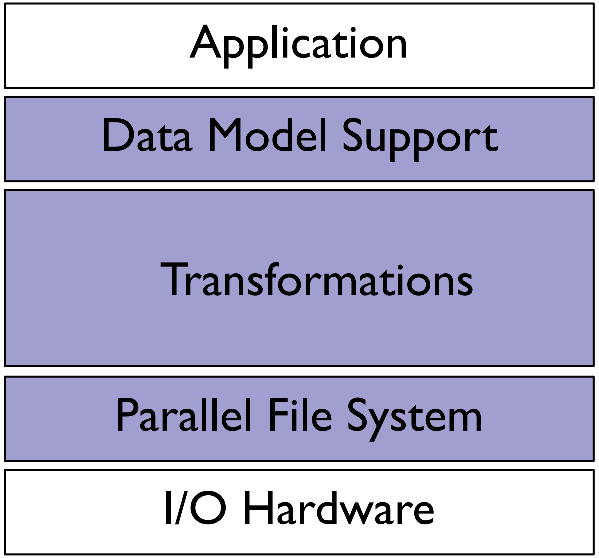


Let's see how Darshan can be leveraged in some practical use cases that demonstrate general best practices in tuning HPC I/O performance

Tuning the parallel file system

Ensuring storage resources match application I/O needs

For some parallel file systems like Lustre, users have direct control over file striping parameters

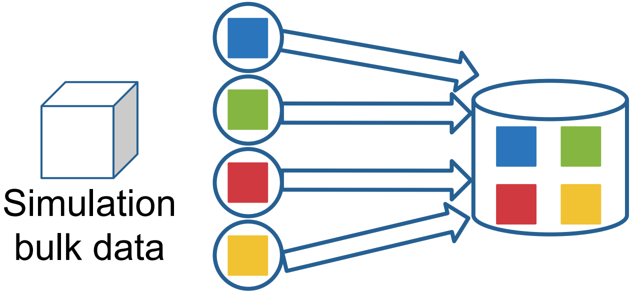
Bad news: Users may have to have some knowledge of the file system to get good I/O performance

Good news: Users can often get higher I/O performance than system defaults with thoughtful tuning -- file systems aren't perfect for every workload!

Tuning the parallel file system

Ensuring storage resources match application I/O needs

Tuning decisions can and should be made independently for different file types



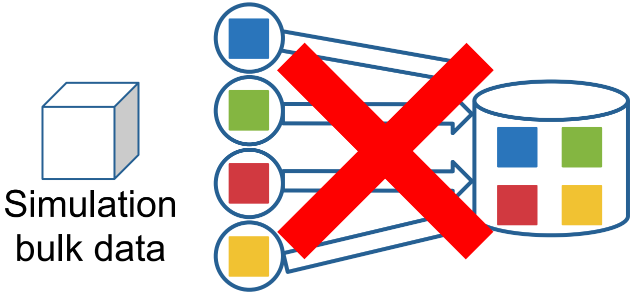
Simulation clients write
data to 1 storage server

Tuning the parallel file system

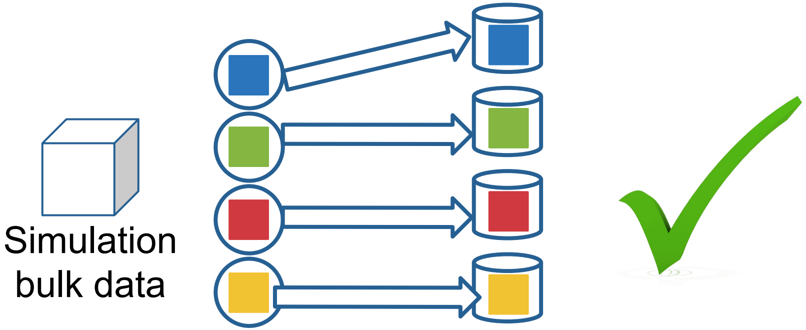
Ensuring storage resources match application I/O needs

Tuning decisions can and should be made independently for different file types

Large application datasets should ideally be distributed across as many storage resources as possible



Simulation clients write data to 1 storage server



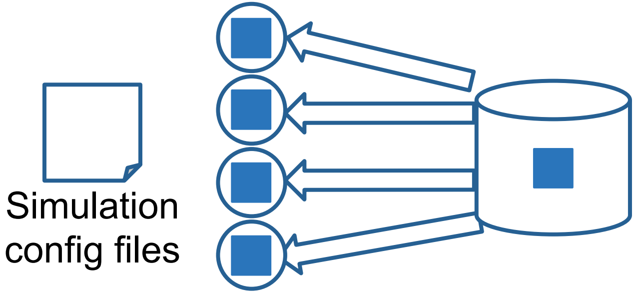
Simulation clients load balance writes across multiple servers

Tuning the parallel file system

Ensuring storage resources match application I/O needs

Tuning decisions can and should be made independently for different file types

On the other hand, smaller files often benefit from being stored on a single server



Simulation clients read config data from 1 storage server

Tuning the parallel file system

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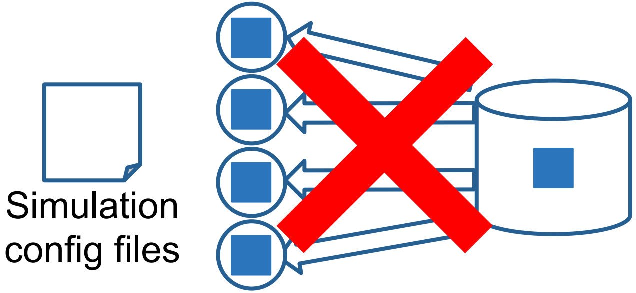
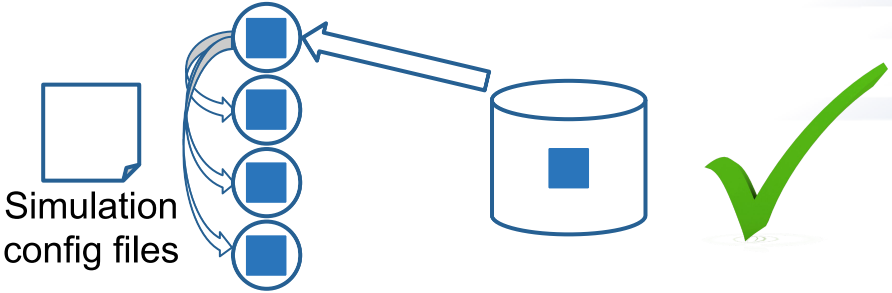


Simulation clients read config data from 1 storage server



Better yet, limit storage contention by having 1 client read data and distribute using communication (e.g., MPI)

Tuning the parallel file system

Ensuring storage resources match application I/O needs

Be aware of what file system settings are available to you and don't assume system defaults are always the best… you might be surprised what you find

- ALCF Theta and NERSC Cori scratch file systems both have a default Lustre stripe width of 1 (i.e., files are stored on one server by default)

Darshan output from a simple 10-process (10-node) POSIX I/O workload to a shared file on a Cori's Lustre scratch volume:

jobid: 32840482	uid: 69628	nprocs: 10	runtime: 6 seconds

I/O performance *estimate* (at the POSIX layer): transferred 1000.0 MiB at 210.38 MiB/s

```
LUSTRE_STRIPE_SIZE  1048576 /global/cscratc
LUSTRE_STRIPE_WIDTH 1    /global/cscratch1/s
LUSTRE_OST_ID_0 100 /global/cscratch1/sd/ss
```

Tuning the parallel file system

Ensuring storage resources match application I/O needs

jobid: 32840482	uid: 69628	nprocs: 10	runtime: 6 seconds

I/O performance *estimate* (at the POSIX layer): transferred 1000.0 MiB at 210.38 MiB/s

```
> lfs setstripe -c 10 testFile # change stripe width to 10
```

jobid: 32840482	uid: 69628	nprocs: 10	runtime: 3 seconds

I/O performance *estimate* (at the POSIX layer): transferred 1000.0 MiB at 562.48 MiB/s

```
LUSTRE_STRIPE_SIZE  1048576 /global/cscrat
LUSTRE_STRIPE_WIDTH 10  /global/cscratch1/
LUSTRE_OST_ID_0 220 /global/cscratch1/sd/s
LUSTRE_OST_ID_1 146 /global/cscratch1/sd/s
LUSTRE_OST_ID_2 107 /global/cscratch1/sd/s
LUSTRE_OST_ID_3 181 /global/cscratch1/sd/s
LUSTRE_OST_ID_4 47  /global/cscratch1/sd/s
LUSTRE_OST_ID_5 209 /global/cscratch1/sd/s
LUSTRE_OST_ID_6 244 /global/cscratch1/sd/s
LUSTRE_OST_ID_7 112 /global/cscratch1/sd/s
LUSTRE_OST_ID_8 36  /global/cscratch1/sd/s
LUSTRE_OST_ID_9 154 /global/cscratch1/sd/s
```

~200% performance boost

Tuning low-level (POSIX) file I/O

Making efficient use of a no-frills I/O API

Users may also need to pay close attention to file system alignment when crafting I/O accesses to a file

- Accesses that are not aligned can introduce performance inefficiencies on file systems

Tuning low-level (POSIX) file I/O

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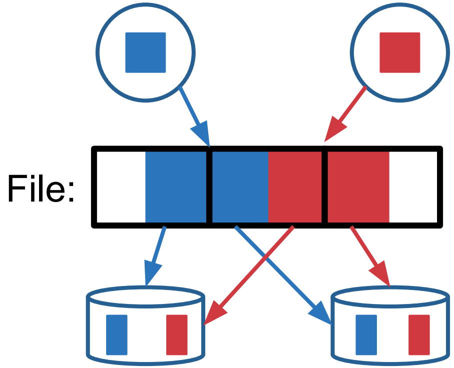
- Accesses that are not aligned can introduce performance inefficiencies on file systems

For Lustre, performance can be maximized by aligning I/O to stripe boundaries:



Unaligned I/O requests can span multiple servers and introduce inefficiencies in storage protocols

Tuning low-level (POSIX) file I/O

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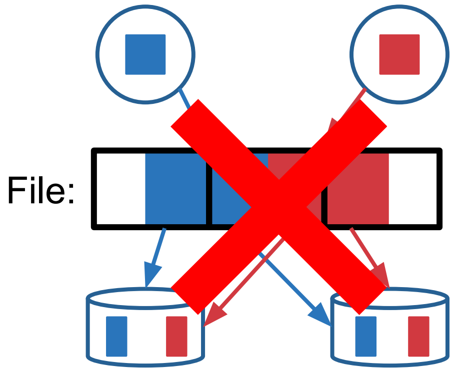
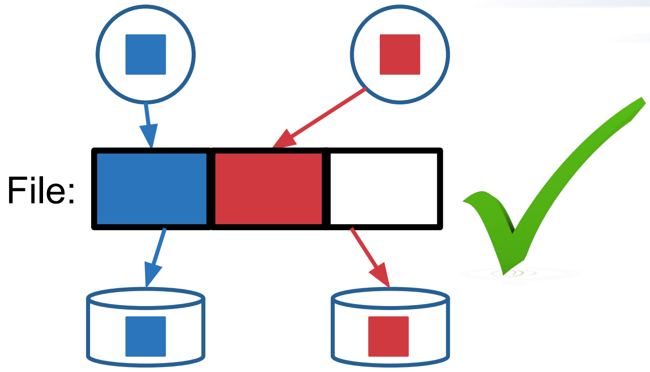


Instead, ensure client accesses are well-aligned to avoid Lustre server contention



Tuning low-level (POSIX) file I/O

Making efficient use of a no-frills I/O API

Repeating our simple 10-client example striping a single file across 10 Lustre OSTs on Cori

Unaligned:

transferred 1000.0 MiB at 310.14 MiB/s

# Module	Rank	Wt/Rd	Segment	Offset	Length	Start(s)	End(s)	[OST]	
X_POSIX	0	write	0	524288	1048576	0.0065	0.0594	[32]	[197]
X_POSIX	1	write	0	1572864	1048576	0.0065	0.0538	[197]	[237]
X_POSIX	2	write	0	2621440	1048576	0.0070	0.0440	[237]	[26]
X_POSIX	3	write	0	3670016	1048576	0.0067	0.0485	[26]	[213]

Hands on exercises: https://github.com/radix-io/hands-on

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```

Aligned:

transferred 1000.0 MiB at 380.28 MiB/s

```
# Module      Rank  Wt/Rd  Segment        Offset       Length     Start(s)      End(s)  [OST]
 X_POSIX         0  write        0             0      1048576       0.0054      0.0066  [197]
 X_POSIX         1  write        0       1048576      1048576       0.0053      0.0064  [102]
 X_POSIX         2  write        0       2097152      1048576       0.0061      0.0072  [106]
 X_POSIX         3  write        0       3145728      1048576       0.0053      0.0064  [120]
```


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Tuning low-level (POSIX) file I/O

Making efficient use of a no-frills I/O API

Even in this small workload, we pay a nearly 20% performance penalty when I/O accesses are not aligned to file stripes (1 MB)

Unaligned:

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Tuning low-level (POSIX) file I/O

Making efficient use of a no-frills I/O API

Accounting for subtle characteristics about I/O performance behavior like file alignment can be a painstaking (or maybe just painful) process…

As highlighted by other presentations, high-level I/O libraries like HDF5 and PnetCDF can help mask much of the complexity needed for transforming scientific computing I/O workloads into performant POSIX-level file system accesses – ***don't reinvent the wheel, use high-level I/O libraries wherever you can****!*

Tuning high-level (HDF5) data access

Optimizing application interactions with the I/O stack

Recall that HDF5 provides a chunking mechanism to partition user datasets into contiguous chunks in the underlying file

- Users can greatly improve performance of partial dataset I/O operations by choosing chunking parameters that match expected access patterns

Tuning high-level (HDF5) data access

Optimizing application interactions with the I/O stack

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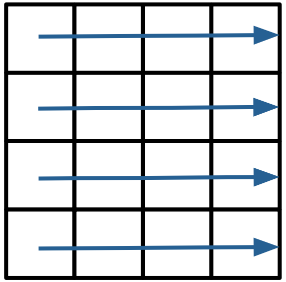

By default, HDF5 will store the dataset contiguously row-by-row (i.e., row-major format) in the file

Tuning high-level (HDF5) data access

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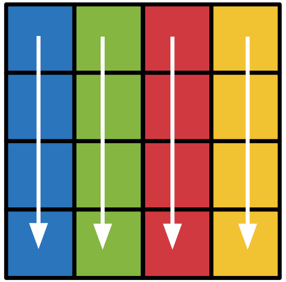
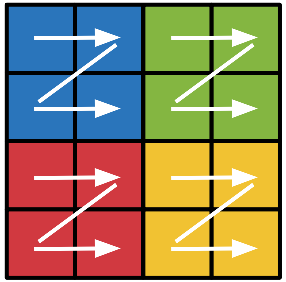


column-based



block-based

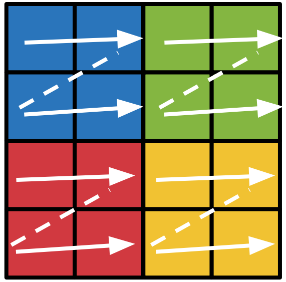
If dataset access patterns do not suit a simple row-major storage scheme, chunking can be applied to map chunks of dataset data to contiguous regions in the file

Tuning high-level (HDF5) data access

Optimizing application interactions with the I/O stack

Consider a 256-process (16-node) example where each process exclusively accesses a block of the dataset

- Each process writes a 2048x2048 block of the dataset (32 MB per-process, 8 GB total)



With no chunking, each process must issue many smaller non-contiguous I/O requests (solid lines) and seek around the file (dashed lines) and, yielding low I/O performance

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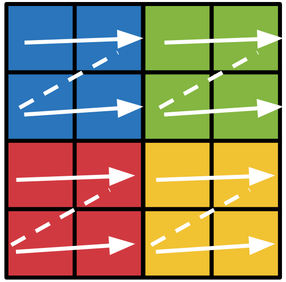
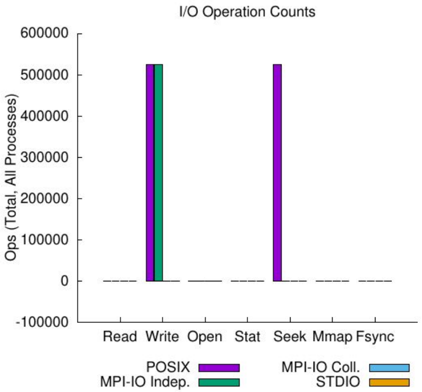


jobid: 32972116	uid: 69628	nprocs: 256	runtime: 143 seconds

I/O performance *estimate* (at the MPI-IO layer): transferred 8192.0 MiB at 57.97 MiB/s



Most Common Access Sizes (POSIX or MPI-IO)

	access size	count
POSIX	16384	524288
	96	2
	544	1
	328	1

256 individual HDF5 writes (1-per-process) yields 500K+ POSIX writes

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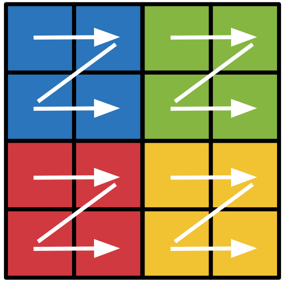

With chunking applied, each process can read their entire data block using one large, contiguous access in the file

Hands on exercises: https://github.com/radix-io/hands-on

Tuning high-level (HDF5) data access

Optimizing application interactions with the I/O stack

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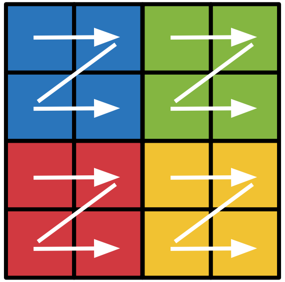
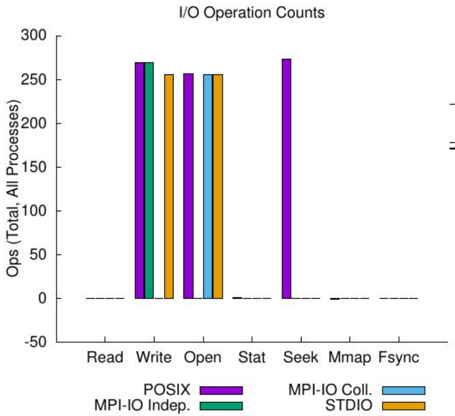


jobid: 32972116	uid: 69628	nprocs: 256	runtime: 52 seconds

I/O performance *estimate* (at the MPI-IO layer): transferred 8192.0 MiB at 164.73 MiB/s



Most Common Access Sizes
(POSIX or MPI-IO)

	access size	count
POSIX	33554432	256
	2616	6
	96	2
	544	1

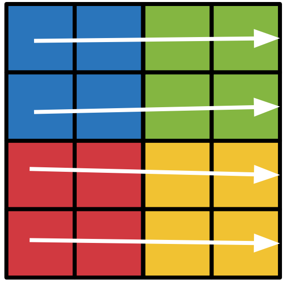
Appropriate chunking selection yields 2.8x performance increase

Tuning high-level (HDF5) data access

Optimizing application interactions with the I/O stack

An alternative optimization uses collective I/O to improve the efficiency of this block-style data access

- Rely on MPI-IO layer collective buffering algorithm to generate contiguous storage accesses and to limit number of clients interacting with storage system



With collective I/O enabled, designated aggregator processes perform I/O on behalf of their peers, and communicate their data using MPI calls

E.g., the green process sends its write data to the blue process (aggregator), who then writes both of their data in one big contiguous chunk

Tuning high-level (HDF5) data access

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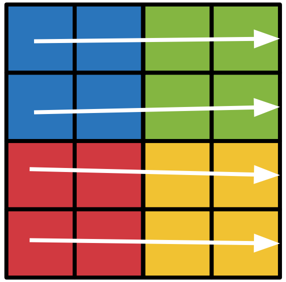
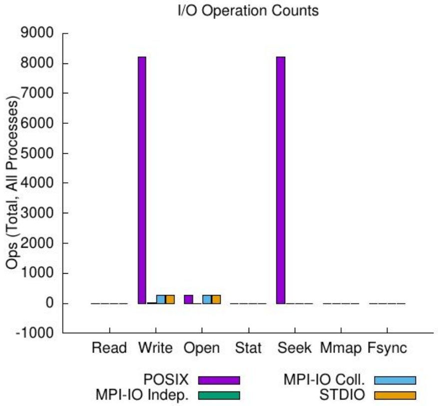


jobid: 32972116	uid: 69628	nprocs: 256	runtime: 32 seconds

I/O performance *estimate* (at the MPI-IO layer): transferred 8192.0 MiB at 268.28 MiB/s



Most Common Access Sizes (POSIX or MPI-IO)

	access size	count
POSIX	1048576	8191
	96	2
	1046528	1
	2048	1

Collective I/O yields 4.6x improvement over no chunking, and 1.6x improvement over chunking

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Using Darshan to analyze HDF5 apps

Collective vs independent I/O behavior

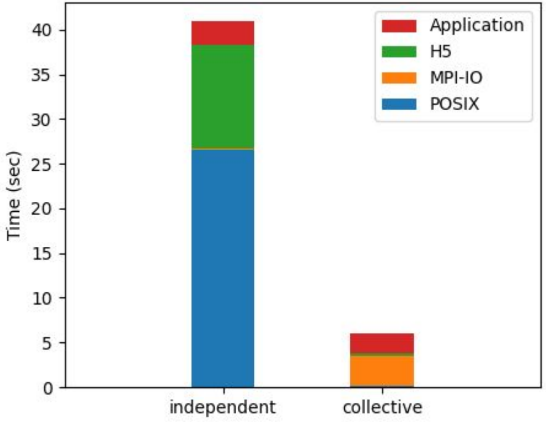
Using the MACSio[1] HDF5 benchmark, run a couple of simple examples demonstrating the types of insights HDF5 I/O instrumentation can enable

- 60-process (5-node) single shared file, 3d mesh, write roughly 1 GiB of cumulative data
- Compare performance of collective and independent 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**



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

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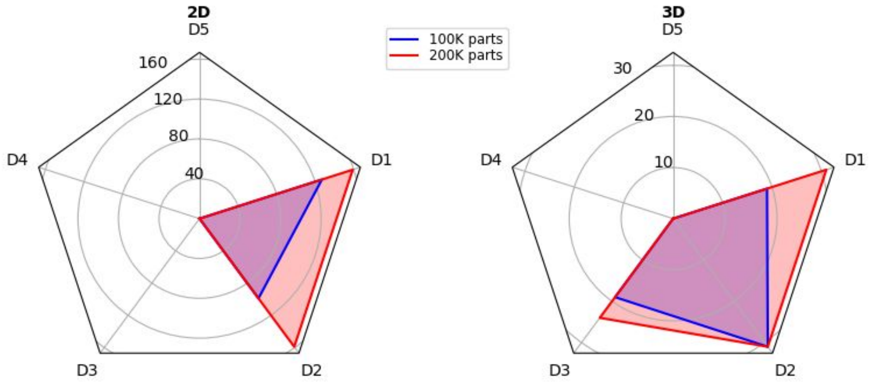
ECP EXASCALE COMPUTING PROJECT

Using Darshan to analyze HDF5 apps

Dataset access patterns

Using the MACSio[1] HDF5 benchmark, run a couple of simple examples demonstrating the types of insights HDF5 I/O instrumentation can enable

- 60-process (5-node) single shared file, 3d mesh, write roughly 1 GiB of cumulative data
- Compare dataset access patterns across different configurations



Number of elements accessed in each dataset dimension for the most common access for each MACSio configuration

Radar plots, or other methods, can be used to help visualize characteristics of HDF5 dataset accesses

Dataset access patterns could be used to help set/optimize chunking parameters to limit accesses to as few chunks as possible

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

Summarizing I/O tuning options

As a user of I/O interface X, what tuning vectors do I have?

I/O Interface	Striping	Alignment	Collective I/O	Chunking
HDF5	✓	✓	✓	✓
PnetCDF	✓	✓	✓	X
MPI-IO	✓	✓	✓	X
POSIX	✓	✓-	X	X

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POSIX	✓	✓ -	X	X

Automatically align application data and library metadata, if user requests so

Collective I/O can be automatically aligned

POSIX I/O requires manually aligning every access

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POSIX	✓	✓-	X	X

Just another reminder that high-level I/O libraries are here to make your life easier

- I/O optimization strategies like collective I/O & chunking can net large performance gains, especially when combined with striping and alignment optimizations

Accounting for a changing HPC landscape

Adapting to technological shifts

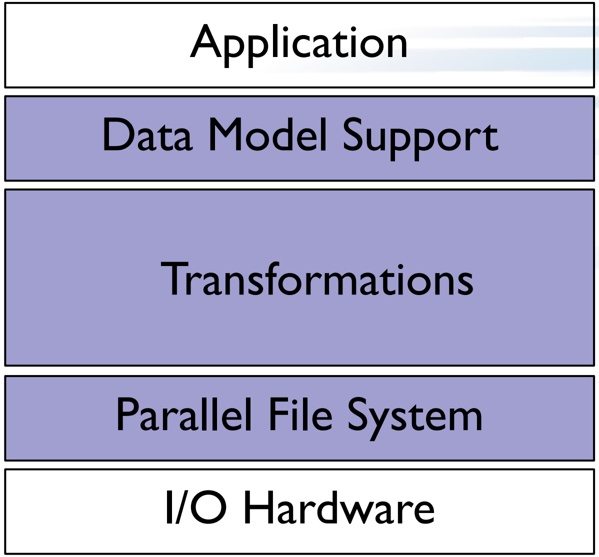
The various technologies covered today form much of the foundation of the traditional HPC data management stack

- Variations on this stack have been deployed at HPC facilities and leveraged by users for high-performance parallel I/O for decades

But, the HPC computing landscape is changing, even if slowly

Changes driven at both ends of the stack

- Newly embraced compute paradigms
- Emerging storage technologies



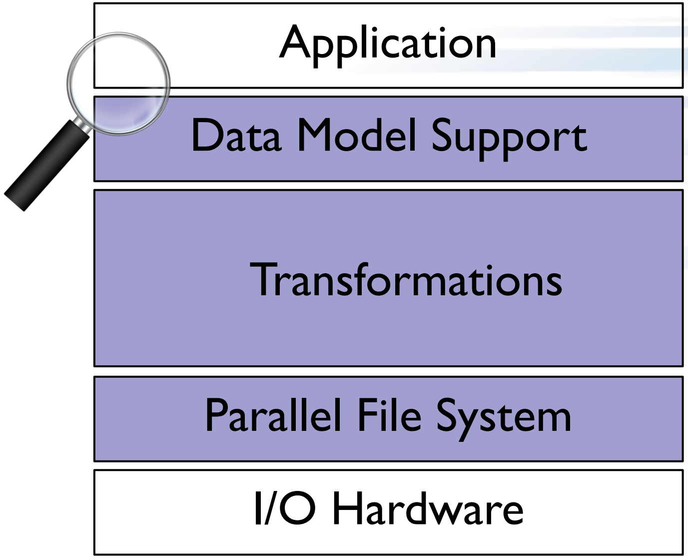
Accounting for a changing HPC landscape

Adapting to technological shifts

Large-scale MPI applications are still the norm at most HPC centers, but other non-MPI compute frameworks are gaining traction:

- Deep learning (TensorFlow, Keras, PyTorch)
- Data analytics frameworks (Spark, Dask)
- Other non-MPI distributed computing frameworks (Legion, UPC)

Many of these frameworks define their own data models and have their own mechanisms for managing distributed tasks



Instrumenting non-MPI applications with Darshan

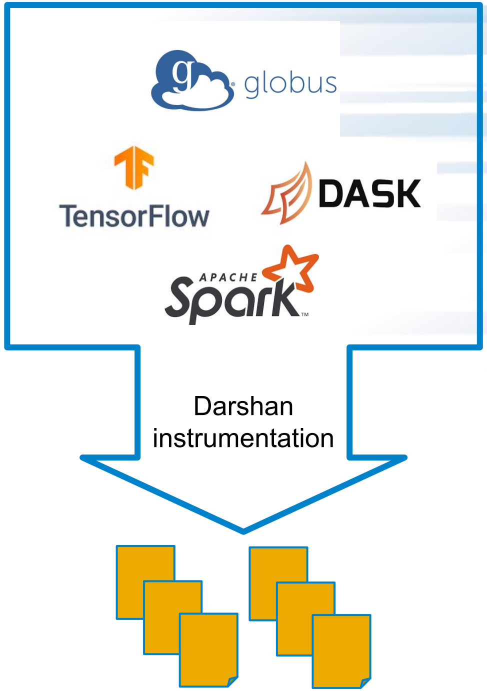
Starting with Darshan version 3.2.0, Darshan supports instrumentation of non-MPI applications*

- Just set DARSHAN_ENABLE_NONMPI environment variable before running

Generates unique Darshan log for each process

Extend Darshan instrumentation from traditional MPI applications to any type of executable

- Python frameworks
- File transfer utilities
- Data service daemons
- Other serial applications



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- Other serial applications

***Caveats:**

- Apps must be dynamically-linked
- Non-MPI mode does not work on Theta's Darshan install, use Spack instead
  - `spack install darshan-runtime~mpi`
  - `spack load darshan-runtime`
  - `LD_PRELOAD` the Darshan shared library
  - Logs stored in `$HOME`

Accounting for a changing HPC landscape

Adapting to technological shifts

HPC storage technology is changing to meet needs of diverse application workloads

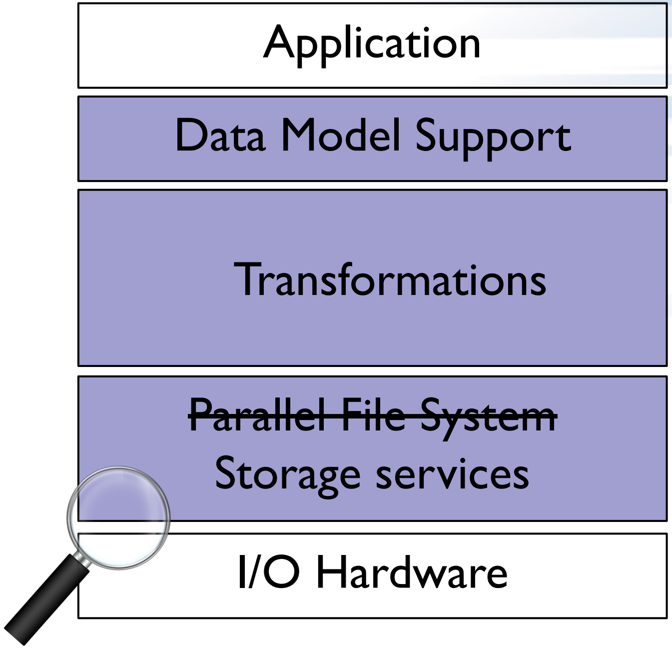
- Users typically have more options than a traditional parallel file system over HDDs

Hardware trends enabling low-latency, high-bandwidth I/O to applications

- Burst buffers, NVM

Novel storage services offer compelling alternatives to traditional file systems

- Unify, DAOS



Recent and ongoing Darshan developments

- New instrumentation modules
  - Heatmap module (*available in 3.4.0*)
    - Provide histograms of I/O activity for different Darshan modules over time
    - Finer-grained accounting of I/O activity without doing a full trace
  - PnetCDF modules (*coming soon*)
    - Support for PnetCDF file and variable interfaces
    - Contributed by Wei-Keng Liao and Claire Lee (Northwestern University)
  - DAOS modules (*coming soon*)
    - Support for DAOS file and object interfaces
- PyDarshan log analysis framework
  - New job summary tool to replace darshan-job-summary.pl (*available in 3.4.0*)
  - Methods to extract actionable I/O insights from logs (coming soon)
    - Can suggest tuning strategies for detected I/O behaviors in Darshan logs
  - Contributions from Nik Awtrey and Tyler Reddy (LANL), and Jakob Luttgau (UTK)

PyDarshan: simplifying Darshan log file analysis

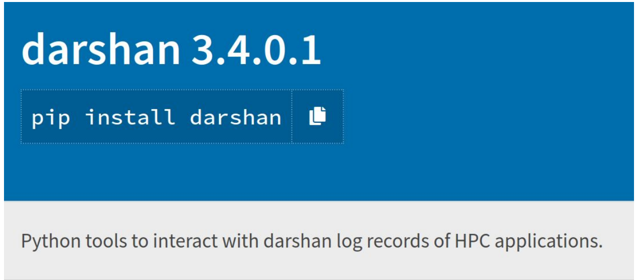
Darshan traditionally offered only the C-based darshan-util library and a handful of corresponding tools to users

- Development of custom Darshan analysis tools was a cumbersome task

PyDarshan developed to simplify the interfacing of analysis tools with log data

- Use Python CFFI module to provide Python bindings to the native darshan-utils C API
- Expose Darshan log data as dictionaries, pandas dataframes, and numpy arrays

Ideally, PyDarshan will lead to a richer ecosystem for Darshan log analysis tools



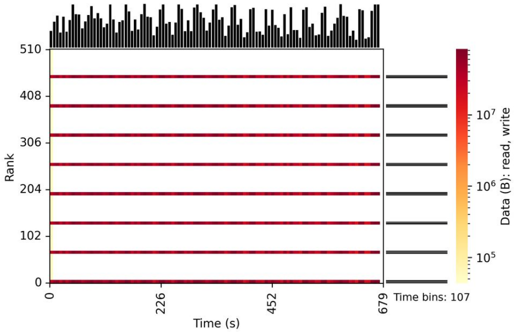
PyDarshan is currently available on PyPI and ready for users to analyze Darshan logs with – use '**`pip install darshan`**'

PyDarshan: simplifying Darshan log file analysis

PyDarshan includes a new job summary tool that produces HTML reports detailing the I/O behavior of applications

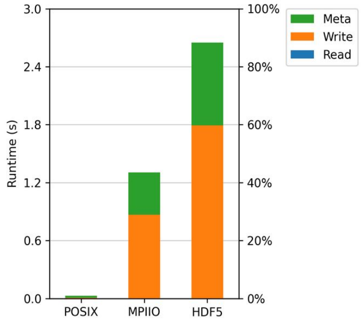
- To generate a report, run ‘`python -m darshan summary <logfile>`’

Heat Map: HEATMAP POSIX



New heatmap module plots highlight app I/O intensity over time, ranks, and interfaces

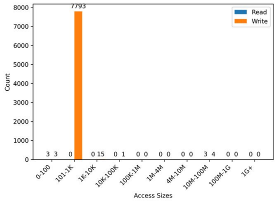
I/O Cost



Old plots have been extended to account for new modules like HDF5

Per-Module Statistics: POSIX

Access Sizes



Common Access Sizes

Access Size	Count
192	7688
128	50
178	35
356	15

Detailed per-module I/O summaries

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ECP EXASCALE COMPUTING PROJECT

Wrapping up

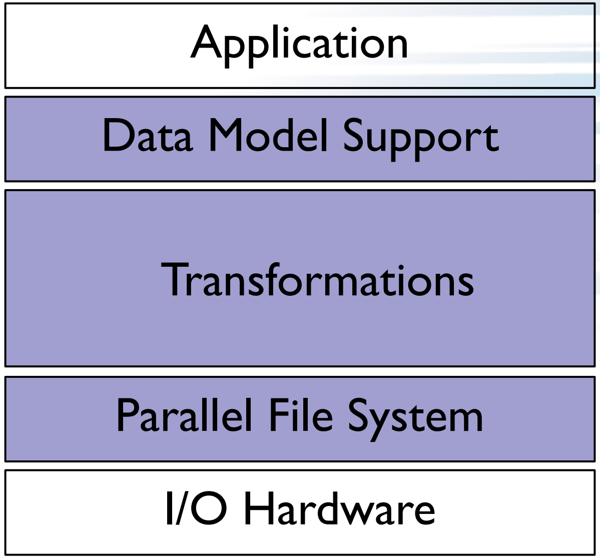
Hopefully this material proves useful in providing a deeper understanding of the different layers of the HPC I/O stack covered today, as well as potential tuning vectors available to you as user

- Optimizing your I/O workload can be challenging, but can potentially offer large performance gains
- Use high-level I/O libraries where you can
- Don't always count on I/O libraries or file systems to automatically provide you the best performance out of the box

Darshan is invaluable for providing understanding of application I/O behavior and informing potential tuning

- https://github.com/darshan-hpc/darshan

Please reach out with questions, feedback, etc.



Thank you!

Bonus

Understanding I/O beyond the application

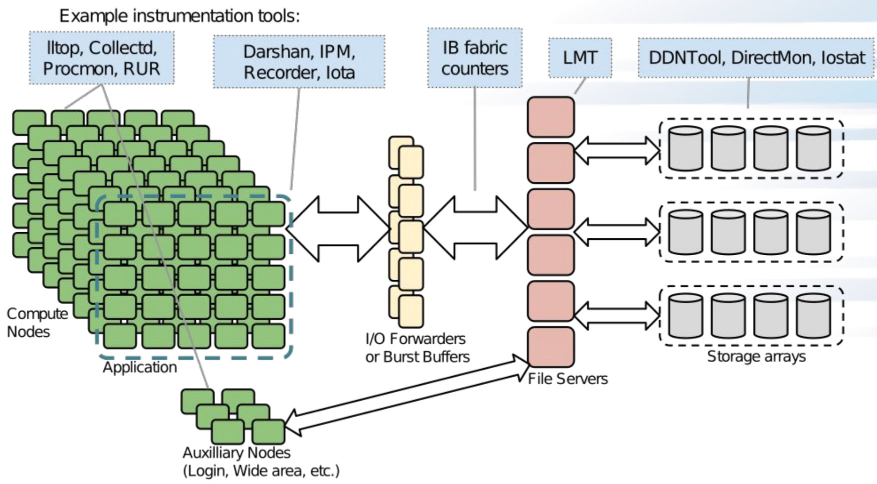
Into the wild...

Many storage resources at HPC facilities are shared between users

- Application-centric analysis can only tell us so much about HPC I/O behavior -- systems-level perspective is needed for complete picture

A more complete understanding of system I/O behavior is critical to reasoning about I/O performance

- How is my performance compared to others?
- What are the performance bottlenecks?
- How much is my I/O affected by contention?



Many existing tools can be used to help compile an accurate system-level view of I/O

Understanding I/O beyond the application

Forming a holistic view

The TOKIO (Total Knowledge of I/O) project aims to provide a framework for holistic characterization and analysis of HPC I/O workloads:

- Collect, integrate, and analyze disparate I/O data
- Define platform-independent blueprint for deploying and utilizing I/O characterization tools, data collection/storage services, and analysis methods
- Provide a trove of relevant data characterizing HPC I/O workloads

Stakeholders:

- Application scientists (productivity)
- Facility operators (efficiency)
- Researchers (optimization)

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

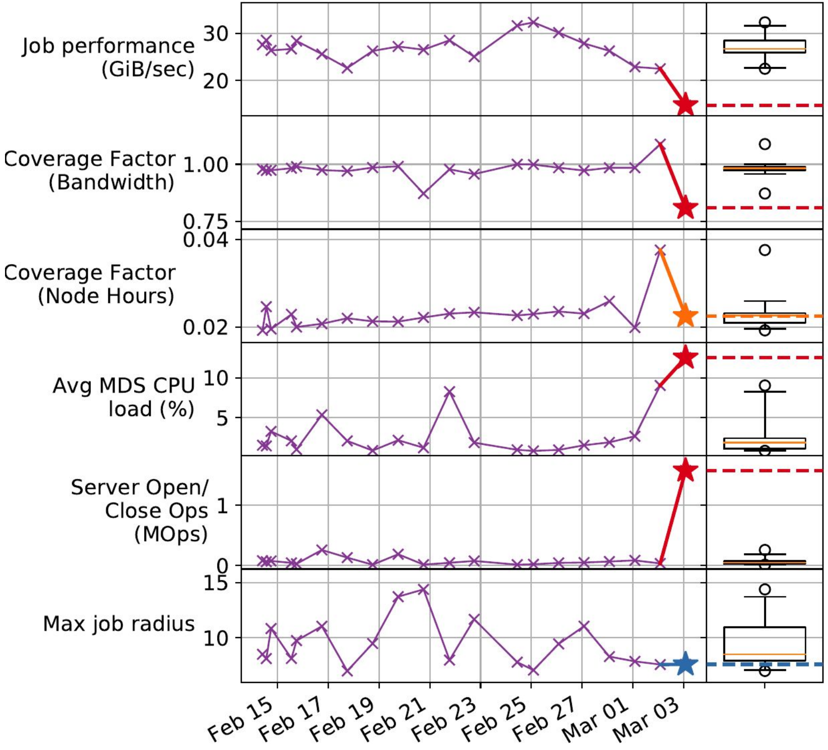
Understanding I/O beyond the application

A TOKIO example

TOKIO utility called UMAMI (Unified metrics and measurements interface) contextualizes application performance measurements with other system measurements

How does my performance compare to previous runs?

Do any metrics stand out that positively/negatively impacted my performance?



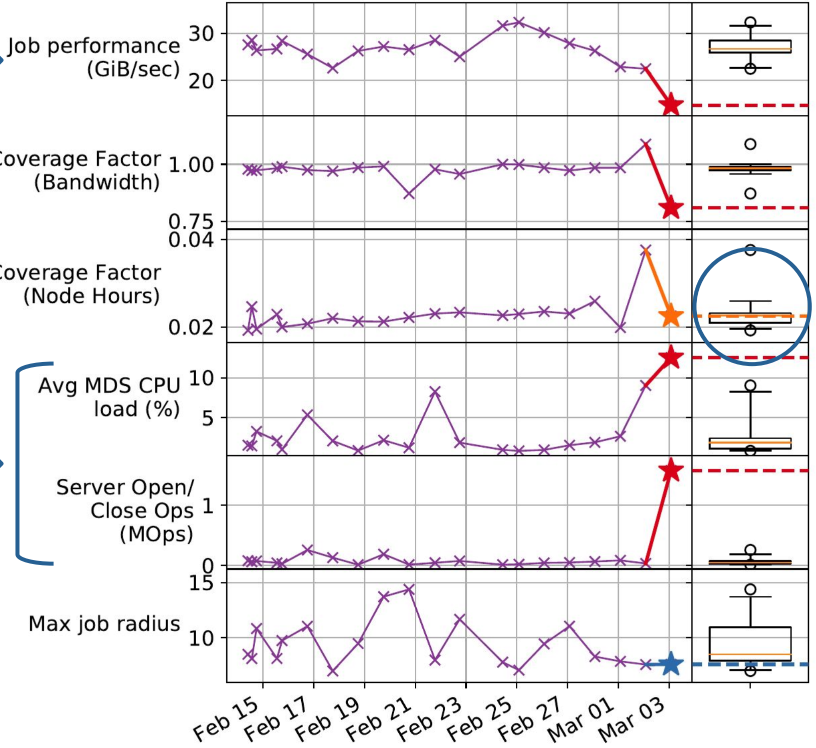
Understanding I/O beyond the application

A TOKIO example

Raw performance

Coverage factor represents contention

Metadata loads

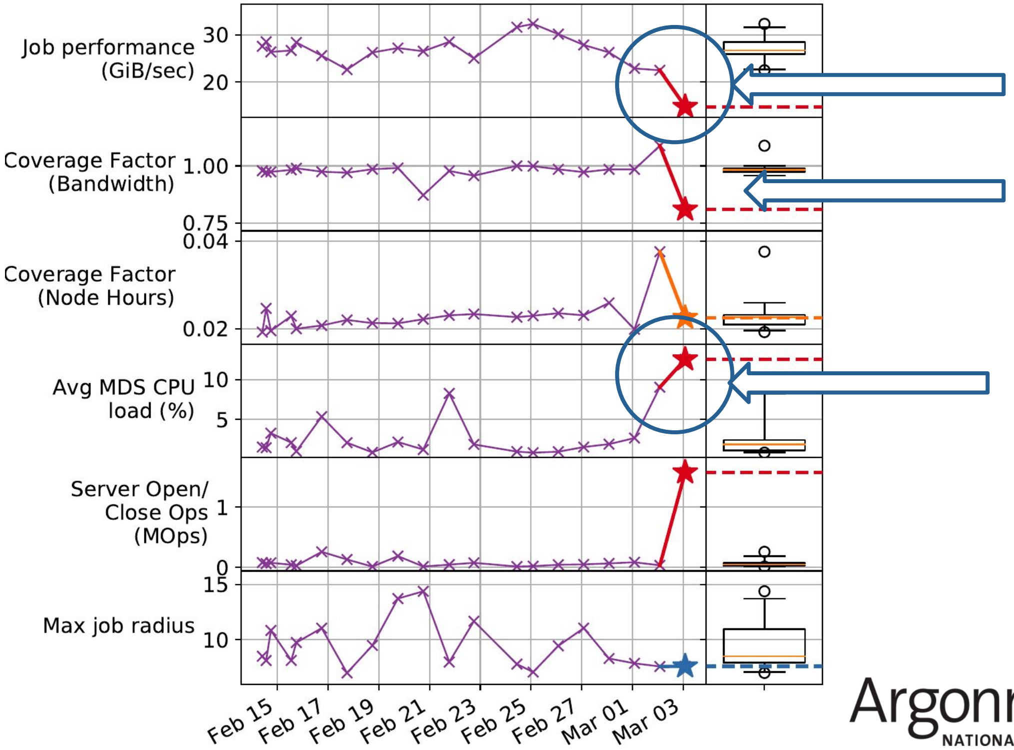


Historical measurements

Box plots to compare against historical measurements

Understanding I/O beyond the application

A TOKIO example



Low performance relative to recent runs

Low coverage factor, meaning other jobs were performing I/O while we were

High metadata server load also likely impacting performance