703308 VO High-Performance Computing
Parallel I/O

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Overview

- Parallel filesystems and I/O concepts
  - Software and hardware characteristics
- MPI I/O
  - How to open, read & write files, performance aspects
- High-level I/O libraries
  - HDF5

TOP500 November '25 update highlights

- No real changes in the top spots
  - El Capitan still no. 1 (though higher Rmax and Rpeak now)
    - Combined AMD CPU+GPU MI300A (similar to Nvidia GH200)
    - Lower power draw than Aurora using Intel…
  - Frontier and Aurora no. 2 and 3
    - Together with El Capitan and JUPITER Booster the only Exascale systems
  - JUPITER Booster same place, but now barely reaching 1 exaflop
  - Expected to be Europe's first Exaflop system
    - New Nvidia Grace Hopper chips, similar to AMD MI300A: combined CPU+GPU with hardware-supported memory coherency
  - European systems on place 4, 6, 8, 9, and 10!

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**El Capitan** - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States	11,340,000	1,809.00	2,821.10	29,685
2	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE Cray OS, HPE DOE/SC/Oak Ridge National Laboratory United States	9,066,176	1,353.00	2,055.72	24,607
3	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	9,264,128	1,012.00	1,980.01	38,698
4	**JUPITER Booster** - BullSequana XH3000, GH Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, RedHat Enterprise Linux, EVIDEN EuroHPC/FZJ Germany	4,801,344	1,000.00	1,226.28	15,794
5	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States	2,073,600	561.20	846.84	

Motivation: kmMountains (PRACE Access project) cont'd

- Simulates mountain climates in European Alps and Himalaya
  - Estimated project duration of 3 years
  - Total amount of data to be written: approx. 400 TB per year

- High I/O requirements
  - Up to 82 GB for checkpointing
  - Up to 1 TB of result data
  - per simulation run!

Run type	#Simulation steps	Wall time per step	#Nodes	Total node hours	Storage needs
Himalayas at 2.2 km	312 months	8.6 h	204	547373	198 TB
Himalayas at 12 km	372 months	1.7 h	8	5059	18.5 TB
Alps at 1.1 km	240 months	16.0 h	104	399360	86 TB
Alps at 2.2 km	240 months	12.0 h	40	115200	21.6 TB
Alps at 12 km	300 months	1.7 h	4	2040	7.8 TB
Processing				100000	
Total Year 1				**1169032**	**332 TB**
Estimated Year 2				**~1300000**	**~400 TB**
Estimated Year 3				**~1300000**	**~400 TB**

Motivation: PRACE technical guidelines

- Lists and describes technical properties and requirements of every PRACE Supercomputer
  - Min/max/average for job lengths, RAM, no. of cores, etc.
  - Also includes storage
    - size and number of files

- https://prace-ri.eu/wp-content/uploads/Technical_Guidelines_Call_24.pdf

Number of Files

In addition to the specification of the amount of data, the number of files also has to be specified. If you need to store more files, the project applicant must contact the centre beforehand for approval.

Field in online form	*Machine*	*Max*	*Remarks*
Number of files (Scratch) <number>	HAWK	n.a.	
	Joliot-Curie	2 million	10 000 files max per directory, without backup, files older than 90 days will be removed automatically
	JUWELS	4 million	Without backup, files older than 90 days will be removed automatically
	Marconi100	2 million	Without backup, files older than 50 days will be removed automatically
	MareNostrum 4	2 million	
	Piz Daint	1 million	No limit while running, but job submission is blocked if the max number of files left on scratch is reached
	SuperMUC-NG	1 million	Without backup, old files are removed automatically, Ideal file size: >100 GB
Number of files (Work) <number>	HAWK	100 000	
	Joliot-Curie	500 000	Extensible on demand, 10 000 files max per directory
	JUWELS	3 million	With backup
	Marconi100	2 million	Without backup
	MareNostrum 4	2 million	
	Piz Daint	50 000 per TB	With backup and snapshots
	SuperMUC-NG	1 million	Ideal file size: >100 GB
Number of files (Home)	HAWK	100 000	

Motivation

- Computation is parallel, why not I/O?
  - Single disks and sequential I/O are slow
  - I/O performance does not automagically scale with compute parallelism
- Why MPI or any other I/O library?
  - You could use e.g. POSIX to manually implement parallel I/O…
  - …but that would mean reinventing the wheel for every new program
- Parallel I/O is very complex!
  - David Henty (EPCC): “IO is the HPC equivalent of printing”
  - Lots of platform-dependent properties, hard to give general advice

Why is I/O in HPC so complex?

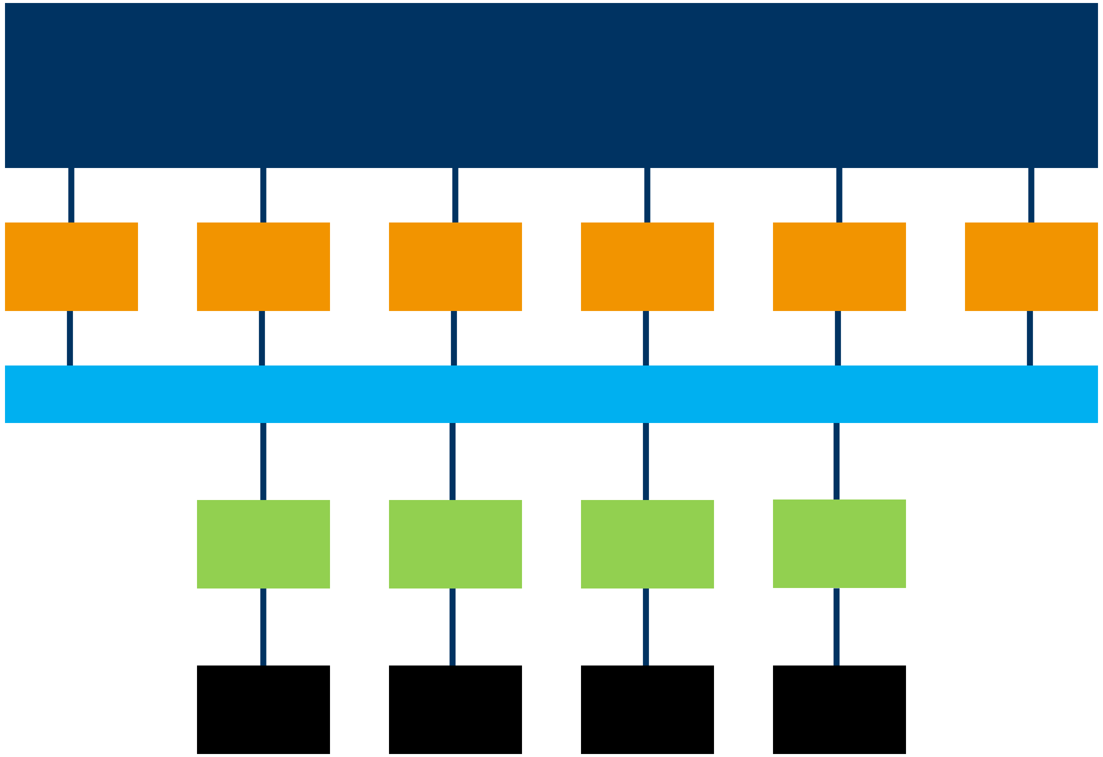
- Data layout issues become much more significant
  - Data is persistent, can outlive job duration
  - Consider checkpoint/restart where the number of nodes changes in-between
  - Pre- or postprocessing using programs other than your main application

- RAM means Random Access Memory
  - Random file access (`fseek()`) is far more inefficient
  - Performance impact of linearization (e.g. depth-first tree indexing, etc.) is aggravated

- I/O software and hardware stacks are very complex
  - Hardware: Multiple components, network interfaces and properties
  - Software: Multiple libraries, I/O behavior patterns and tunable parameters

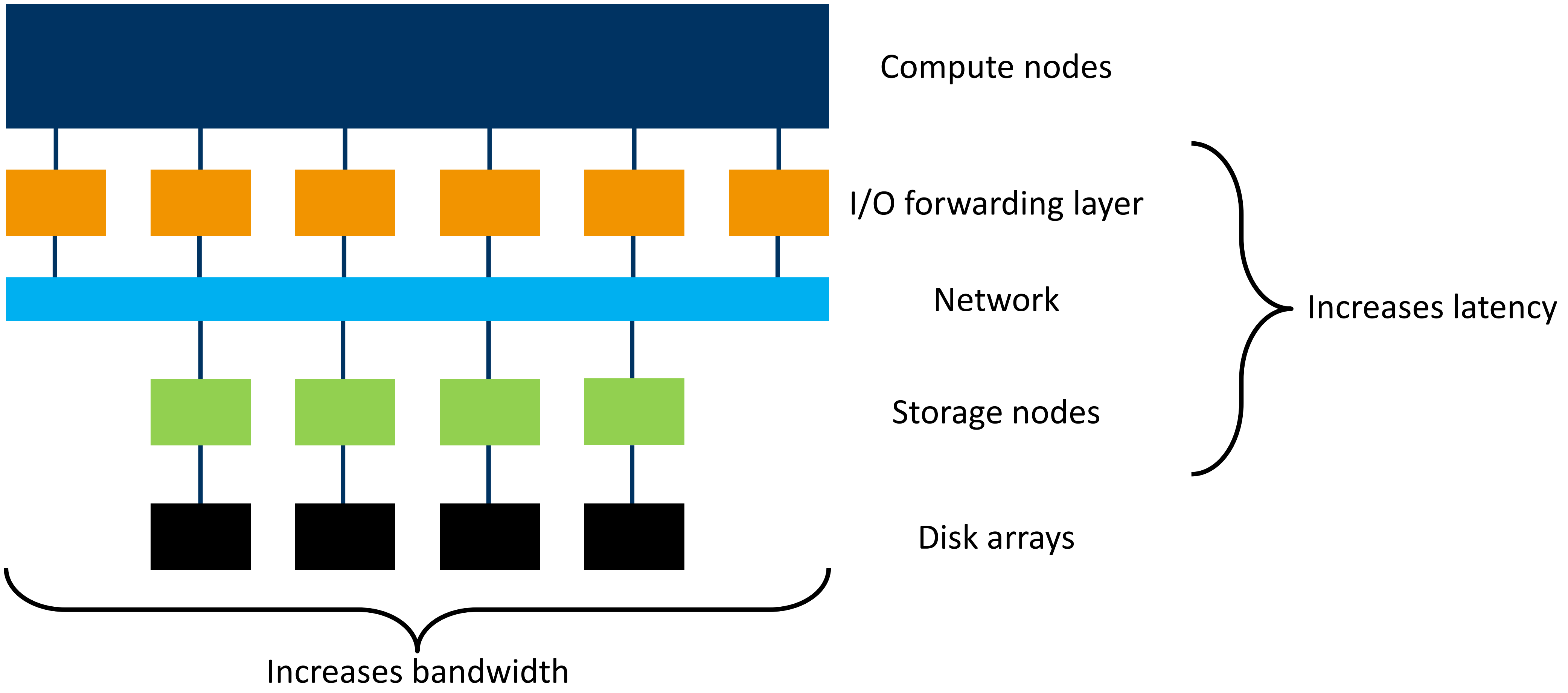
Parallel Filesystems and I/O Concepts

General hardware stack

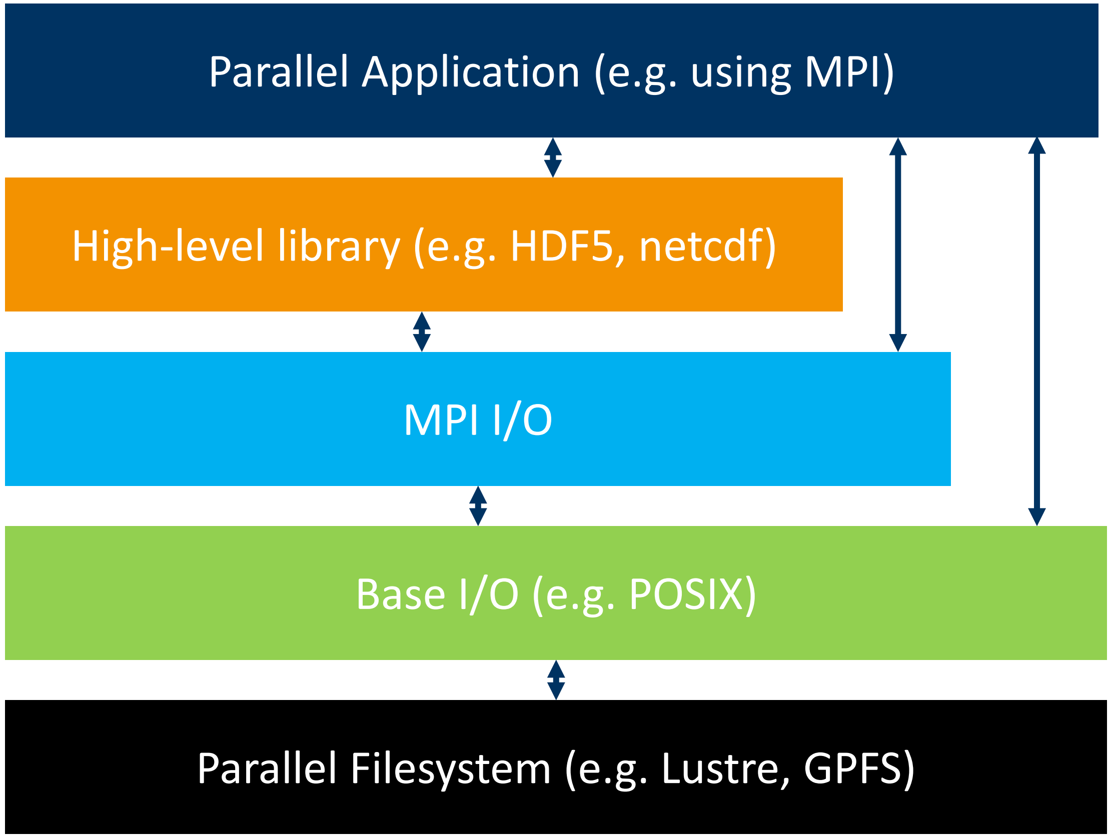


Compute nodes	Run the user application, issue high-level I/O requests (e.g. via MPI), might do data transformations beforehand
I/O forwarding layer	Nodes or routers, connect compute nodes to storage nodes, aggregate requests to optimize and ease workload, can offer optimizations such as RDMA
Network	Can be shared with compute nodes or dedicated for storage only, also multiple, heterogeneous networks possible for some filesystems (e.g. Lustre)
Storage nodes	Run the actual file system and are in charge of controlling the disk arrays
Disk arrays	Each handled as a single entity but usually consisting of multiple disks for improved performance and resilience (e.g. RAID-5/6)

General hardware stack



General software stack



Parallel filesystems

- Provide explicit support for parallel I/O in the application (or library)
- Lots of additional features
  - Load balancing
  - Caching
  - Request aggregation
  - Other performance optimizations
- Many big players, including
  - Lustre
  - DAOS
  - GPFS (IBM Storage Scale / Spectrum Scale)
  - BeeGFS
  - OrangeFS
- Try to adhere to POSIX requirements but are usually not fully compliant
  - Only need to support enough to not break most applications
  - Often unsupported: atomic move/rename, file locks, unlinking open files, symbolic or hard links, etc.

Lustre

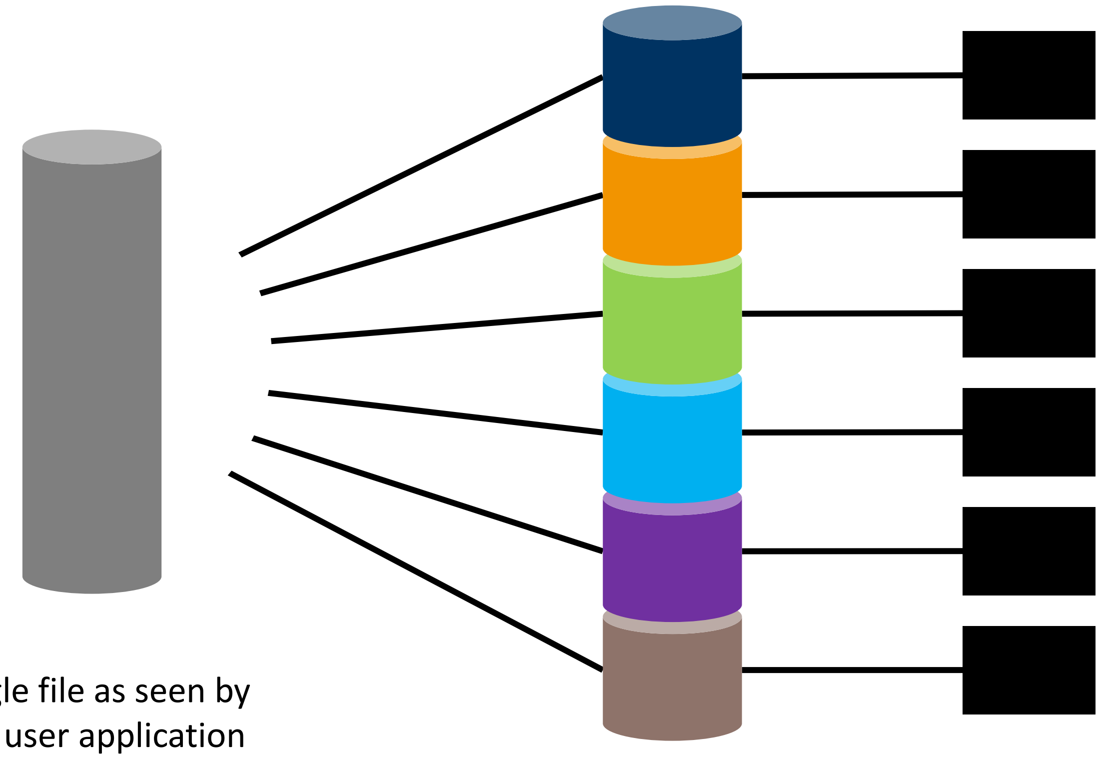
- Many large-scale HPC systems use Lustre
  - Basically all EuroHPC JU systems
  - More than half of the first 100 TOP500 systems
  - Easily achieves TB/s bandwidths if properly provisioned and configured
  - GPLv2
- Uses two main concepts of storage
  - Object storage: stores the actual files
  - Meta data: stores filenames, permissions and which OST holds the file(s)
- Uses ext4 or ZFS as backend storage
  - Invisible to user
  - Enables user-independent optimizations such as compression, deduplication or copy-on-write
  - But no support for resilience!

	Server	Target (disk arrays)
Meta data	MDS	MDT
Object storage (=user data)	OSS	OST

Lustre terminology

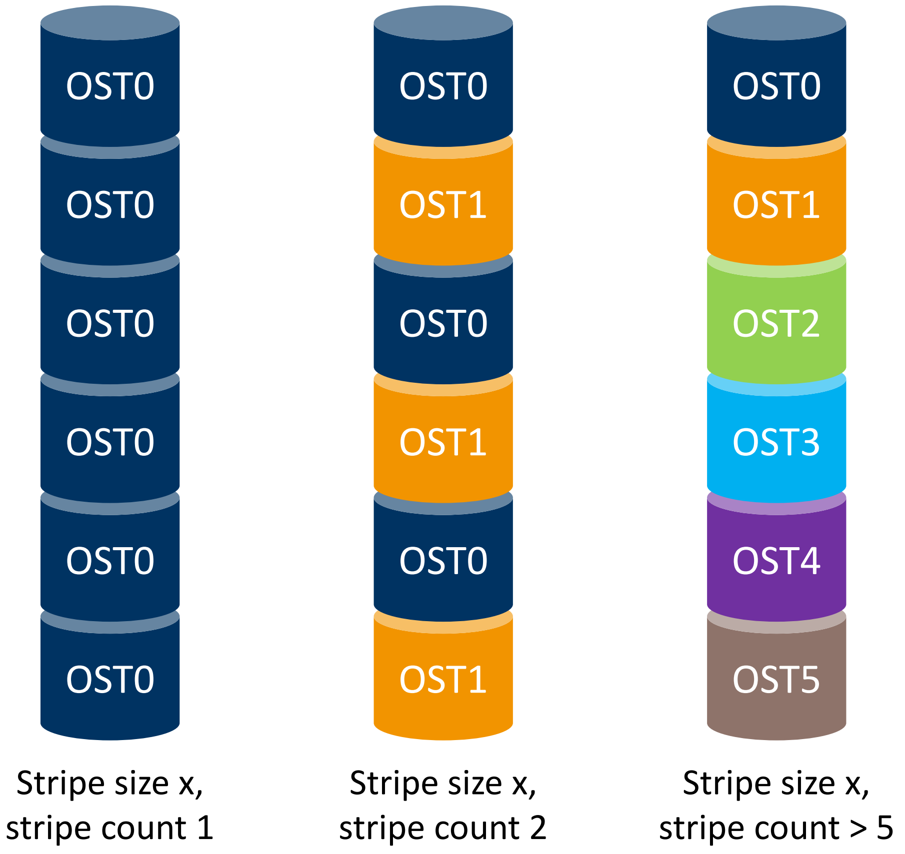
Lustre striping

- Performance gain derived through "striping"
  - File is split by the file system in e.g. 2 MB stripes
  - Size can be controlled at runtime, per file/path (usually between 1 and 32 MB)
- Enables parallel file access without requiring application support
  - Careful: no resilience in Lustre, losing an OST means losing all files on it
  - Resilience must be handled within OST (e.g. RAID-5/6), also: backups



Lustre stripe size and stripe count

- Stripe Size
  - The length of a single stripe
  - A single stripe is always located contiguously on an OST
- Stripe Count
  - The number of OSTs to use per file
- Note: most parallel filesystems use such an approach, with different terminology (GPFS: “blocks”) and slight differences in semantics



Common Lustre tools

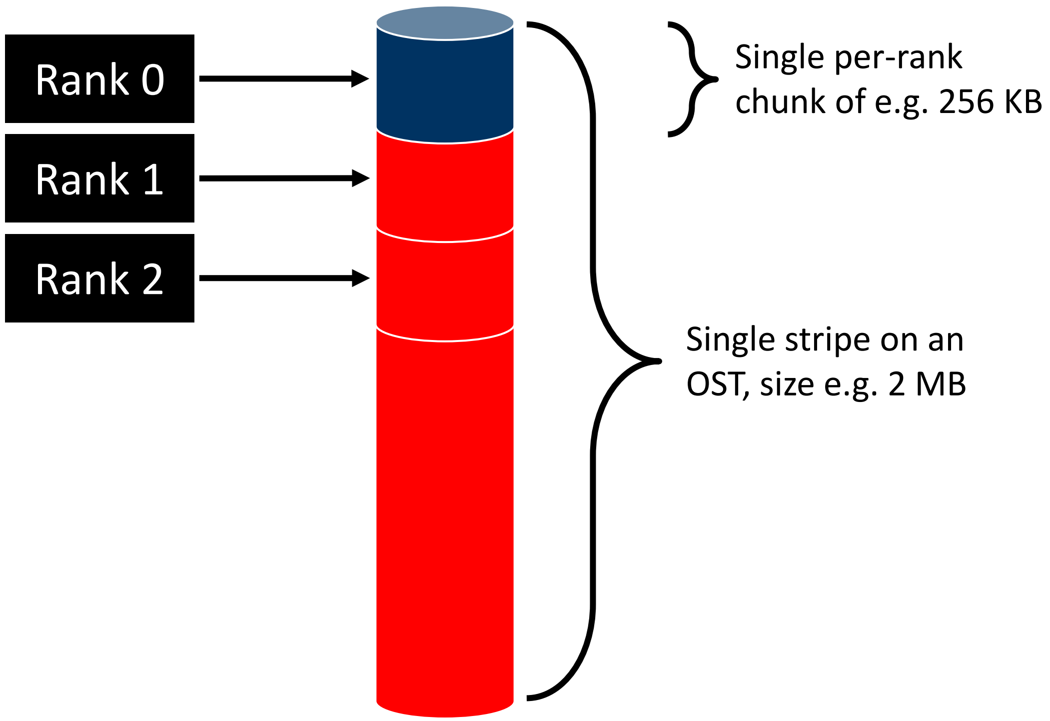
- `lfs osts <path>`
  - List name and status of OSTs for given file path
- `lfs getstripe <path>`
  - Get striping information
- `lfs setstripe <args> <path>`
  - Set striping information
- `lfs df`
  - Get disk usage statistics

Performance pitfall: false sharing

- Similar to false sharing in multi-threaded programs
  - Cache line ~ stripe
  - Also: lock contention

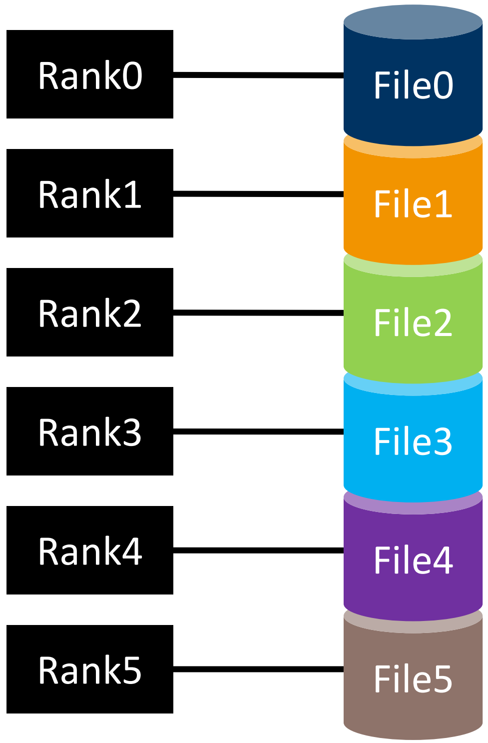
- Rank 0 issues 256 KB write request to Lustre
  - "No Problem! Let me lock the file on OST X, read the full 2 MB stripe, update 256 KB of it, write the 2 MB back to disk, and release the lock"
- Rank 1 issues 256 KB write request to Lustre
  - "No Problem! Let me lock the file on OST X, read the full 2 MB stripe, update 256 KB of it, write the 2 MB back to disk, and release the lock"
- …

- Stripe-aligned I/O access is vital for good performance!
  - User-controlled (domain decomposition and/or I/O request granularity)!
- Also: Consider overstriping (stripe count > no. of OSTs)



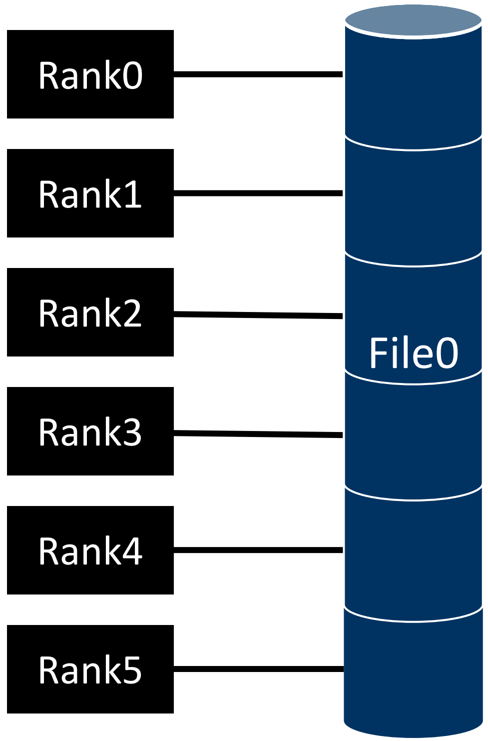
File access patterns: file-per-rank

- Advantages
  - Simple to implement
  - No coordination between processes needed
  - No false sharing of stripes/blocks
- Disadvantages
  - Number of files quickly becomes unmanageable
  - More difficult to change number of ranks for checkpoint/restart; postprocessing required
  - Files often need to be merged to create a canonical dataset for post-processing
  - Meta data handling bottleneck (e.g. some systems only have one MDS for all users)



File access patterns: file-per-app

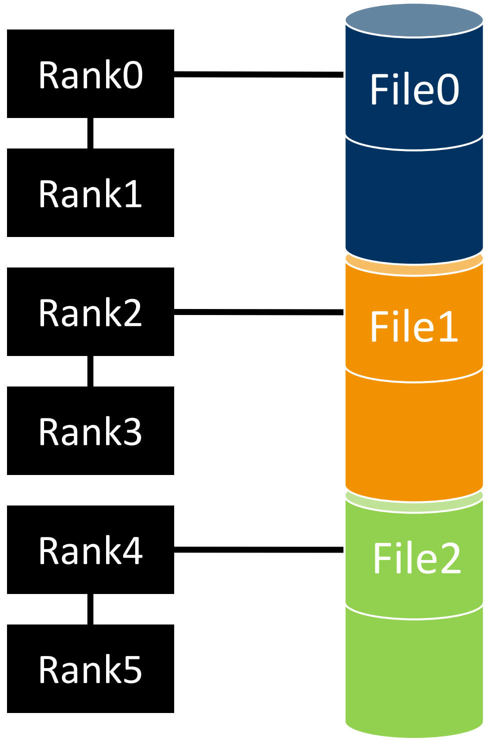
- Advantages
  - Number of files is independent of number of processes
  - Files can be in canonical representation (no post-processing)
- Disadvantages
  - Uncoordinated client requests might induce performance penalties
  - File layout may induce false sharing of file system blocks
  - Implementation overhead



File access patterns: file-per-subset

- Advantages
  - Number of files only depends on e.g. number of nodes
  - Possibly reduces strain on I/O subsystem

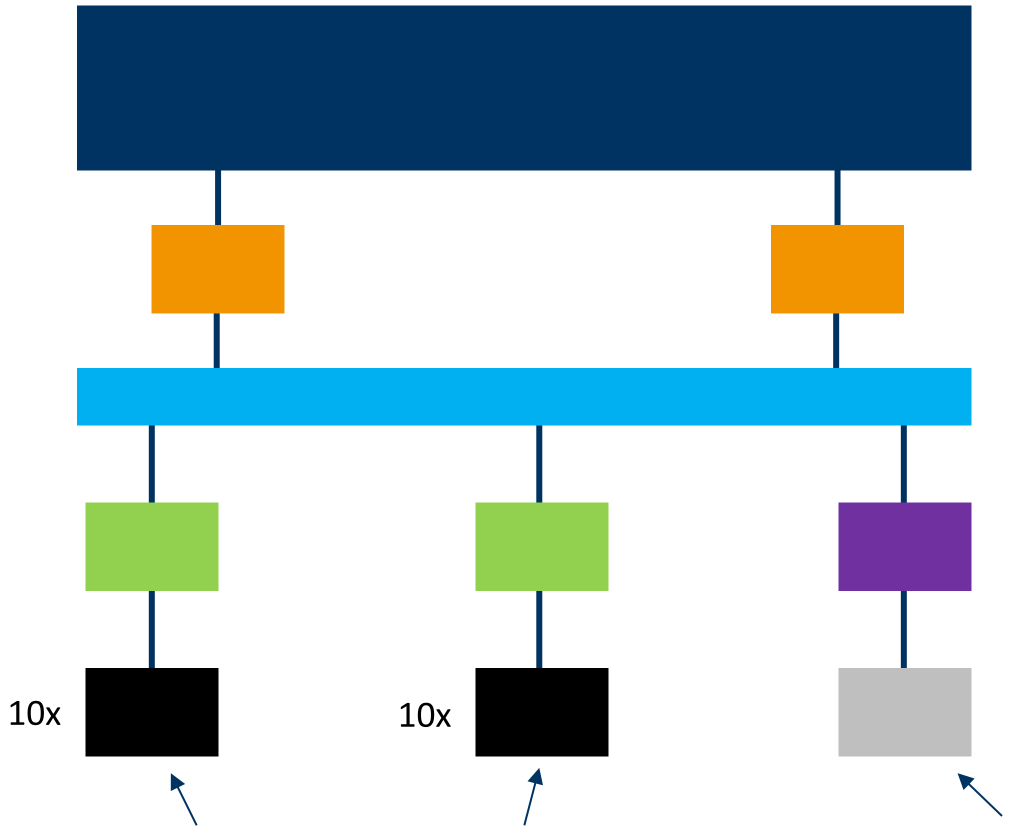
- Disadvantages
  - Requires application-side tuning for optimal results
  - Postprocessing required
  - Additional implementation overhead



UIBK I/O infrastructure

- LCC3 ($SCRATCH)
  - 100 Gbit/s Infiniband (consolidated compute nodes + storage), GPFS
- LEO4 + LEO5
  - GPFS / IBM Storage Scale / IBM Spectrum Scale
  - Flash storage for meta data user data
  - RAID5 disk arrays for performance and resilience

Local example: LEO4 @ UIBK (GPFS)



Each: RAID5 with 8+1 SAS-HDDs,
Shared per storage node: 6 hot spares

RAID5 with 8 SSDs

2 file servers, each: 1x 100 Gbit/s Infiniband to compute nodes and 4x 16 Gbit/s Fibre Channel (FC) to storage

2x SAS storage, each: 8x 16 Gbit/s FC to I/O layer, total ~65 TB, user data

1x flash storage: 8x 16 Gbit/s FC to I/O layer, total ~16 TB, meta data + user data

IO500

- Similar to TOP500 but for storage performance
  - https://io500.org/

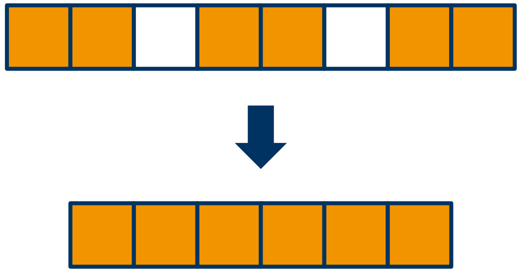
	INFORMATION							IO500			
# ↑	BOF	INSTITUTION	SYSTEM	STORAGE VENDOR	FILE SYSTEM TYPE	CLIENT NODES	TOTAL CLIENT PROC.	SCORE ↑	BW (GIB/S)	MD (KIOP/S)	REPRO.
1	SC23	Argonne National Laboratory	Aurora	Intel	DAOS	300	62,400	32,165.90	10,066.09	102,785.41	✓
2	SC23	LRZ	SuperMUC-NG-Phase2-EC	Lenovo	DAOS	90	6,480	2,508.85	742.90	8,472.60	✓
3	ISC25	Erlangen National High Performance Computing Center	Helma	MEGWARE	Lustre	186	18,600	838.99	438.62	1,604.84	✓
4	ISC25	Samsung Electronics	SSC-24	WekaIO	WekaIO	291	16,005	826.86	248.67	2,749.41	✓
5	SC23	King Abdullah University of Science and Technology	Shaheen III	HPE	Lustre	2,080	16,640	797.04	709.52	895.35	✓

MPI I/O

Characteristics

- Provides "high-level" interface for
  - Data partitioning
  - Asynchronous I/O operation
  - Strided read & write access

- Interfaces with derived datatypes
  - Reading and writing files similar to exchanging messages
  - Allows MPI-idiomatic message transfer and file I/O
  - Allows to aggregate strided file accesses
    - Remember MPI vector derived datatype
    - Storage media like contiguous accesses!
    - Also remember `MPI_Type_contiguous`!

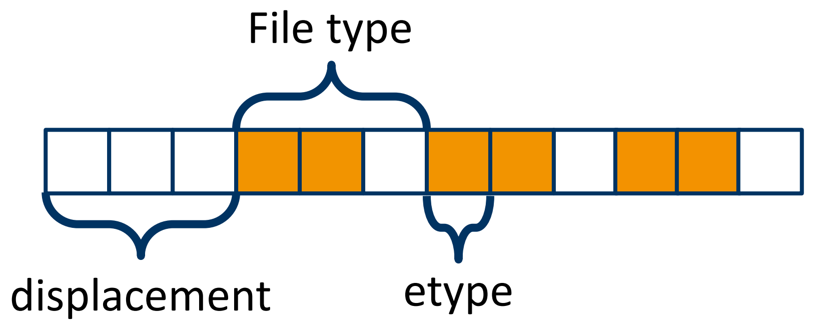


Basics

- Very similar to POSIX (and most other) I/O
  - `fopen() == MPI_File_open()`
  - `fwrite() == MPI_File_write()` (and a lot of others)
  - `fclose() == MPI_File_close()`

- Features could be implemented manually with POSIX, but complicated
  - Parallel access, buffering, offsets, flushes, etc.

- Basic building blocks & terminology
  - etype: type of individual elements
  - filetype: which portion of file is visible to current rank
  - displacement: number of bytes to be skipped from the start of the file
  - view: tuple of (etype, filetype, displ.)



Example

```
int main(int argc, char** argv) {
    MPI_Init(&argc, &argv);

    MPI_File fh;
    MPI_File_open(MPI_COMM_WORLD, "my_file", MPI_MODE_RDWR | MPI_MODE_CREATE, MPI_INFO_NULL, &fh);

    char* buf = ... // data to be written
    int size = ...; // size of data to be written
    MPI_Offset offset = ...; // e.g. compute a rank-dependent file offset

    MPI_File_write_at(fh, offset, buf, size, MPI_CHAR, MPI_STATUS_IGNORE);

    MPI_File_close(&fh);
    free(buf);
    MPI_Finalize();

    return EXIT_SUCCESS;
}
```

Opening and closing files

- `MPI_File_open(comm, filename, amode, info, fh)`
  - Is a collective call
  - Filename is implementation-dependent but must reference same file on all ranks
  - Allows specifying access modes and info hints
  - Internally, MPI maintains individual and shared file pointers after opening a file
    - subsequent operations decide which of those are used and/or updated
  - Can use `MPI_COMM_SELF` for rank-local files

- `MPI_File_close(fh)`
  - Is a collective call
  - Will delete file if open mode included `MPI_DELETE_ON_CLOSE`
    - Useful for temporary files

File open access modes

- `MPI_MODE_RDONLY`: read-only
- `MPI_MODE_WRONLY`: write-only
- `MPI_MODE_RDWR`: read and write
- `MPI_MODE_CREATE`: create if file does not exist
- `MPI_MODE_EXCL`: fail if file already exists
- `MPI_MODE_DELETE_ON_CLOSE`: delete on close
- `MPI_MODE_UNIQUE_OPEN`: file not opened concurrently (even outside MPI; removes need for locks)
- `MPI_MODE_SEQUENTIAL`: file is only accessed sequentially: mandatory for sequential stream files (pipes, tapes, ...); mutually exclusive with `MPI_MODE_RDWR`
- `MPI_MODE_APPEND`: all file pointers set to end of file

- Must be the same for all ranks participating in the same `MPI_File_open()` call

File info: hints for MPI

- Used in `MPI_File_open()`, `MPI_File_set_view()`, or `MPI_File_set_info()`
  - collective buffering
    - `collective_buffering`: specifies whether the application may benefit from coalescing small I/O requests of multiple ranks to form larger blocks on fewer ranks for the storage layer
    - `cb_block_size`: data access in chunks of this size
    - `cb_buffer_size`: on each node, usually a multiple of stripe/block size
    - `cb_nodes`: number of nodes to be used for collective buffering
  - disk striping (only relevant in `MPI_FILE_OPEN()`)
    - `striping_factor`: number of I/O devices used for striping
    - `striping_unit`: length of a chunk on a device (in bytes)

- Use `MPI_INFO_NULL` if no hints

Writing and reading data

positioning	(non)blocking	coordination	
		noncollective	collective
explicit offsets	blocking	MPI_File_read_at()	MPI_File_read_at_all()
		MPI_File_write_at()	MPI_File_write_at_all()
	nonblocking	MPI_File_iread_at()	MPI_File_iread_at_all()
		MPI_File_iwrite_at()	MPI_File_iwrite_at_all()
individual file pointers	blocking	MPI_File_read()	MPI_File_read_all()
		MPI_File_write()	MPI_File_write_all()
	nonblocking	MPI_File_iread()	MPI_File_iread_all()
		MPI_File_iwrite()	MPI_File_iwrite_all()
shared file pointer	blocking	MPI_File_read_shared()	MPI_File_read_ordered()
		MPI_File_write_shared()	MPI_File_write_ordered()
	nonblocking	MPI_File_iread_shared()	
		MPI_File_iwrite_shared()	

File pointer semantics

- Explicit offsets
  - Most basic I/O, like POSIX
  - read/write location is always computed using start of file + offset, no file pointers are changed
- Individual file pointers
  - Allows use of derived data types
  - File pointer is advanced when used in an operation
  - Each operation on a file pointer only affects this rank's individual file pointer
- Shared file pointers
  - Same as individual FP, but single, shared file pointer is advanced
  - Non-collective: concurrent calls by multiple ranks are serialized in nondeterministic order
  - Collective: concurrent calls by multiple ranks are serialized in-order

File Views

- Provide a visible and accessible set of data from an open file
- `MPI_File_set_view(fh, disp, etype, filetype, datarep, info)`
  - collective operation
  - Allows to change the rank's view of the data, even repeatedly
    - local and shared file pointers are reset to zero
  - `datarep` argument is a string that specifies the format in which data is written to a file: `native`, `internal`, `external32`, or `user-defined`
  - same `etype` extent and same `datarep` on all processes
  - mainly useful for custom, non-contiguous data access within a file

General guidelines

- Lustre
  - Keep stripe count above 1 but below total number of OSTs (allows Lustre to avoid slow OSTs)
- MPI I/O
  - Explicit offsets, non-collective: similar to independent POSIX calls, (often) bad performance
  - Explicit offsets, collective: exploits parallelism in filesystem, better performance
  - Individual file pointers, non-collective: exploits request aggregation due to derived data types, better performance
  - Individual file pointers, collective: best of both worlds, best performance
- A ton of tuning involved, dependent on: filesystem semantics; number of storage and I/O forwarding nodes; size, bandwidth and latency of disk arrays; buffer sizes; network contention; application characteristics; etc.

Error Handling

- File handles have their own error handler
  - Default is MPI_ERRORS_RETURN (c.f. message passing: MPI_ERRORS_ARE_FATAL)
- Changing the default:
  - MPI_File_set_errhandler(MPI_FILE_NULL, MPI_ERRORS_ARE_FATAL);
- Note: MPI behavior is undefined after first erroneous MPI call
  - But a high-quality implementation will support I/O error handling facilities

High-level I/O libraries

HDF5 / NetCDF4

- Hierarchical Data Format / Network Common Data Form
- Libraries for efficiently writing and reading scientific data
  - MPI is quite low-level, does not provide any higher-level file structure
- Are somewhat compatible
  - NetCDF4 uses a subset of HDF5 file structure + some additions
- Provide API and tools for reading and manipulating files
  - HDF5: C, C++, Fortran 90, Python, Java, Command line (and probably others)
  - E.g. `h5diff`

HDF5 Structure

- Provides a unix-like path structure
  - E.g. `/Group1/Group5/DataSet9`

- Terminology:
  - File: Container for storing data
  - Group: Structure that can contain HDF5 objects (datasets, attributes)
  - Attribute: Describes datasets (e.g. experiment parameters, git commit versions, etc.)
  - Dataspace: Describes shape of dataset (e.g. dimensionality)
  - Dataset: Multi-dimensional arrays of data

HDF5 File Operations

H5Fcreate(), H5Fopen()

File level

H5Screate_simple(), H5Sopen()

Dataspace level

H5Dcreate(), H5Dopen()

Dataset level

H5Dread(), H5Dwrite()

H5Dclose()

H5Sclose()

H5Fclose()

HDF5 Features

- Parallelism
  - Supports collective or non-collective MPI I/O, controlled by user through HDF5 API
- Compression
  - Data can be automatically compressed in transit
- Hyperslabs
  - Select a subset of data corresponding to e.g. a certain dimension
  - Facilitates extracting e.g. a 2D plane from 3D data

Summary

- Parallel I/O is very complex
- Getting high performance means knowing the platform and its settings
  - Stripe/block sizes, counts, individual disk array performance, etc.
- MPI I/O offers standardized I/O interface
  - Higher-level libraries exist, use them if suitable!

Sources

- Rolf Rabenseifner, HLRS
- Richard J Zamora, ANL
- David Henty, EPCC
- …