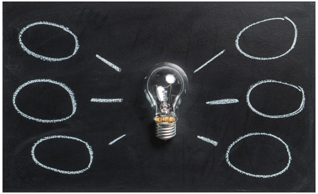
Julian Kunkel

Data Storage



Learning Objectives

- Sketch a typical I/O stack
- Develop a NetCDF data model for a given use case
- Compare the performance of different storage media
- Sketch application types and access patterns
- Justify the use for I/O benchmarks
- Describe an I/O performance optimization technique
- Describe a strategy for trustworthy benchmark result

Outline

Reminder: High-Performance Computing (HPC)

Definitions

- HPC: Field providing massive compute resources for a computational task
  - Task needs too much memory or time on a normal computer
  - $\Rightarrow$ Enabler of complex scientific simulations, e.g., weather, astronomy
- Supercomputer: aggregates power of 10,000 compute devices
- Storage system: provides some kind of storage with some API
- File system: provides a hierarchical namespace and “file” interface
- Parallel I/O: multiple processes can access distributed data concurrently

Supercomputers Host Costly Storage

- Compute performance growth by 20x each generation (∼5 years).
- Storage throughput/capacity improves by just 6x.

Exascale Storage Systems – An Analytical Study of Expenses

	2004	2009	2015	2020	2025	Exascale (2020)
Performance	1.5 TF/s	150 TF/s	3 PF/s	60 PF/s	1.2 EF/s	1 EF/s
Nodes	24	264	2500	12,500	31,250	100k-1M
Node performance	62.5 GF/s	0.6 TF/s	1.2 TF/s	4.8 TF/s	38.4 TF/s	1-15 TF/s
System memory	1.5 TB	20 TB	170 TB	1.5 PB	12.8 PB	3.6-300 PB
Storage capacity	100 TB	5.6 PB	45 PB	270 PB	1.6 EB	0.15-18 EB
Storage throughput	5 GB/s	30 GB/s	400 GB/s	2.5 TB/s	15 TB/s	20-300 TB/s
Disk drives	4000	7200	8500	10000	12000	100k-1000k
Archive capacity	6 PB	53 PB	335 PB	1.3 EB	5.4 EB	7.2-600 EB
Archive throughput	1 GB/s	9.6 GB/s	21 GB/s	57 GB/s	128 GB/s	-
Power consumption	250 kW	1.6 MW	1.4 MW	1.4 MW	1.4 MW	20-70 MW
Investment	26 M€	30 M€	30 M€	30 M€	30 M€	$200 M[4]

Real Values – 2018

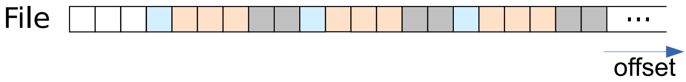
	Mistral
Characteristics	Value
Performance	3.1 PF/s
Nodes	2882
Node performance	1.0 TF/s
System memory	200 TB
Storage capacity	52 PB
Storage throughput	700 GB/s
Disk drives	10600
Archive capacity	500 PB
Archive throughput	18 GB/s
Compute costs	15.75 M EUR
Network costs	5.25 M EUR
Storage costs	7.5 M EUR
Archive costs	5 M EUR
Building costs	5 M EUR
Investment	38.5 M EUR
Compute power	1100 kW
Network power	50 kW
Storage power	250 kW
Archive power	25 kW
Power consumption	1.20 MW

Application Data vs. File

Applications work with (semi)structured data

- Vectors, matrices, n-Dimensional data

A file is just a sequence of bytes!



Applications/Programmers must serialize data into a flat namespace

- Uneasy handling of complex data types
- Mapping is performance-critical
- Vertical data access unpractical (e.g., to to pick a slice of multiple files)

The I/O Stack

- Parallel application
  - Is distributed across many nodes
  - Has a specific access pattern for I/O
  - May use several interfaces
    File (POSIX, ADIOS, HDF5), SQL, NoSQL
- Middleware provides high-level access
- POSIX: ultimately file system access
- Parallel file system: Lustre, GPFS, PVFS2
- File system: EXT4, XFS, NTFS
- Block device: utilizes storage media to export a block API
- Operating system: (orthogonal aspect)

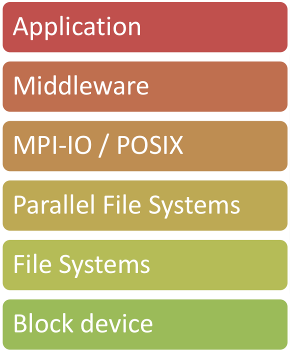


Figure: Example I/O stack

Storage Media

- Many technologies are available with different characteristics
- Block-accessible or byte-addressable (NVRAM)

	Memristor	PCM	STT-RAM	DRAM	Flash	HD
Chip area per bit (F^2)	4	8–16	14–64	6–8	4–8	n/a
Energy per bit (pJ)[2]	0.1–3	2–100	0.1–1	2–4	10^1–10^4	10^6–10^7
Read time (ns)	<10	20–70	10–30	10–50	25,000	5–8x10^6
Write time (ns)	20–30	50–500	13–95	10–50	200,000	5–8x10^6
Retention	>10 years	<10 years	Weeks	<Second	~10 years	~10 years
Endurance (cycles)	~10^{12}	10^7–10^8	10^{15}	>10^{17}	10^3–10^6	10^{15} ?
3D capability	Yes	No	No	No	Yes	n/a

Figure: Source: ZDNet [100]

Zoo of Interfaces

Multitude of data models

- POSIX File: Array of bytes
- HDF5: Container like a file system
  - Dataset: N-D array of a (derived) datatype
  - Rich metadata, different APIs (tables)
- Database: structured (+arrays)
- NoSQL: document, key-value, graph, tuple

Choosing the right interface is difficult – a workflow may involve several

Properties / qualities

- Namespace: Hierarchical, flat, relational
- Access: Imperative, declarative, implicit (`mmap()`)
- Concurrency: Blocking vs. non-blocking
- Consistency semantics: Visibility and durability of modifications

Application I/O Types

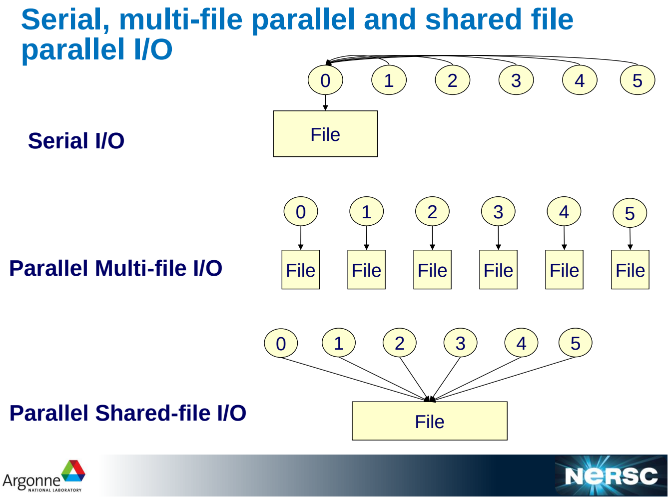


Figure: Source: Lonnie Crosby [101]

Application I/O Access Patterns

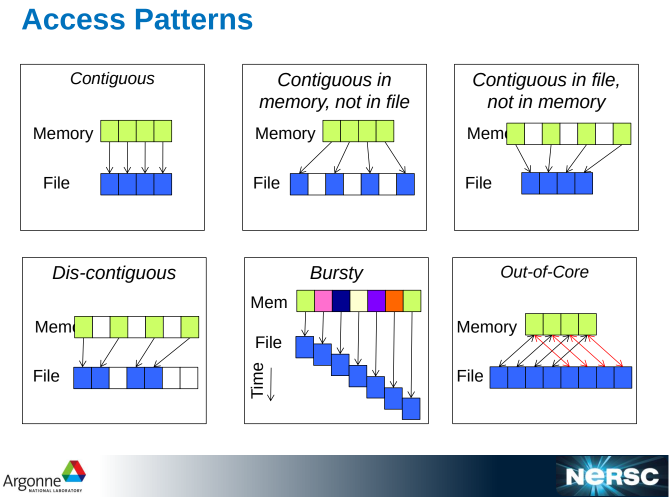


Figure: Source: Lonnie Crosby [101]

File Striping: Distributing Data Across Devices

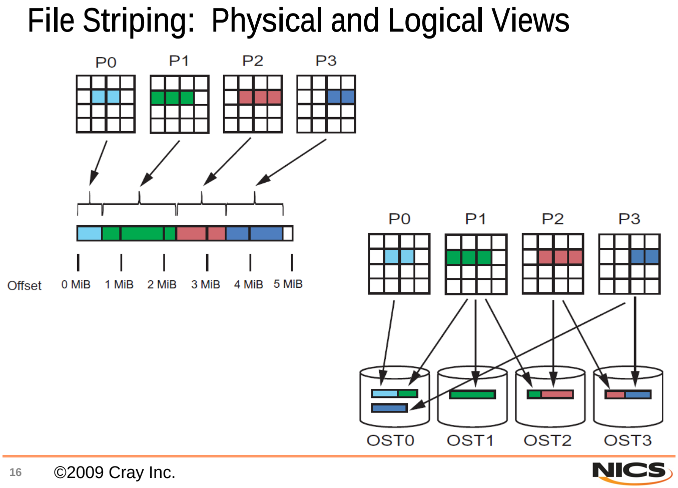


Figure: Source: Lonnie Crosby [101]

Parallel I/O Efficiency

- I/O intense science requires good I/O performance
- DKRZ file systems offer about 700 GiB/s throughput
  - However, I/O operations are typically inefficient: Achieving 10% of peak is good
  - Unfortunately, prediction of performance is barely possible
- Influences on I/O performance
  - Application's access pattern and usage of storage interfaces
  - Communication and slow storage media
  - Concurrent activity – shared nature of I/O
  - Tenable optimizations deal with characteristics of storage media
  - Complex interactions of these factors
- The I/O hardware/software stack is very complex – even for experts
- Requires tools and methods for
  - diagnosing causes
  - predicting performance, identification of slow performance
  - prescribing tunables/settings

Illustration of Performance Variability

- Measured at DKRZ (max. 700 GiB/s)
- Optimal performance:
  - Small configuration: 6 GiB/s per node
  - Large configurations: 1.25 GiB/s per node
- Best-case benchmark: optimal application I/O
  - Independent I/O with 10 MiB chunks of data
  - Real-world I/O is sparse and worse
- Configurations on user-side vary:
  - Number of nodes the benchmark is run
  - Processes per node
  - Read/Write accesses
  - Tunable: stripe size, stripe count
- Best setting depends on configuration!

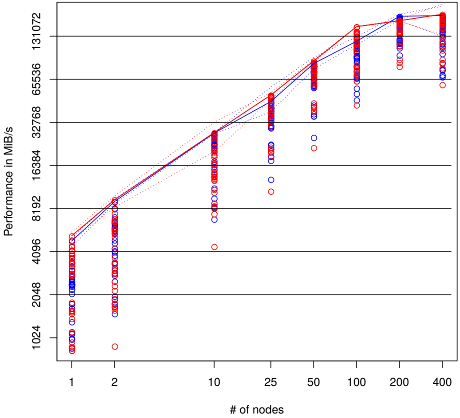


Figure: A point represents one configuration

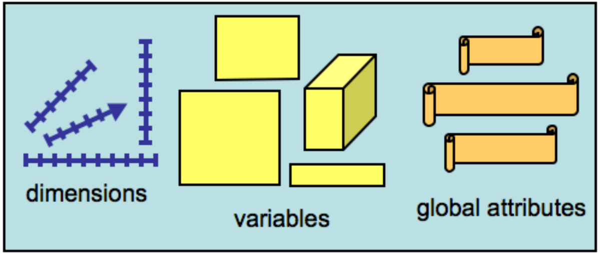
Outline

NetCDF

- NetCDF is an example for a "high-level" I/O-API and ecosystem
- In a simple view, NetCDF is:
  - A data model
  - A file format
  - A set of APIs and libraries for various programming languages
- Together, the data model, file format, and APIs support
  - creation, access, and **sharing** of scientific data
- Allows to describe multidimensional data and include metadata which further characterizes the data
- APIs are available for most programming languages used in geo-sciences

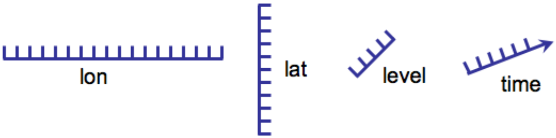
The Classic NetCDF Model

- NetCDF files are containers for Dimensions, Variables, and Global Attributes.
- A NetCDF file (dataset) has a path name and possibly some dimensions, variables, global (file-level) attributes, and data values associated with the variables.



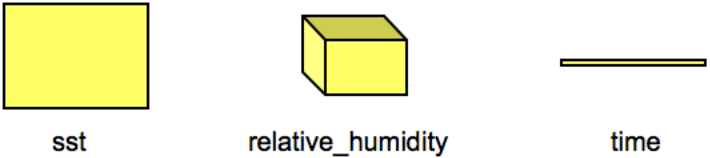
The Classic NetCDF Model – Dimensions

- Dimensions are used to specify variable shapes, grids, and coordinate systems.
- A dimension has a name and a length.
- A dimension can be used to represent a real physical dimension
  - Example: time, latitude, longitude, or height
- A dimension can also be used to index other quantities
  - Example: station or model run number
- The same dimension can be used in multiple variables.



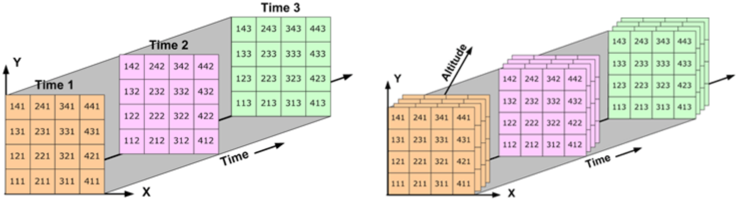
The Classic NetCDF Model – Variables

- A variable holds a multidimensional array of values of the same type
- A variable has a name, type, shape (according to dimensions), attributes, and values
- In the classic data model, the type of a variable is the external type of its data as represented on disk, one of: `char` (text character), `byte` (8 bits), `short` (16 bits), `int` (32 bits), `float` (32 bits), `double` (64 bits)



The Classic NetCDF Model – Data

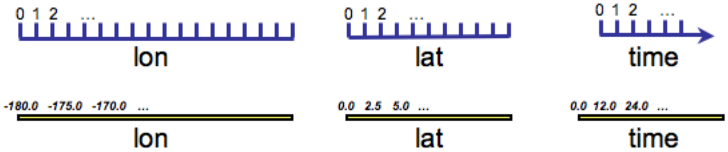
- The data in a NetCDF file is stored in the form of arrays. For example:
  - Temperature varying over time at a location is stored as a **one-dimensional array**
  - Temperature over an area for a given time is stored as a **two-dimensional array**
  - Three-dimensional (3D) data, like temperature over an area varying with time, or four-dimensional (4D) data, like temperature over an area varying with time and altitude, is stored as a **series of two-dimensional arrays**



Reference: https://pro.arcgis.com/en/pro-app/help/data/multidimensional/fundamentals-of-netcdf-data-storage.htm

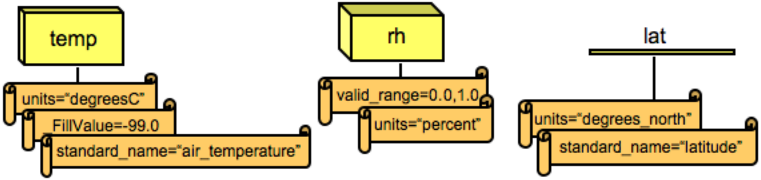
The Classic NetCDF Model – Coordinate Variables

- A 1D variable with the same name as a dimension is a **coordinate variable**
- The coordinate variable is associated with a dimension of one or more data variables and typically defines a physical coordinate corresponding to that dimension
- Many programs that read NetCDF files recognize coordinate values they find



The Classic NetCDF Model – Attributes

- Attributes hold metadata (data about data)
- An attribute contains information about properties of a variable or the whole dataset
- Attributes are scalars or 1-D arrays
- An attribute has a name, type, and values. Attributes are used to specify such properties as units, standard names (that identify types of quantity), special values, maximum and minimum valid values, scaling factors, offsets, ...



Common Data form Language (CDL)

- Notation used to describe NetCDF object is called CDL (network Common Data form Language)
  - Provides a convenient way of describing NetCDF datasets
- Utilities allow producing CDL text files from binary NetCDF datasets and vice-versa
- File contains dimensions, variables, and attributes
- Components are used together to capture the meaning of data and relations among data fields

```
netcdf filename {
dimensions:
        lat = 3 ;
        lon = 4 ;
        time = UNLIMITED ; // (2 currently)

variables:
        float lat(lat) ;
                lat:long_name = "Latitude" ;
                lat:units = "degrees_north" ;
        float lon(lon) ;
                lon:long_name = "Longitude" ;
                lon:units = "degrees_east" ;
        int time(time) ;
                time:long_name = "Time" ;
                time:units = "days since 1895-01-01" ;
                time:calendar = "gregorian" ;
        float rainfall(time, lat, lon) ;
                rainfall:long_name = "Precipitation" ;
                rainfall:units = "mm yr-1" ;
                rainfall:missing_value = -9999.f ;

// global attributes:
                :title = "Historical Climate Scenarios" ;
                :Conventions = "CF-1.0" ;

data:
 lat = 48.75, 48.25, 47.75;
 lon = -124.25, -123.75, -123.25, -122.75;
 time = 364, 730;
 rainfall =
   761, 1265, 2184, 1812, 1405, 688, 366, 269, 328, 455, 524, 877,
   1019, 714, 865, 697, 927, 926, 1452, 626, 275, 221, 196, 223;
}
```

Coordinate variable

Variable attribute

Global attribute

The Classic NetCDF Model – UML Diagram

- The classic NetCDF can be represented in an UML diagram

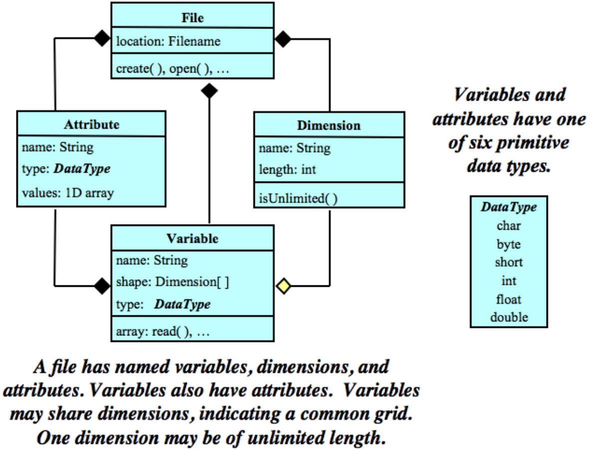
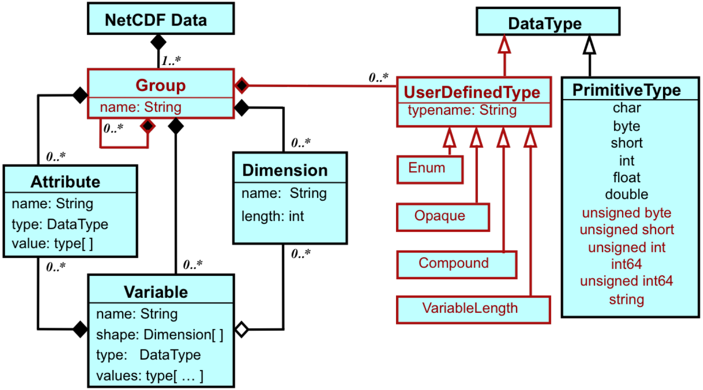


Figure: Source [102]: NetCDF UML Diagram

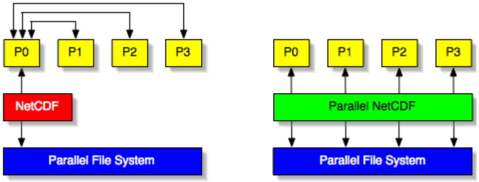
NetCDF Data Models

- Classic: Simplest model – Dimensions, variables, attributes
- Enhanced: More powerful model – Adds groups, types, nesting



Parallel I/O in NetCDF-4

- NetCDF-4 provides parallel file access to both classic and NetCDF-4/HDF5 files
- The parallel I/O to classic files is achieved through PNetCDF while parallel I/O to NetCDF-4 files is through HDF5 or ESDM, ZARR format support is coming
- NetCDF-4 exposes the parallel I/O features of HDF5
  - HDF5 provides easy-to-use parallel I/O feature



Outline

Understanding of I/O Behavior and Systems

How can we understand system behavior?

- Observation
  - Measurement of runs on the system
  - Can be many cases to run
  - Slight bias since measurement perturbs behavior
  - Benchmarking: applications geared to exhibit certain system behavior
- Monitoring: system/tool-provided observation creation
- Theory: Performance models
  - Used to determine performance for a system/workload
  - Behavioral models

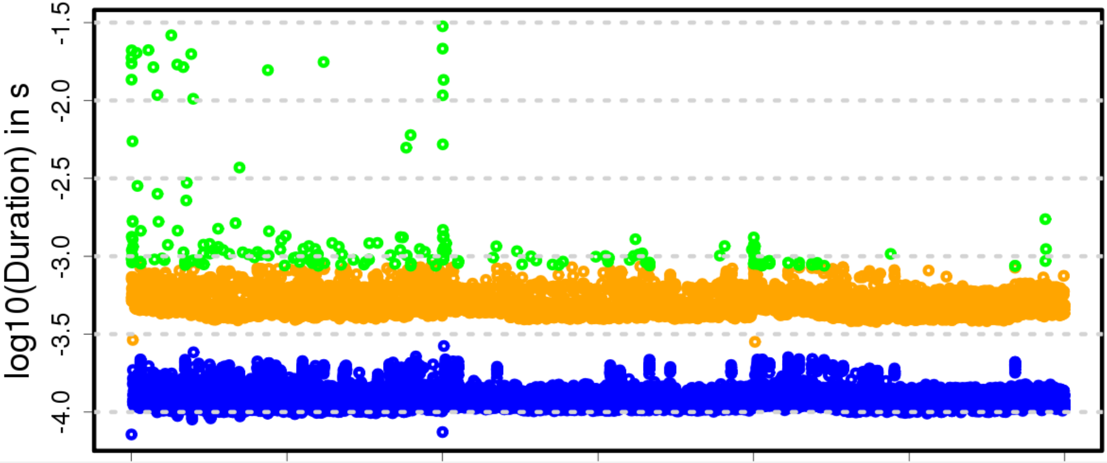
    Build models based on ensemble of observations
- System/application simulation
  - Based on system and workload models

Monitoring I/O

- To understand variability better, must analyze and understand behavior
- We need to capture I/O behavior, options
  - System-level, i.e., analyze OS-observable statistics such as bytes read
  - Application-level, record individual operations performance
- There are many interesting metrics that can be recorded
- Many tools exists that aid this analysis

Performance Variability for Single Operations

- Rerunning the same operation (access size, ...) leads to performance variation
- Individual measurements – 256 KiB sequential write (outliers purged)



Understanding Performance Variability

Issue

- Measuring operation repeatedly results in different runtime
- Reasons:
  - Sometimes a certain optimization is triggered, shortening the I/O path
  - Example strategies: read-ahead, write-behind
- Consequence: Non-linear access performance, time also depends on access size
- It is difficult to assess performance of even repeated measurements!

Goal

- Predict likely reason/cause-of-effect by just analyzing runtime
- Estimate best-case time, if optimizations would work as intended

Comparing Density Plot with the Individual Data Points

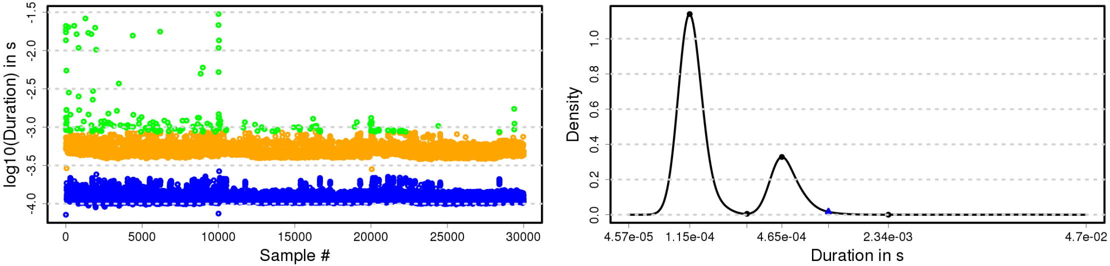


Figure: Duration for sequential reads with 256 KiB accesses (off0 mem layout)

Algorithm for determining classes (color schemes)

- Create density plot with Gaussian kernel density estimator
- Find minima and maxima in the plot
- Assign one class for all points between minima and maxima
- Rightmost hill is followed by cutoff (blue) close to zero ⇒ outliers (unexpected slow)

Write Operations

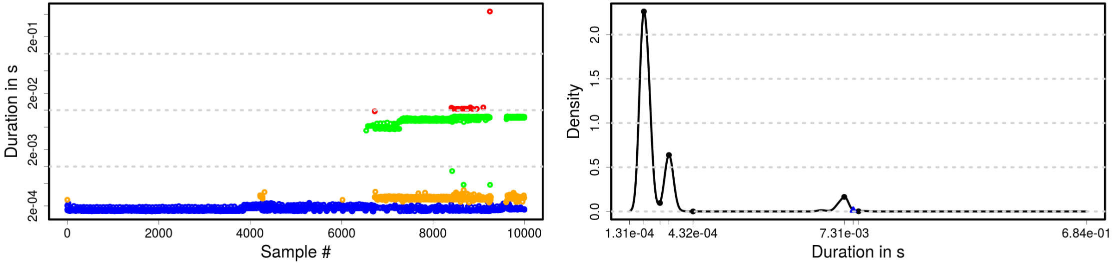


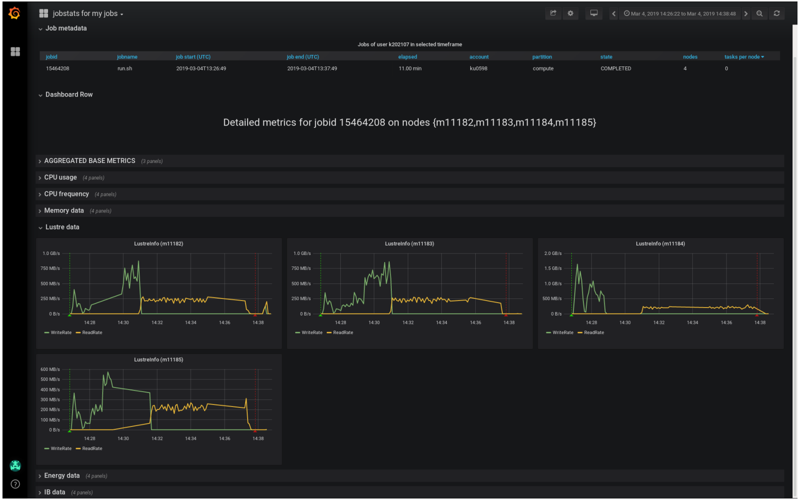
Figure: Results for one write run with sequential 256 KiB accesses (off0 mem layout).

Known optimizations for write

- Write-behind: cache data first in memory, then write back
- Write back is expected to be much slower

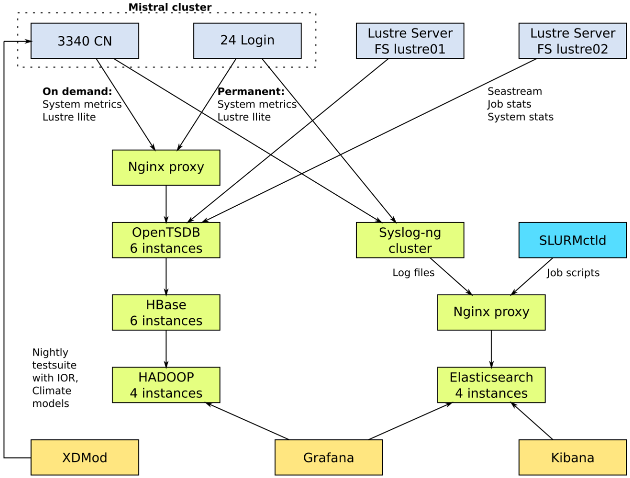
This behavior can be seen in the figure !

System-Wide Monitoring



- Grafana visualization
- Read/write shown
- Metrics supported
  - md_file_create
  - md_file_delete
  - md_read (only)
  - md_mod(ify)
  - md_other
  - read_bytes
  - read_calls
  - write_bytes
  - write_calls

DKRZ Monitoring System



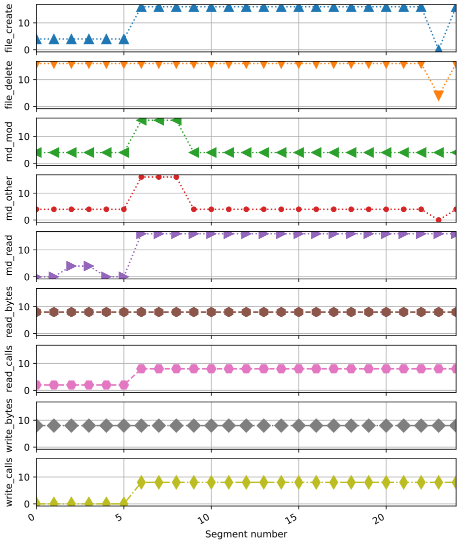
Details

- Periodicity: 10s
- Record metrics
  - From /proc
  - 9 aggregated
- Jobs are linked to the data

Mistral Supercomputer

- 3,340 Nodes
- 2 Lustre file systems
- 52 PByte capacity
- 100+ OSTs per fs

Visualizing Job Behavior and Comparing different jobs



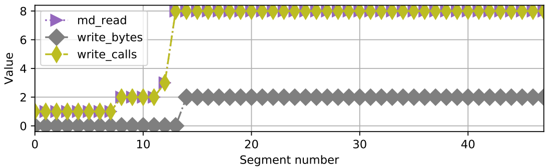


Figure: For this job, other metrics == 0

- Different jobs differ significantly
- We can compare jobs
- Metrics categorized based on categories
  - 0 = non-IO
  - 1 = intense
  - 4 = extreme
- Segments represent 10 min

Outline

How Can Benchmarks Help to Analyze I/O?

- Benefits of benchmarks
  - Can use simple/understandable sequence of operations
    - Ease comparison with theoretic values (that requires understandable metrics)
  - May use a pattern like a realistic workloads
    - Provides performance estimates or bounds for workloads!
  - Sometimes only possibility to understand hardware capabilities
    - Because the theoretic analysis may be infeasible
- Benefits of benchmarks vs. applications
  - Are easier to code/understand/setup/run than applications
  - Come with less restrictive "license" limitations
- Flexible testing (strategies)
  - Single-shot: e.g., acceptance test
  - Periodically: regression tests

Benchmarks

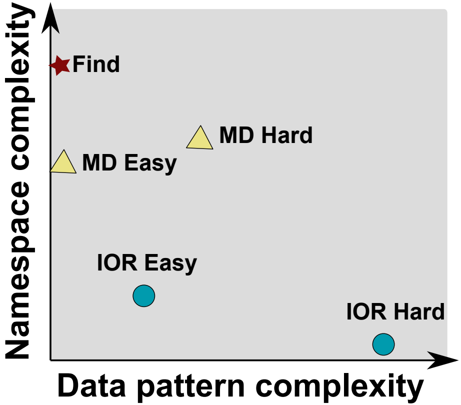
- Benchmarks measure system behavior and implement (simple) well-known behavior
- Many I/O benchmarks exist covering various aspects
  - APIs used
  - Data access pattern
  - Memory access pattern
  - Parallelism and concurrency
- Let's talk about the IO-500 benchmark suite; it is
  - **Representative**: for optimized and naive workloads
  - **Inclusive**: cover various storage technology and non-POSIX APIs
  - **Trustworthy**: representative results and prevent cheating
  - **Cheap**: easy to run and short benchmarking time (in the order of minutes)
  - Favors a single metric to simplify the comparison across dimensions

Goals of the IO-500 Benchmarking Effort

- Bound performance expectations for realistic workloads
- Track storage system characteristics behavior over the years
  - Foster understanding of storage performance development
  - Support to identify potent architectures for certain workloads
- Document and share best practices
  - Tuning of the system is encouraged
  - Submitters must submit detailed run parameters
- Support procurements, administrators and users

https://io500.org

Covered Access Patterns



- IOR-easy: large seq on file(s)
- IOR-hard: small random shared file
- MD-easy: mdtest, per rank dir, empty files
- MD-hard: mdtest, shared dir, 3900 byte
- find: query and filter files based on name and creation time
- Executing concurrent patterns not covered (another dimension)

Predictability and Latency Matters

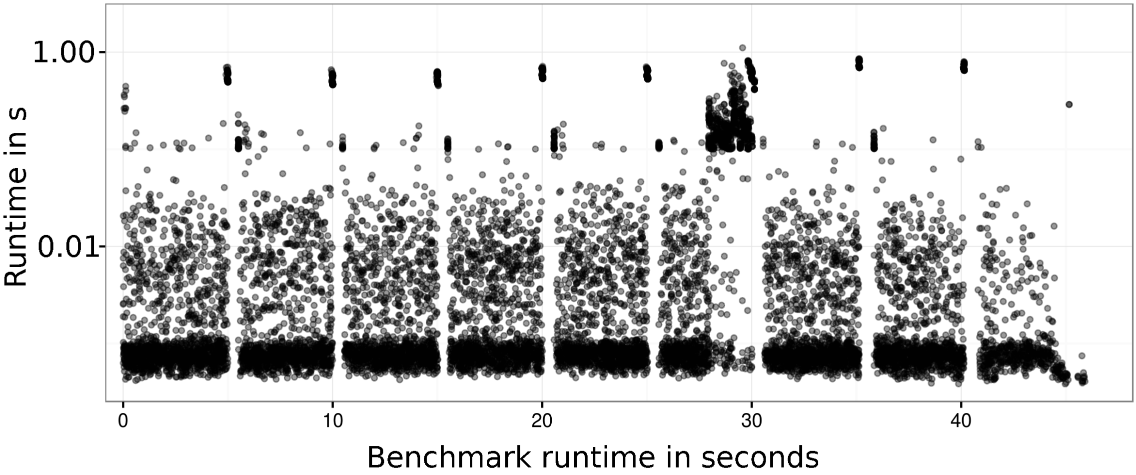
Performance Predictability

- How long does an I/O / metadata operation take?
- Important to predict runtime
- Important for bulk-synchronous parallel applications
  - The slowest straggler defines the performance

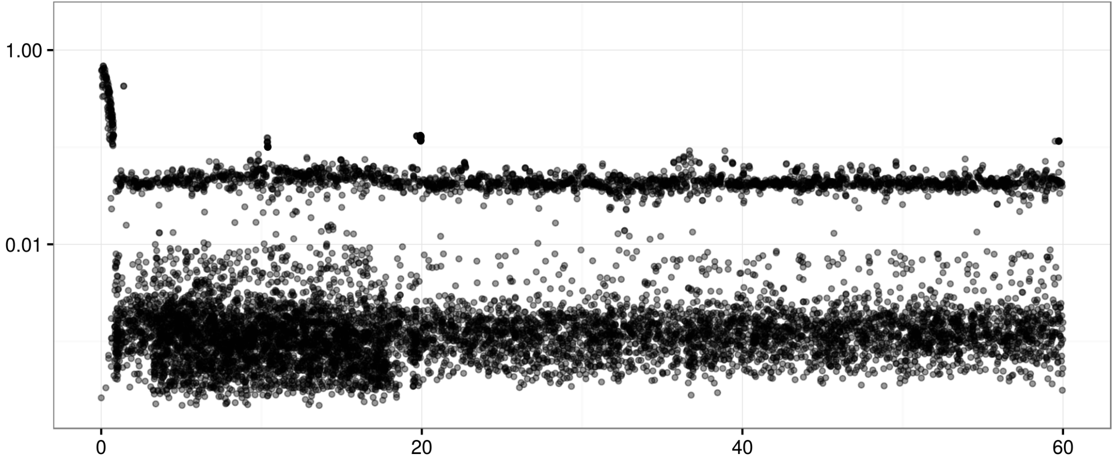
Measurement

- In the following, we plot the timelines of metadata create operations
  - Sparse plot with randomly selected measurements
  - Every point above 0.1s is added
- All results obtained on 10 Nodes using MD-Workbench
  `https://github.com/JulianKunkel/md-workbench`
  - Options: 10 PPN, D=1, I=2000, P=10k, precreation phase

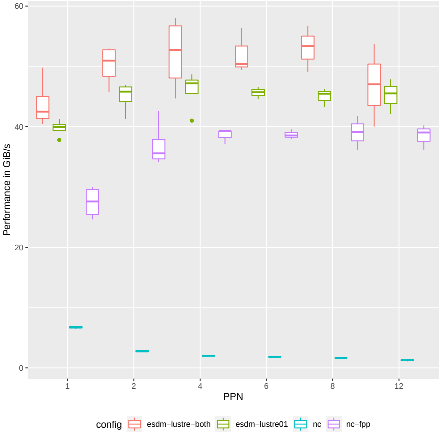
Latencies: Lustre / Mistral at DKRZ



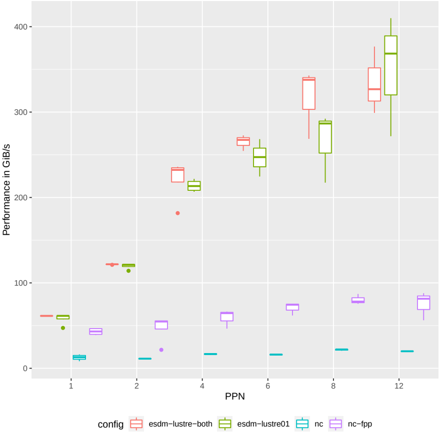
Latencies: GPFS / Cooley at ALCF



Performance of the NetCDF-Bench 100 Nodes@Mistral



Write



Read

- Better performance than FPP but looks for users like a single file

Importance of Choosing the Right Mean Value

- We must repeat a benchmark run to obtain trustworthy data
  - Reduce impact of random errors due to background activity
- How do we weight input when repeating a benchmark run?

Tuning for improving the Geom-Mean value

Description	Input (11 values)	**Geom**	Arithmetic	Harmonic
Balanced system	10 . . . 10 10 **10**	10	10	10
One slow bench	10 . . . 10 10 **1**	8.1	9.2	5.5
Tuning worst 2x	10 . . . 10 10 **2**	8.6	9.3	7.3
Tuning good 2x	10 . . . 10 **20 1**	8.6	10.1	5.6
Tuning good 100x	10 . . . 10 **100 1**	10	17.4	5.8

- Avoid arithmetic mean
- May use box-plots to visualize variability
- Geom mean honors tuning equally, insensitive to “outliers”
- Harmonic mean favors balanced systems (complex to scale results)

Probing Approach

- Many sites run periodic regression tests, e.g., nightly
  - Helps to identify performance regressions with updates
- Instead, we run a non-invasive benchmark (a probe) with a high frequency
  - Mimic the user-visible client behavior
  - Measuring latency for metadata and data operations
- Generate and analyze generated statistics
- Derive a slowdown factor (file system load)

Probing: Performance Measurement

Preparation

- Data: Generate a large file (e.g., $>$ 4x main memory of the client)
- Metadata: Pre-create a large pool of small files (e.g., 100k+ files)

Benchmarks

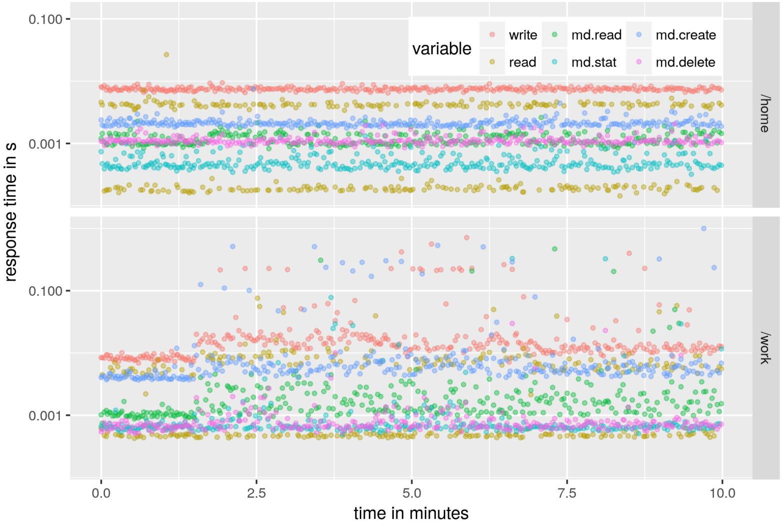
- Repeat the execution of the two patterns every second
- DD: Read/Write a random 1 MB block
- MD-Workbench: stat, read, delete, write a single file per iteration
  - Allows regression testing, i.e., retain the number of files
  - *J. Kunkel, G. Markomanolis. Understanding Metadata Latency with MDWorkbench.*

Executed as Bash script or an integrated tool: `https://github.com/joobog/io-probing`

Test Systems

- JASMIN, the data analysis facility of the UK
  - Precreation: 200k files, 200 GB data file
  - 60 days of data
  - Script runs exclusively on a node
- Archer, the UK national supercomputer service
  - Precreation: 200k files, 200 GB data file
  - 30 days of data
  - Script runs on a shared interactive node
- Mistral, the HPC system at the German Climate Computing Center
  - Precreation: 100k files, 1.3 TB data file
  - 18 days of data
  - Tool runs on a shared interactive node

Understanding the Timeseries



- Every probe (1s) for 10 min
- For two file systems
- Home is stable
- Work shows irregularities

IO-500 Response Time on Archer

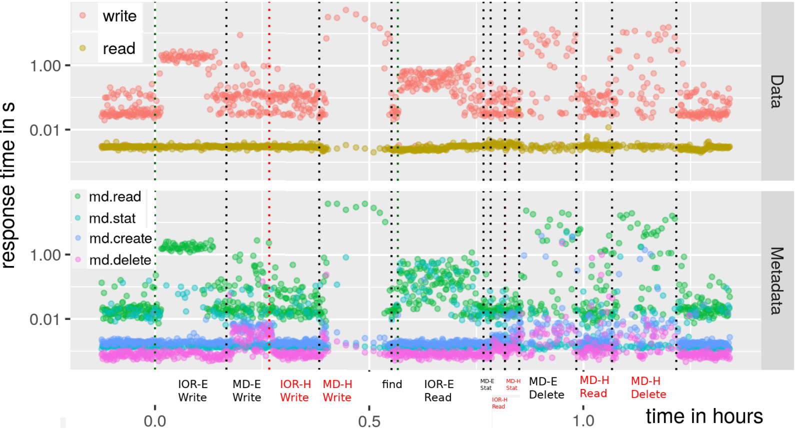


Figure: Response time (all measurements)

- Run on 100 nodes
  score 8.45
- The IO-500 various phases
  Data and metadata heavy
- First, all measurements

Validating Slowdown on All Measurements

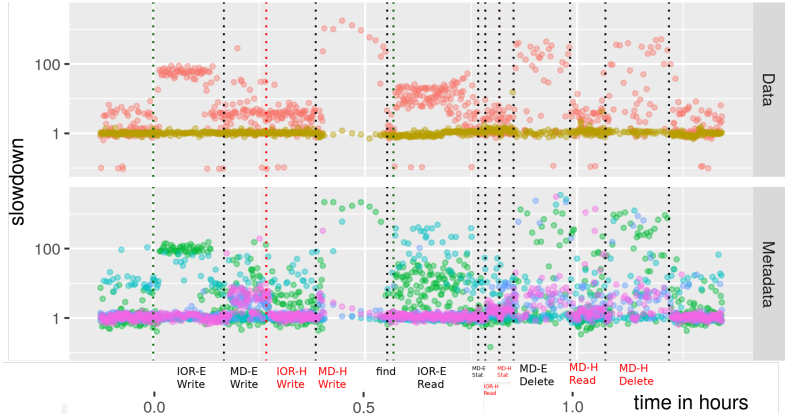


Figure: Slowdown (all measurements)

- Computed median slowdown
  Expected: median of 30 days
- Influence of phases is visible
- MDHard 1000x slowdown
  Influences data latency!
  10s of seconds latency
- IOREasy 100x slowdown
- IORHard not too much
- Data read is stable

Validating Slowdown: Reduced Data

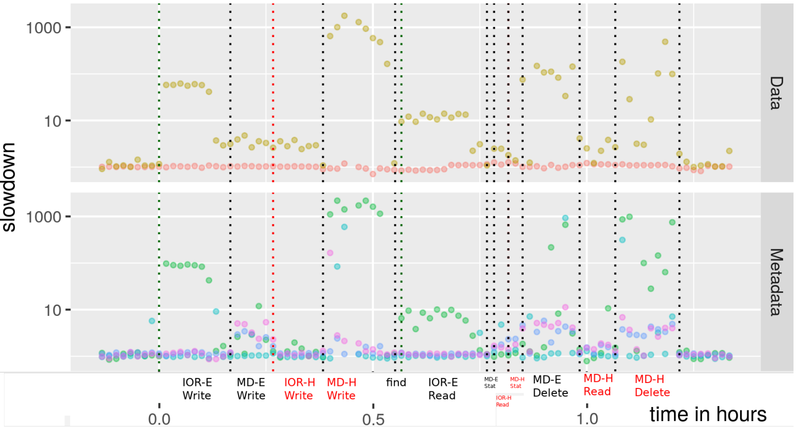


Figure: Slowdown (60s mean statistics)

- Data reduction: 60s mean
- More robust, clearer to see

Timelines of 4h Statistics

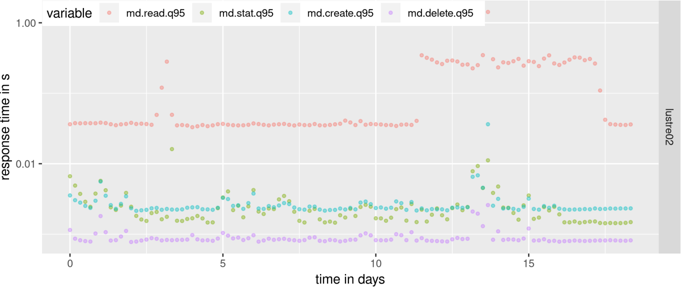


Figure: Mistral metadata timeline

- Use Q95, 5% ops are slower
- Change in behavior at day 12
  Reason: unknown

Slowdown for 4h Statistics

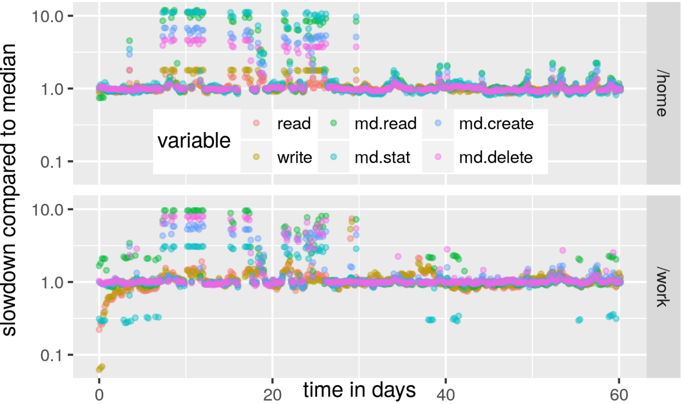


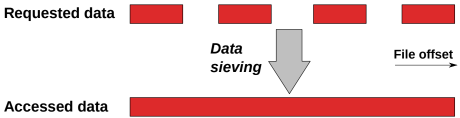
Figure: JASMIN, computed on 4 hour intervals

- Slowdown: Using the median
- Typically value is 1
- Sometimes a system is 10x slower
  - Due to user interactions
  - Concurrent application execution
- Values below 1, unusual (caching)
- Good to see long-term issues

Outline

Optimizations

- There are too many tunables and optimizations for I/O
  - Read-ahead, write-behind, async I/O
  - Distribution of data across servers (e.g., Lustre stripe size)
  - We will investigate the complexity of one example...
- Performance benefit of I/O optimizations is non-trivial to predict
- Non-contiguous I/O supports data-sieving optimization
  - Transforms non-sequential I/O to large contiguous I/O
  - Tunable with MPI hints: enabled/disabled, buffer size
  - Benefit depends on system AND application



- Data sieving is difficult to parameterize
  - What should be recommended from a data center's perspective?

Experiments

- Simple single threaded benchmark, vary access granularity and hole size
- Captured on DKRZ porting system for Mistral
- Vary Lustre stripe settings
  - 128 KiB or 2 MiB
  - 1 stripe or 2 stripes
- Vary data sieving
  - Off or On (4 MiB)
- Vary block and hole size (similar to before)
- 408 different configurations (up to 10 repeats each)
  - Mean arithmetic performance is 245 MiB/s
  - Mean can serve as baseline “model”

System-Wide Defaults

- Comparing a default choice with the best choice
- All default choices achieve 50-70% arithmetic mean performance
- Picking the best default for stripe count/size: 2 servers, 128 KiB
  - 70% arithmetic mean performance
  - 16% harmonic mean performance ⇒ some bad choices result in very slow performance

Default Choice			Best	Worst	Arithmetic Mean			Harmonic Mean	
Servers	Stripe	Sieving	Freq.	Freq.	Rel.	Abs.	Loss	Rel.	Abs.
1	128 K	Off	20	35	58.4%	200.1	102.1	9.0%	0.09
1	2 MiB	Off	45	39	60.7%	261.5	103.7	9.0%	0.09
2	**128 K**	**Off**	87	76	**69.8%**	209.5	92.7	8.8%	0.09
2	2 MiB	Off	81	14	72.1%	284.2	81.1	8.9%	0.09
1	128 K	On	79	37	64.1%	245.6	56.7	15.2%	0.16
1	2 MiB	On	11	75	59.4%	259.2	106.1	14.4%	0.15
2	**128 K**	**On**	80	58	**68.7%**	239.6	62.6	**16.2%**	0.17
2	2 MiB	On	5	74	62.9%	258.0	107.3	14.9%	0.16

Table: Performance achieved with any default choice

Applying Machine Learning

- Building a classification tree with different depths
- Even small trees are much better than any default
- A tree of depth 4 is nearly optimal; avoids slow cases

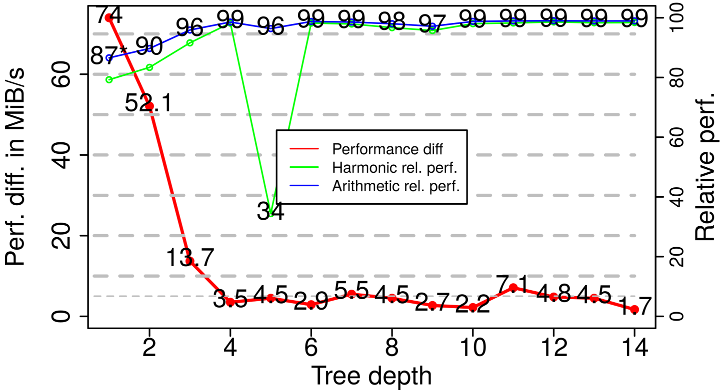


Figure: Perf. difference between learned and best choices, by maximum tree depth, for DKRZ's porting system

Decision Tree & Rules

Extraction of knowledge from a tree

- For writes: Always use two servers; For holes below 128 KiB ⇒ turn DS on, else off
- For reads: Holes below 200 KiB ⇒ turn DS on
- Typically only one parameter changes between most frequent best choices

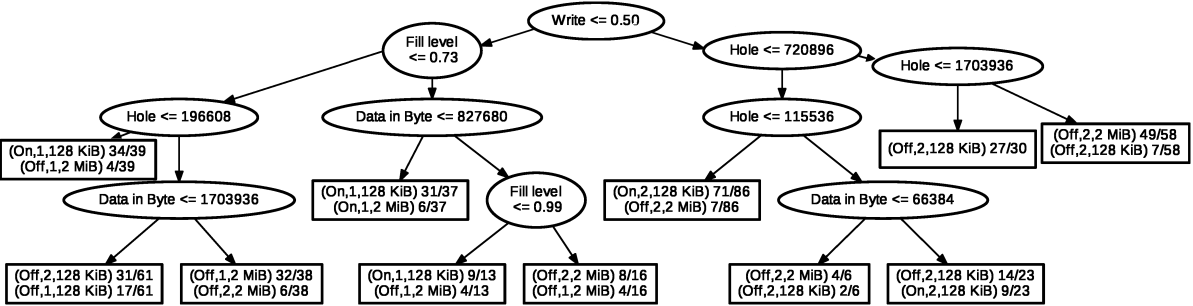
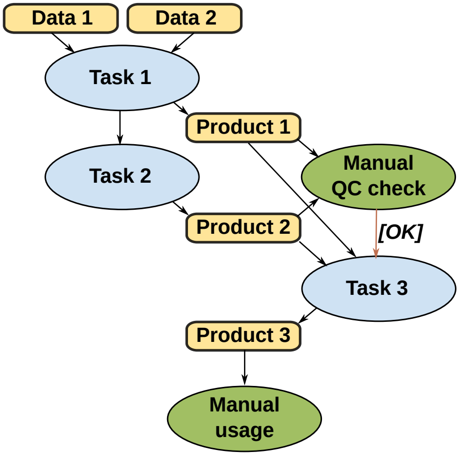


Figure: Decision tree with height 4. In the leaf nodes, the settings (Data sieving, server number, stripe size) and number of instances for the two most frequent best choices

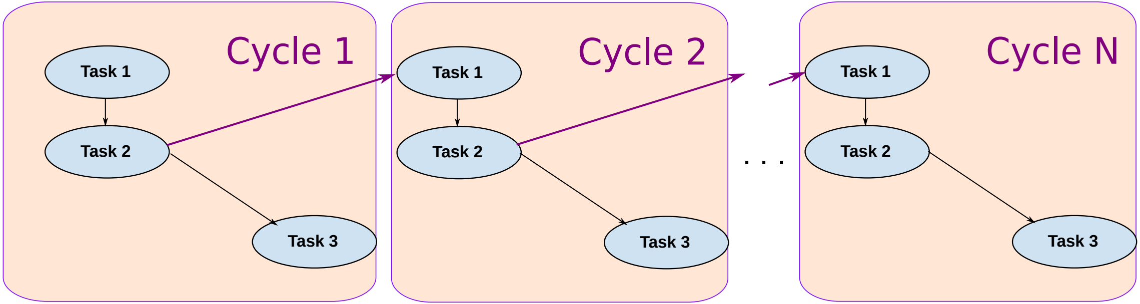
Outline

Workflows

- Insight: What users are interested in
- Consider workflow from 0 to insight
  - Needs input
  - Produces output data
  - Uses tasks
    - Parallel applications
    - Big data tools
    - Manual analysis / quality control
  - May need month to complete
  - Manual tasks are unpredictable



A (Science) Workflow Description



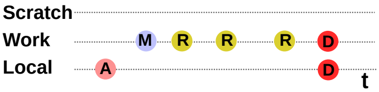
- Current practice (in climate/weather)
- Dependencies between tasks are described
- Assume a calculation that repeats for multiple cycles/iterations

Complexity of Data Placement Scheduling

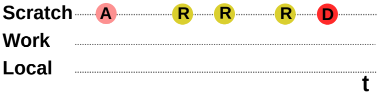
Scenario

- Consider three file systems: local, scratch, and work
  - Local is a compute-node local storage system
- Data can be stored on any of these storage systems
- Users need to manually optimize data placement to hardware throughout life cycle
- Could the system do more knowing details about the workflow?

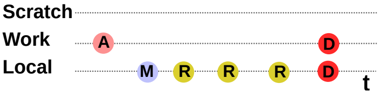
Alternative life cycles for mapping a dataset (Selection)



Local and work file systems



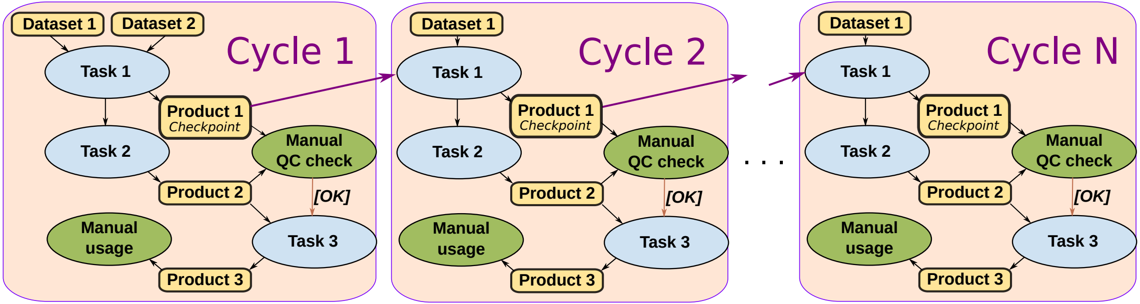
Scratch file system only



Local and work file systems

Allocation, **M**igration, **R**eading, and **D**eleting

Possible Extended (Science) Workflow Description



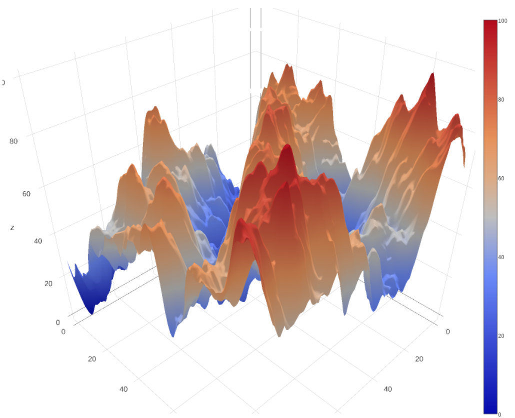
- Workflow description with IO characteristics
  - Input required
  - Needed input
  - Generated output and its characteristics
  - Information Lifecycle (data life)
  - ⇒ Explicit input/output definition (dependencies) instead of implicit

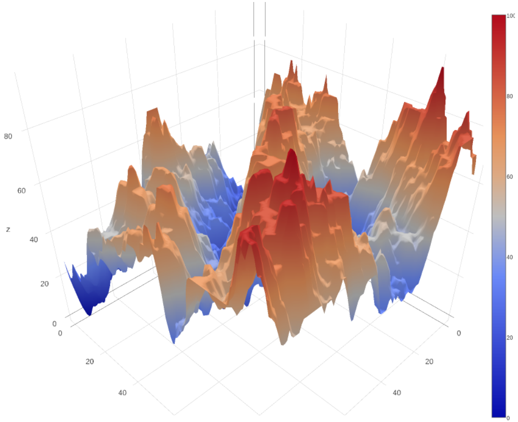
Data-Reduction

- Issues
  - Storing data for a long time is expensive
  - Performance is an issue
- Data can be stored in various formats on storage media
- Data-Reduction techniques aim to reduce storage requirements
- Strategies
  - Avoiding output - challenge: need data for analysis!
  - Re-computation - recreate data upon need using the same computing
  - Lossless compression - compress data such that bit-identical data can be recreated
    - Examples: bzip, zip, WAV (audio)
  - Lossy compression - (some, configurable) data loss upon recreation
    - Example: MP3, video files
- Typically measured as compression ratio, e.g., 10:1 (means 10% capacity remains)

Example Data

Visualization of Simplex noise (2D: 100x100 points)





Right picture compressed storing just 3 most significant bits (ratio 11.3:1)

Example Study Using Compression on two Systems

Algorithm	Ratio	Compr MiB/s	Decom. MiB/s
csc33-5	0.485	3.4	16.7
lzlib17-9	0.491	1.4	17.0
xz522-9	0.493	2.1	20.8
lzma938-5	0.493	2.2	24.2
brotli052-11	0.510	0.2	110.6
lzma938-2	0.526	7.9	23.1
zstd100-22	0.526	2.2	294.3
xpack2016-06-02-9	0.548	12.3	282.9
brotli052-5	0.549	16.5	156.6
xpack2016-06-02-6	0.549	16.9	278.9
zstd100-11	0.549	13.8	394.0
zstd100-2	0.574	177.6	455.3
lz4hcr131-16	0.640	3.1	1522.2
lzsse22016-05-14-16	0.640	7.7	1341.6
lz4hcr131-12	0.640	9.4	1519.5
lz4hcr131-9	0.640	17.2	1511.5
lz4hcr131-4	0.649	30.0	1477.8
lz515	0.673	229.2	858.6
density0125beta-2	0.683	419.4	496.5
pithy2011-12-24-9	0.694	305.9	1131.4
lzo1x209-1	0.726	606.7	833.7
lz4r131	0.726	469.8	1893.1
lz4fastr131-3	0.741	646.1	2001.1
lz4fastr131-17	0.772	1132.7	2263.1
blosclz2015-11-10-3	0.872	494.4	2612.6
blosclz2015-11-10-1	0.900	819.4	2496.9
memcpy	1.000	4449.1	4602.0

(a) WR data

Algorithm	Ratio	Compr MiB/s	Decom. MiB/s
lzlib17-9	0.426	1.5	22.0
xz522-9	0.427	2.2	24.3
lzma938-5	0.431	2.9	29.1
lzham10-d26-1	0.445	1.4	113.3
csc33-3	0.445	6.5	23.3
brotli052-11	0.451	0.3	124.5
lzma938-0	0.473	13.0	28.2
zstd080-22	0.476	1.1	260.7
brotli052-5	0.489	18.4	165.6
zstd080-18	0.496	3.9	434.4
xpack2016-06-02-9	0.498	19.3	386.8
xpack2016-06-02-1	0.504	53.5	362.0
zstd080-5	0.511	69.4	560.8
brotli052-2	0.512	126.6	168.7
zstd080-2	0.518	220.9	594.0
zstd080-1	0.523	355.0	633.9
lzo1c209-999	0.566	13.5	939.5
lz5hc15-4	0.574	126.3	1410.1
lz515	0.576	326.9	1934.9
lz4hcr131-16	0.577	3.1	2720.6
lz4hcr131-12	0.577	12.4	2700.8
lz4hcr131-9	0.577	28.4	2670.3
lzo1b209-6	0.578	143.3	992.5
lz4r131	0.599	951.4	3037.4
lz4fastr131-3	0.603	1272.6	3215.6
pithy2011-12-24-3	0.613	1787.5	3535.2
lz4fastr131-17	0.614	1904.8	3610.3

(b) DKRZ data

- Running 162 algos
- Best algos shown left
- Developed tool: SFS
- DKRZ: 3 TByte of 50 PB data scanned
  - 5 Weeks, one node
  - LZ4Fast faster than memcpy
- WR: 38.1 GByte of 1.1 TByte scanned

Outline

Research Activities & Interest

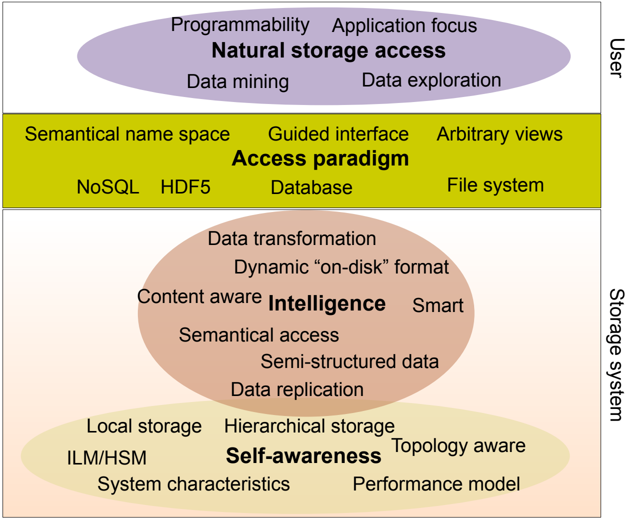
High-performance storage for HPC

- Efficient I/O
  - Performance analysis methods, tools and benchmarks
  - Optimizing parallel file systems and middleware
  - Modeling of performance and costs
  - Tuning: Prescribing settings
  - Management of (data-driven/big data) workflows
- Data reduction: compression library, algorithms, methods
- Interfaces: towards domain-specific solutions and novel interfaces

Other research interests

- Application of big data analytics (e.g., for humanities, medicine)
- Cost-efficiency for data centers in general
- Scientific Software Engineering

Personal Vision: Towards Intelligent Storage Systems and Interfaces



- Abstract data interfaces
- Enhanced data management
- Integrated compute/storage
- Flexible views on data

- Smart hardware/storage
  - Self-aware systems
  - AI optimized placement
  - Bring-your-own-behavior model
- Across sites and cloud

Summary

- Achieving efficient I/O is challenging due to
  - complex systems
  - deep software stack
  - performance variability
  - optimizations
- Monitoring, performance analysis and benchmarking is needed
- There are many optimization strategies
- The NetCDF data model manages n-Dimensional data

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