# Advanced Message-Passing Programming

Efficient use of the Lustre Filesystem











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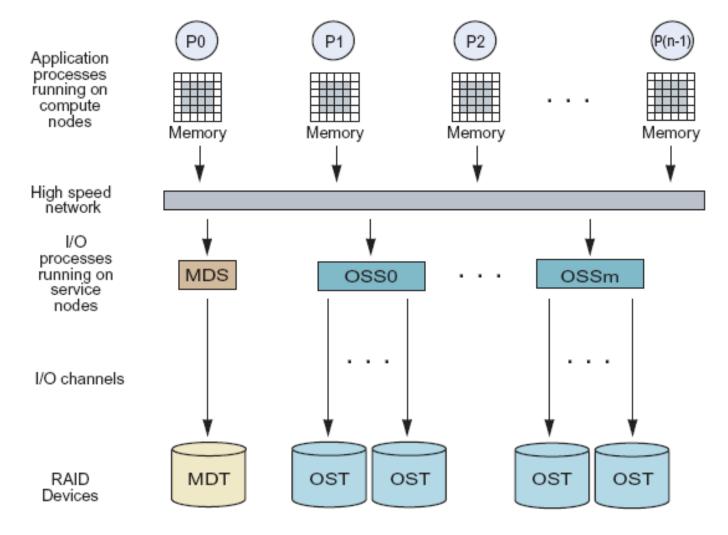
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#### Lustre: where are the bottlenecks?







#### Caution!

- IO benchmarking is very difficult and can be nonreproducible
  - 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 but not necessarily 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 nodes
- Uses MPI collectives (e.g. scatter/gather) to aggregate data to these nodes
  - 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

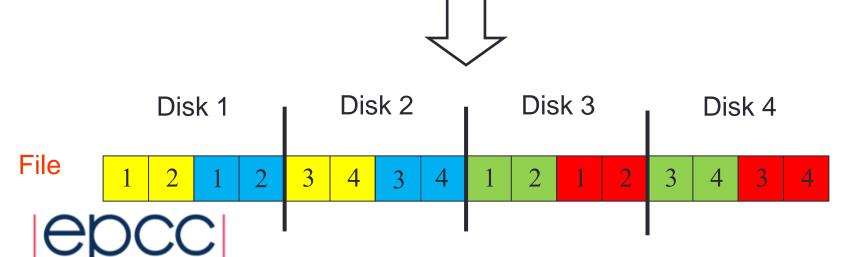




# 4x4 array on 2x2 Process Grid

**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 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: 1fs 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



