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CRUK CI cluster introduction (III of III)

Some advanced topics

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Reference Genomes (new cluster)

- Path to reference data:

  /scratchb/bioinformatics/reference_data/reference_genomes/
- Path to assembly:

  …/*organism*/*assembly*/
- What we maintain:
  - Genome sequence (fasta)
  - Alignment indices: BWA, TopHat, Bowtie (1,2)
  - Annotations:
    - GTF format gene model
    - RefFlat format gene model
    - Signal artifact list (if available)

Working with Lustre

1. Revisit architecture

2. Stripes

3. Avoiding I/O Bottlenecks

4. Using System Cache

Lustre: Quick Review

Lustre is a massively parallel distributed file system

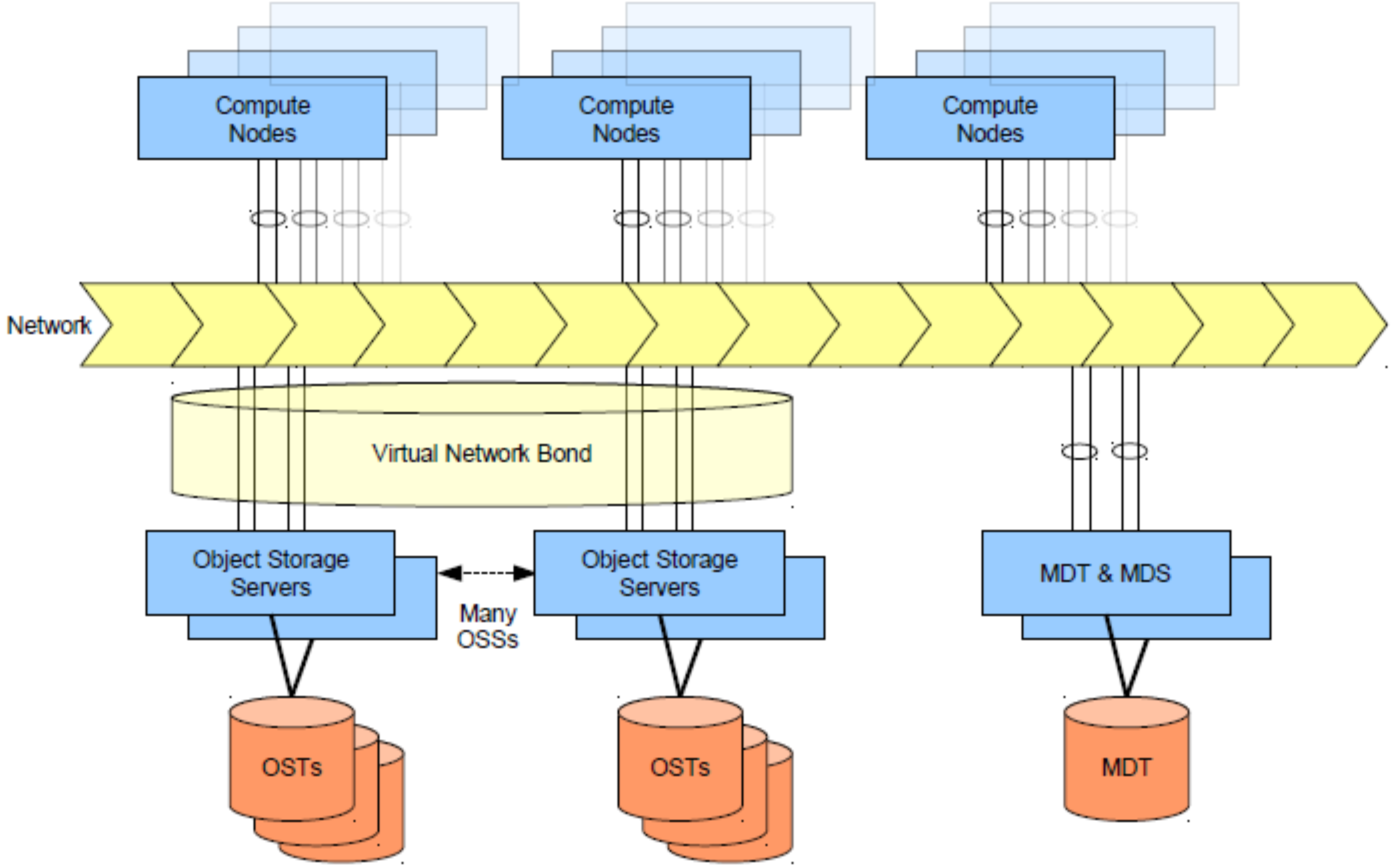
- Deployed in 7 out of 10 most powerful supercomputers
- POSIX compliant

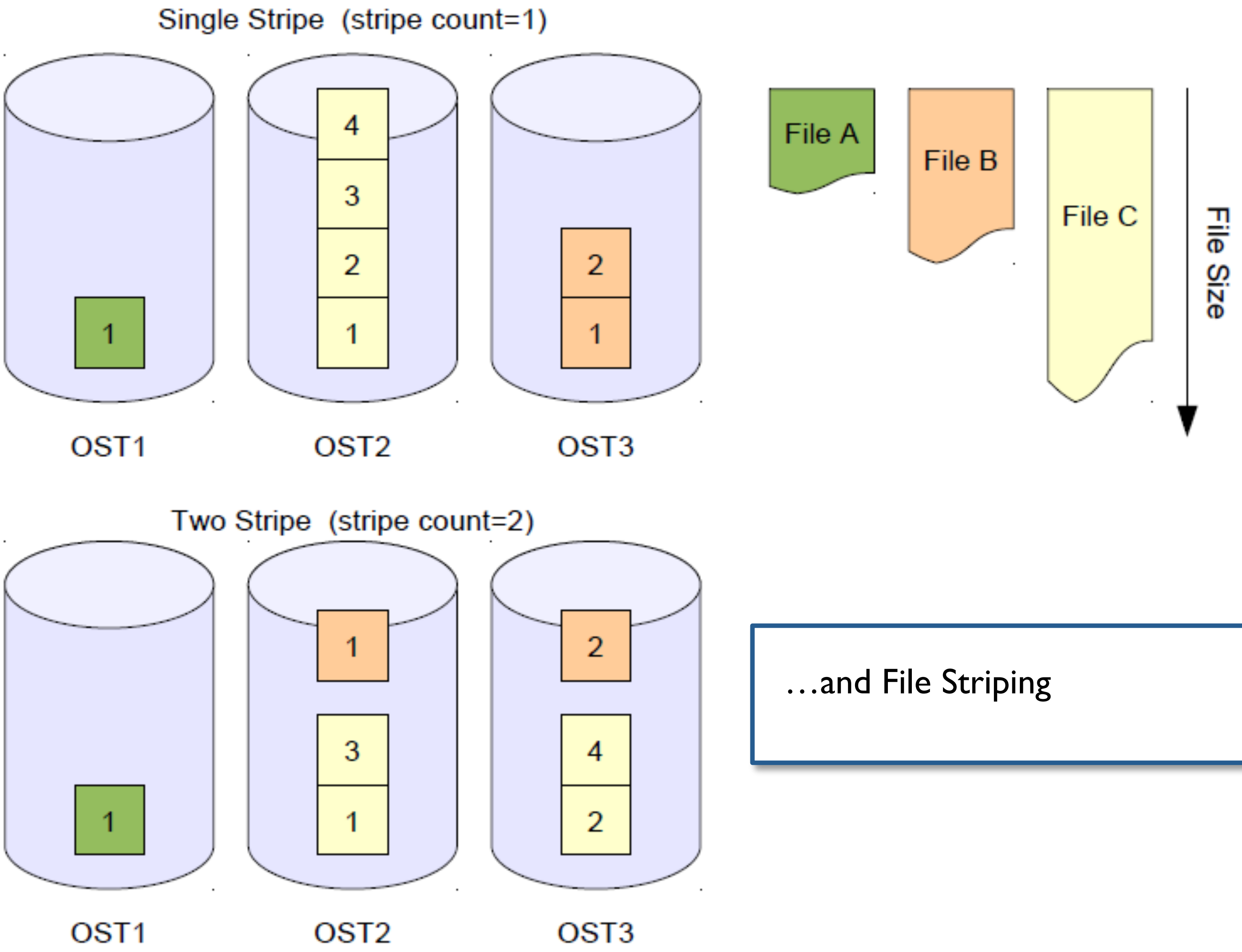
Lustre design paradigm concepts

- Separation of file meta-data and storage allocation
- Scalable data serving through parallel data striping
- Aggregates network bandwidth
- Distributed operation

’**scratch**’ storage we (deliberately) don't back it up

Lustre Architecture …





…and File Striping

File Striping Large Files

Striping allows file size to exceed single OST size

Performance benefit

- Aggregates I/O bandwidth to single large file
- In general, more strips improves performance
- Small overhead associated with open/closing striped files

Many jobs reading single file

- For example blastdb and maq reference data
- /lustre/reference_data/genomes

Many jobs reading & writing multiple large files

- Requires benchmarking

Many jobs writing to single file

- High bandwidth but requires careful coding (can be disastrous)

Set Stripe Information

Set per file or directory

Default is not to stripe

Only newly created files will be stripes

- Use cp (not mv) to migrate existing files

```
uk-cri-lcst01 ~ $ lfs setstripe <file|dir> --size <stripe_size>
--count <count> --index <index>
```

Where,

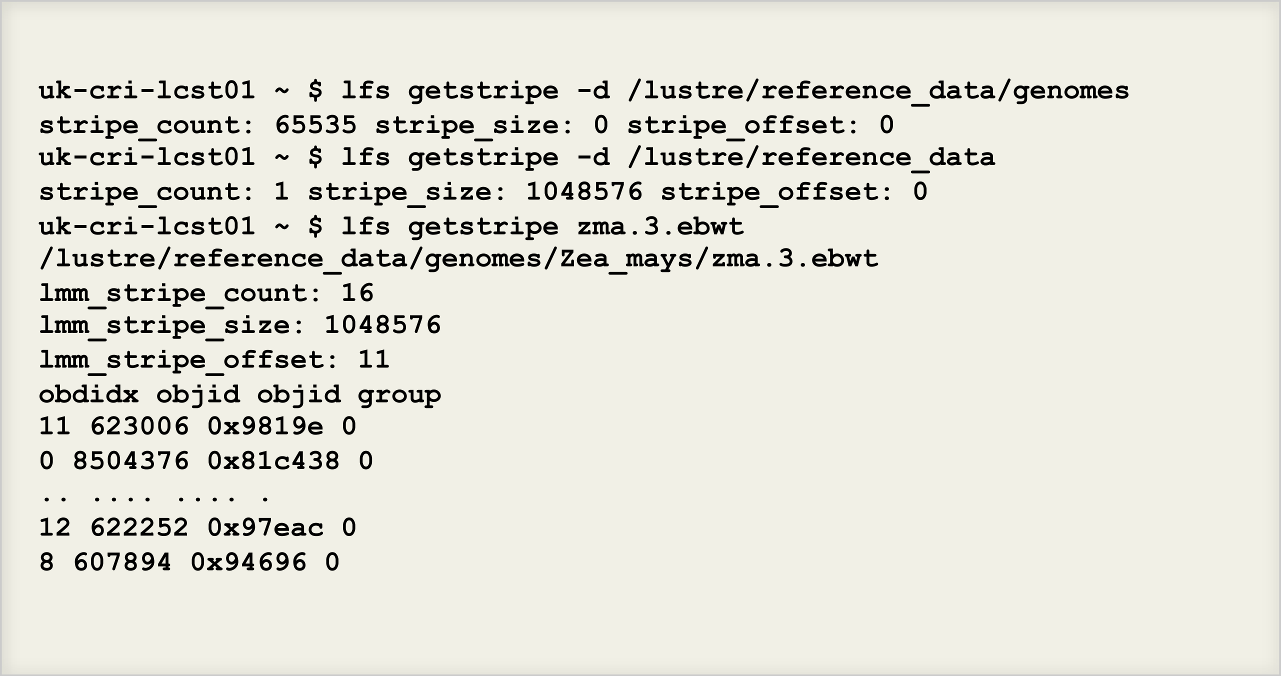
size = stripe size specified in k, m or g (0 default 1MB)

count = OST stripe count (0 defaults 4 OST and -1 over all OSTs)

index = OST index of first stripe (-1 indicating default)

Read Stripe Information

Inspect file and directory stripe information with **lsf getstripe**



```
uk-cri-lcst01 ~ $ lfs getstripe -d /lustre/reference_data/genomes
stripe_count: 65535 stripe_size: 0 stripe_offset: 0
uk-cri-lcst01 ~ $ lfs getstripe -d /lustre/reference_data
stripe_count: 1 stripe_size: 1048576 stripe_offset: 0
uk-cri-lcst01 ~ $ lfs getstripe zma.3.ebwt
/lustre/reference_data/genomes/Zea_mays/zma.3.ebwt
lmm_stripe_count: 16
lmm_stripe_size: 1048576
lmm_stripe_offset: 11
obdidx objid objid group
11 623006 0x9819e 0
0 8504376 0x81c438 0
.. ..... ..... .
12 622252 0x97eac 0
8 607894 0x94696 0
```

Using System Cache

Disk access is slow (no escape from this!)

- Memory access measured in a few nanoseconds
- Disc access measured in 10s of milliseconds

Linux uses free memory as cache

- Memory reclaimed as least used files expunged

“Pre-warming” cache

- Can dramatically increase I/O performance

```
uk-cri-lcst01 ~ $ cat largefile > /dev/null
uk-cri-lcst01 ~ $ grep searchString largefile
```

Avoiding Cache misses

Say you want to compare 3 sequences against 3 large databases:

“Out of the box” example

- sequence 1 vs database 1 **No cache: disk read required**
- sequence 1 vs database 2 **Cache miss: disk read required**
- sequence 1 vs database 3 **Cache miss: disk read required**
- sequence 2 vs database 1 **No cache: data expunged from cache**
- sequence 2 vs database 2 **Cache miss: disk read required**

Re-ordering to avoid cache misses

- sequence 1 vs database 1 **No cache: disk read required**
- sequence 2 vs database 1 **Cache hit: data in cache**
- sequence 3 vs database 1 **Cache hit: data in cache**
- sequence 1 vs database 2 **No cache: disk read required**
- sequence 2 vs database 2 **Cache hit: data in cache**

Avoiding Bad Performance

· Interactive use

- Statting files can be slow (common with shared file systems)
- Avoid directly editing small files on lustre (keep to /home)
- Turn off "color ls" (stat required for each file/directory)

Random seeks

- Small random I/O extremely slow on lustre
- Avoid, as much as possible, running databases on lustre

e.g. mysql, sqlite, Berkeley DB etc

Limit number of files in directory

- 100,000s files in single directory bad (avoid, if possible)
- Use lfs setstripe to confine all files to single OST

```
uk-cri-lcst01 ~ $ lfs setstripe --count 1 directory
```

Parallel Workloads

What happens when you increase your dataset size?

- O(n), O(n log n), O(n^2), O(n^9)
- Runtime & memory increase (O) with problem size (n)

Calculations are carried out in parallel

- Operating on principle that large calculations can often be divided into N smaller tasks
- These tasks are solved concurrently
- Time reduces to a function of O(n^x)/N

Parallel overheads

- communication, concurrency, parallel I/O introduce new overheads
- O(N), O(N log N), O(N^2)

Amdahl's Law

- Speed up of parallel application is ultimatley limited by the fixed runtime of any sequence sections
- There's no magic bullet for this, you may have to change your algorithm, or mix parallel and single node sections.

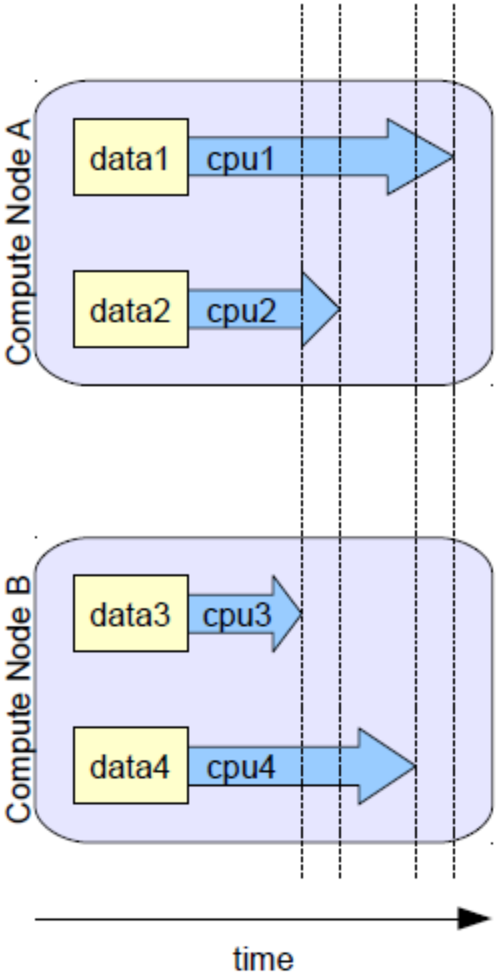
Simple Parallel

(‘*Embarassing*’ or ‘*Trivial*’ in the computing science literature)

Solving many similar and independent tasks

- Analysis split into tasks
- Task assigned to one cpu
- No inter-task communication
- More throughput by running more tasks
- Task runtime varies

90% of bioinformatics codes fall into this model



Shared Memory

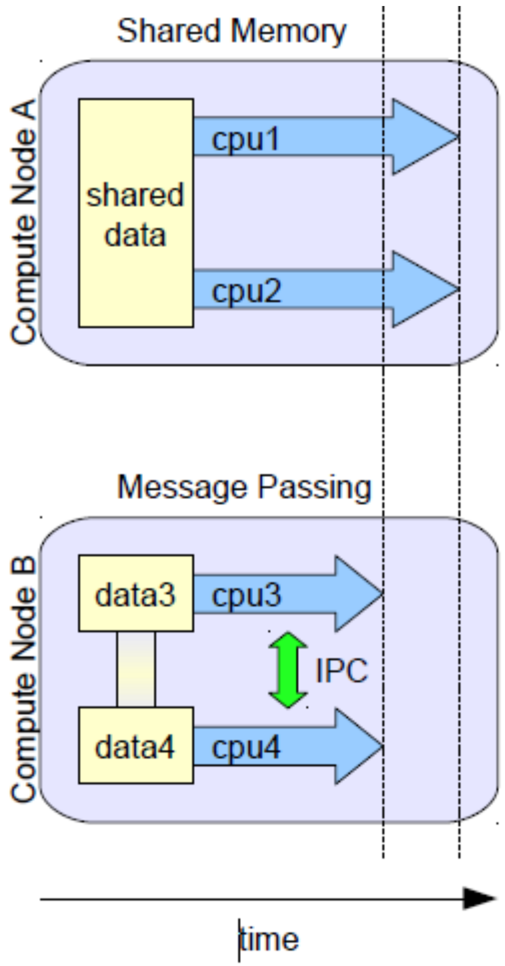
Shared tasks and memory

- Tasks assigned to cpus or cores
- Inter-task communication via shared memory
- Runtime decreases by adding more threads

Message Passing - local

Multiple processes communicate using O/S level systems. Code must be specifically written to exploit parallelism

- OpenMP/OpenMPI/etc



Message passing over network

Single task split across many compute nodes

- inter-machine communication (IMC)
- through MPI/OpenMP libraries again

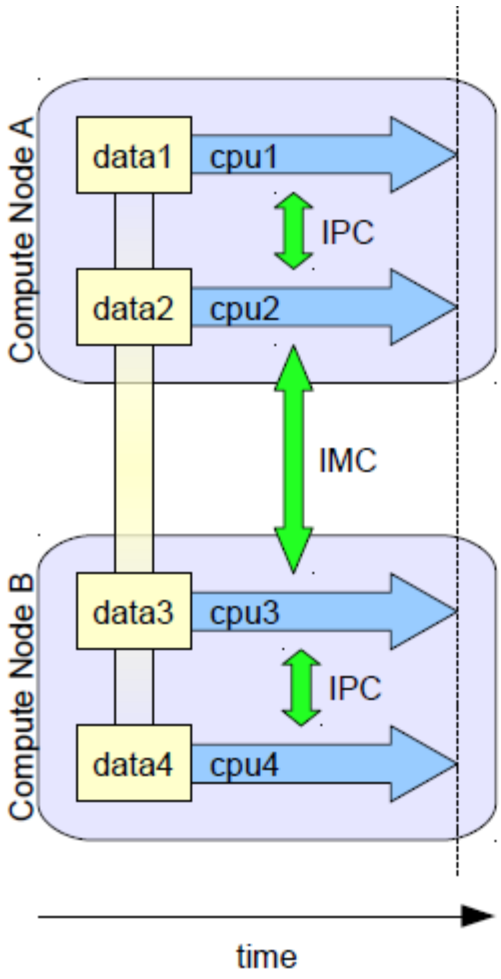
Hybrid models

Single task split across many compute nodes

- Mix SMP, local MP, network MP

Can be tricky to predict performance.

Your code may get quite complex…



Acknowledgements

Peter Maccallum
Marc O'Brien
Mark Dunning
Ann Pajon