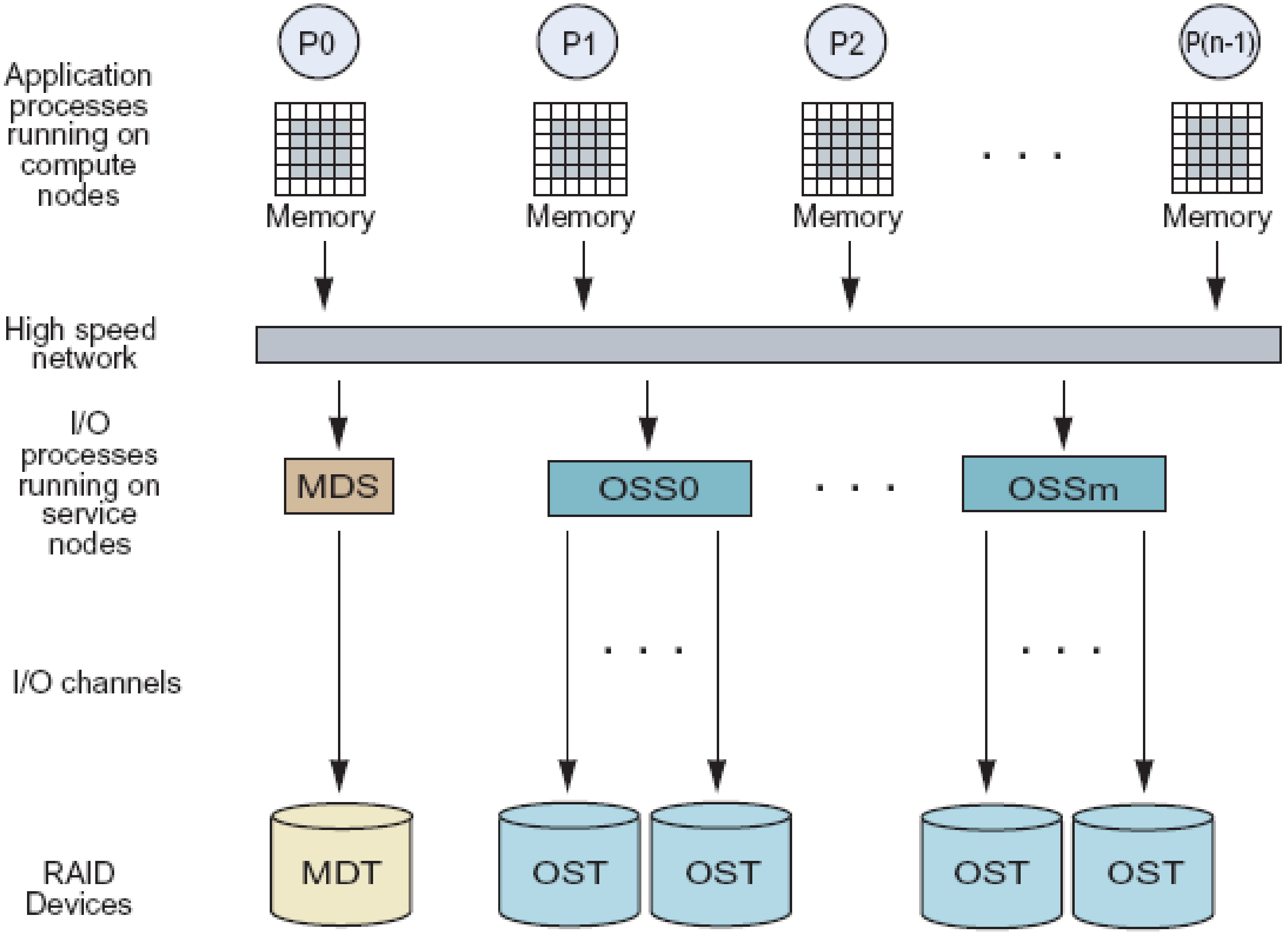
Advanced Message-Passing Programming

Efficient use of the Lustre Filesystem

Reusing this material

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

- Four 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
  - expect better performance for small I/O transactions
  - better latency and maybe better bandwidth
- Each disk system 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!

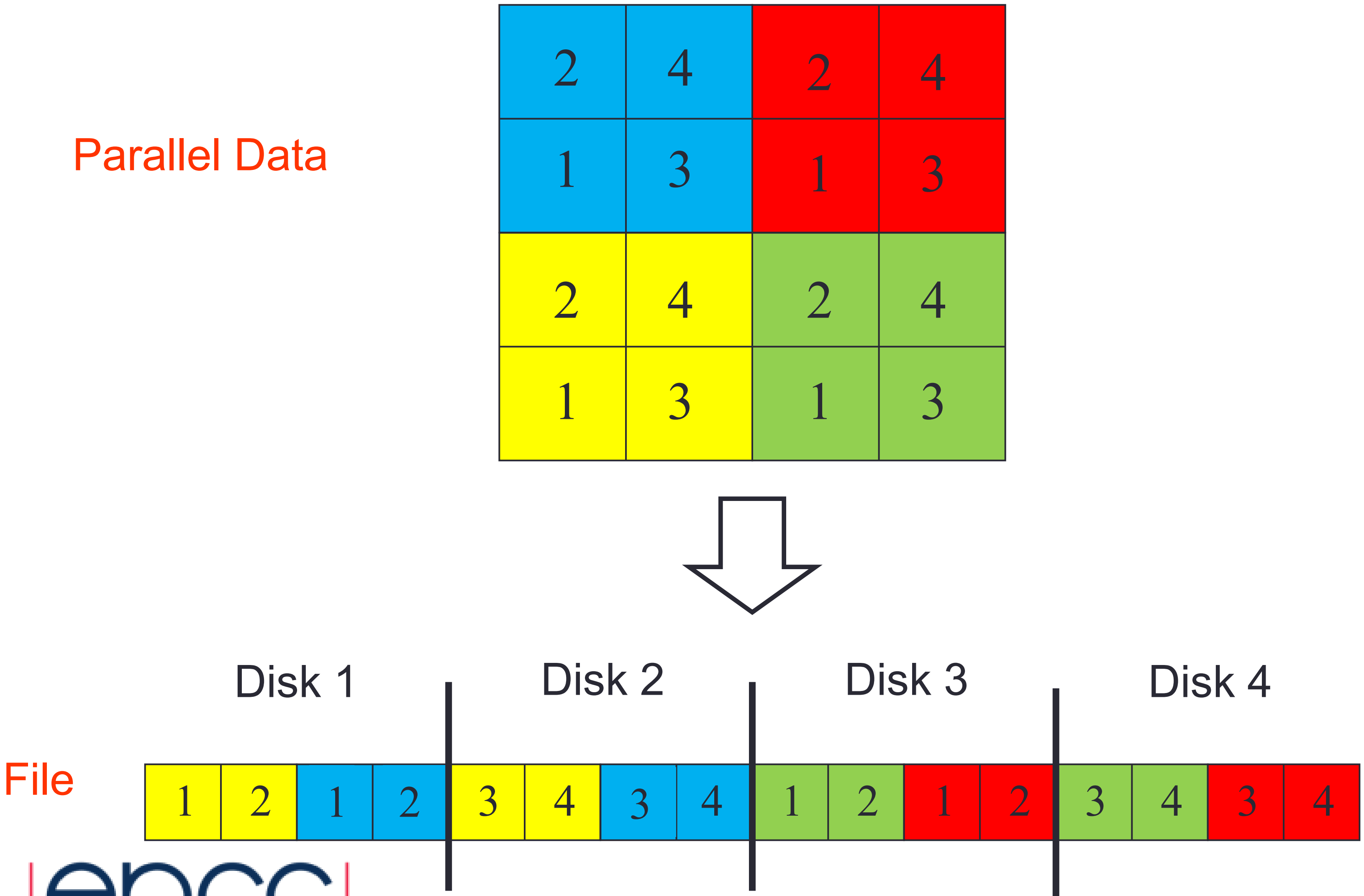
How does parallel IO work?

- 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

File

Disk 1				Disk 2				Disk 3				Disk 4			
🟨 1	🟨 2	🟦 1	🟦 2	🟨 3	🟨 4	🟦 3	🟦 4	🟩 1	🟩 2	🟥 1	🟥 2	🟩 3	🟩 4	🟥 3	🟥 4

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 four times as many aggregators (four per node)

```
export MPICH_MPIIO_HINTS=*:cray_cb_nodes_multiplier=4
```

- This causes multiple processes to write to the same OST
  - default locking approach is very inefficient
  - try using `*:cray_cb_write_lock_mode=2,*:cray_cb_nodes_multiplier=4`

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 in excess of 10 GiB/s for parallel write

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

Every node writes one file at a time

```
// Create communicator per node so only one process on a node does IO at any one time

 MPI_Comm_split_type(MPI_COMM_WORLD, MPI_COMM_TYPE_SHARED, rank, MPI_INFO_NULL, &nodecomm);

 int noderank, nodesize, rankloop;
 MPI_Comm_rank(nodecomm, &noderank);
 MPI_Comm_size(nodecomm, &nodesize);

 for (rankloop = 0; rankloop < nodesize; rankloop++)
 {
     // Do the IO one at a time
     if (rankloop == noderank)
       {
         write_file_from_this_process();
       }
     // Wait your turn
     MPI_Barrier(nodecomm);
 }

 MPI_Comm_free(&nodecomm);
```