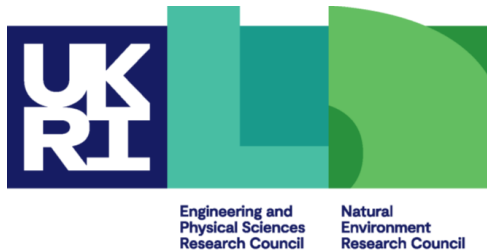


Advanced Message-Passing Programming

Efficient use of the Lustre Filesystem



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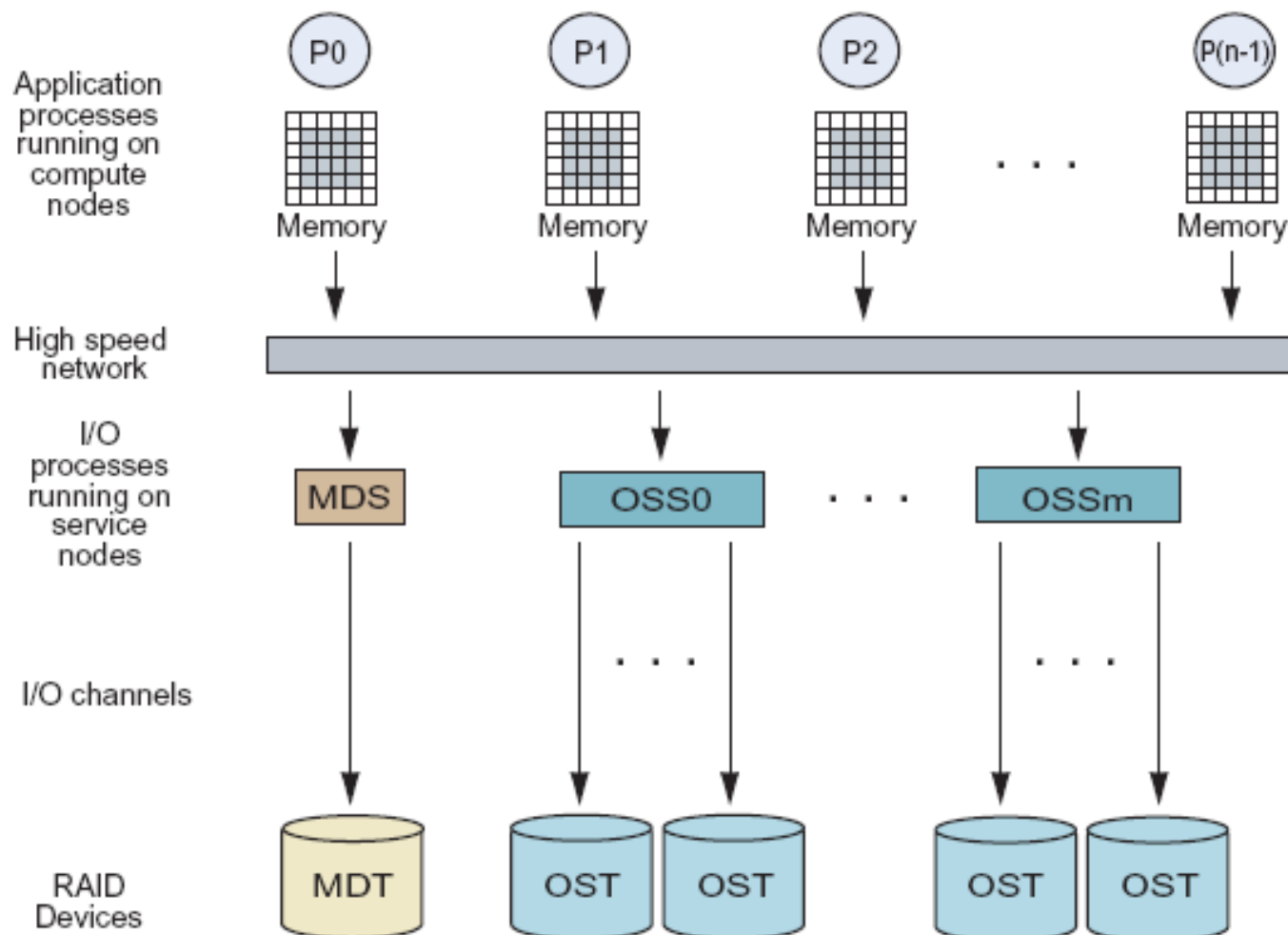
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Lustre: where are the bottlenecks?



Caution!

- IO benchmarking is very difficult and can be non-reproducible
 - you are sharing the ARCHER2 system with other users
 - someone else may also be writing to the same OSTs
 - someone else may be using the same network links
- Caching can give very high IO rates
 - especially with small files
- Ensure benchmarks run for a reasonable time
 - e.g. a few seconds (i.e. large amounts of data)
 - and repeat them several times

ARCHER2 hardware

- Three separate /work filesystems
 - each has 12 OSTs and one MDS
 - consortia assigned to different partitions to share the load
- Additional filesystem with SSDs not spinning disks
 - still to be configured
 - expect better performance for small I/O transactions
 - better latency and maybe better bandwidth
- Each has around 3.3 PiB of storage
 - total of 13.2 PiB (which is 14.5 PB !)

Serial IO

- You are not using parallel libraries
 - single file with controller IO (a single writer)
 - file-per-process (many independent writers)
- Little point in striping the file
 - single file: performance bottlenecks appear to be elsewhere
 - multiple files: already parallel as we are using many disks
- This is why a single stripe is the default
- Ballpark figure: single process can achieve about 1 GiB/s
 - in the absence of caching, i.e. writing very large files

MDS performance

- The MDS can become overloaded
 - e.g. opening and closing a file requires MDS access
 - this is therefore a serial operation
 - and you share the MDS with all users on the same filesystem
 - do not do multiple “open/seek/close” operations on the same file
- Tricks
 - try not to write too many files
 - a simple trick is file-per-node rather than file-per-process
- If you must have lots of files, consider multiple directories
 - e.g. a directory per node
 - decreases lookup times for files

Stripe size

- Default is 1 MiB
 - seems quite small for very large datasets
 - experiment with larger settings:
`lfs setstripe -S 4m <dir/file>`
- Do not set too large
 - as you won't be using all of the OSTs!

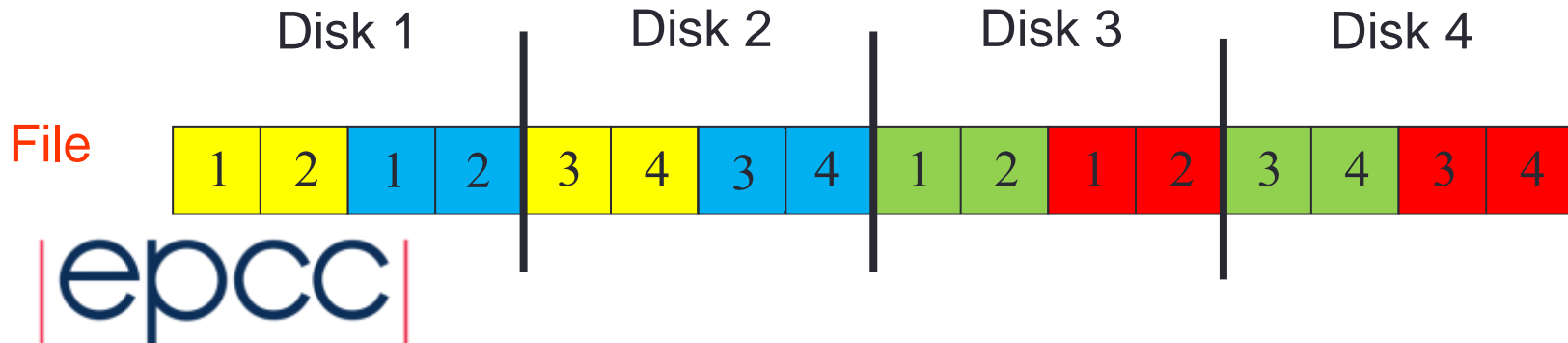
How does parallel IO work?

- MPI-IO auto-configures to the Lustre settings
- Identifies a small number of aggregator processes
 - spread across nodes if possible
- Uses MPI collectives (e.g. scatter/gather) to aggregate data to these processes
 - then performs a small number of large write operations
 - minimises overheads of locking etc.
- Only possible with collective IO calls
- Can get useful runtime statistics by setting
 - `export MPICH_MPIIO_STATS=1`
 - in your SLURM script

4x4 array on 2x2 Process Grid

Parallel Data

2	4	2	4
1	3	1	3
2	4	2	4
1	3	1	3



Aggregators

- By default, Cray MPI uses one aggregator per stripe
 - does not seem optimal as single-process IO is slow
- This default can be changed
- E.g. to use twice as many aggregators

```
export MPICH_MPIIO_HINTS=:cray_cb_nodes_multiplier=2
```

Switching MPI versions

- Default low-level network layer: OFI, Open Fabrics Interface
 - can sometimes have poor MPI collective performance
 - fix (which is already in the default script) is:

```
export FI_OFI_RXM_SAR_LIMIT=64K
```

- Can switch MPI to use UCX, developed by Mellanox
 - UCX seems to be better for collectives with heavy comms loads
 - no need to recompile – just alter your SLURM script

```
module swap craype-network-ofi craype-network-ucx  
module swap cray-mpich cray-mpich-ucx
```

Common mistakes

- Serial IO mistakes
 - text data files
 - multiple accesses to a large number of small files
 - using striping for serial IO
- Parallel IO mistakes
 - using a parallel IO library but not striping the file
 - I would recommend full striping across all OSTs
 - using non-collective (i.e. individual) IO to a single file
 - you must quantify performance in terms of GiB/s
 - you should be able to achieve around 10 GiB/s for parallel IO

Conclusions

- For parallel IO to a single shared file
 - use a high-level parallel IO library
 - use collective calls
 - stripe file across all OSTs: `lfs setstripe -c -1 <output_dir>`
- For serial IO (single or multiple files)
 - do not stripe the files (e.g. accept defaults on ARCHER2)
 - consider writing file per node
 - controller IO: only uses a single disk
 - file-per-process: may overload the MDS, especially with many users
 - consider file-per-node, or multiple files-per-node to utilise full bandwidth