PERFORMANCE OF PARALLEL IO ON LUSTRE AND GPFS

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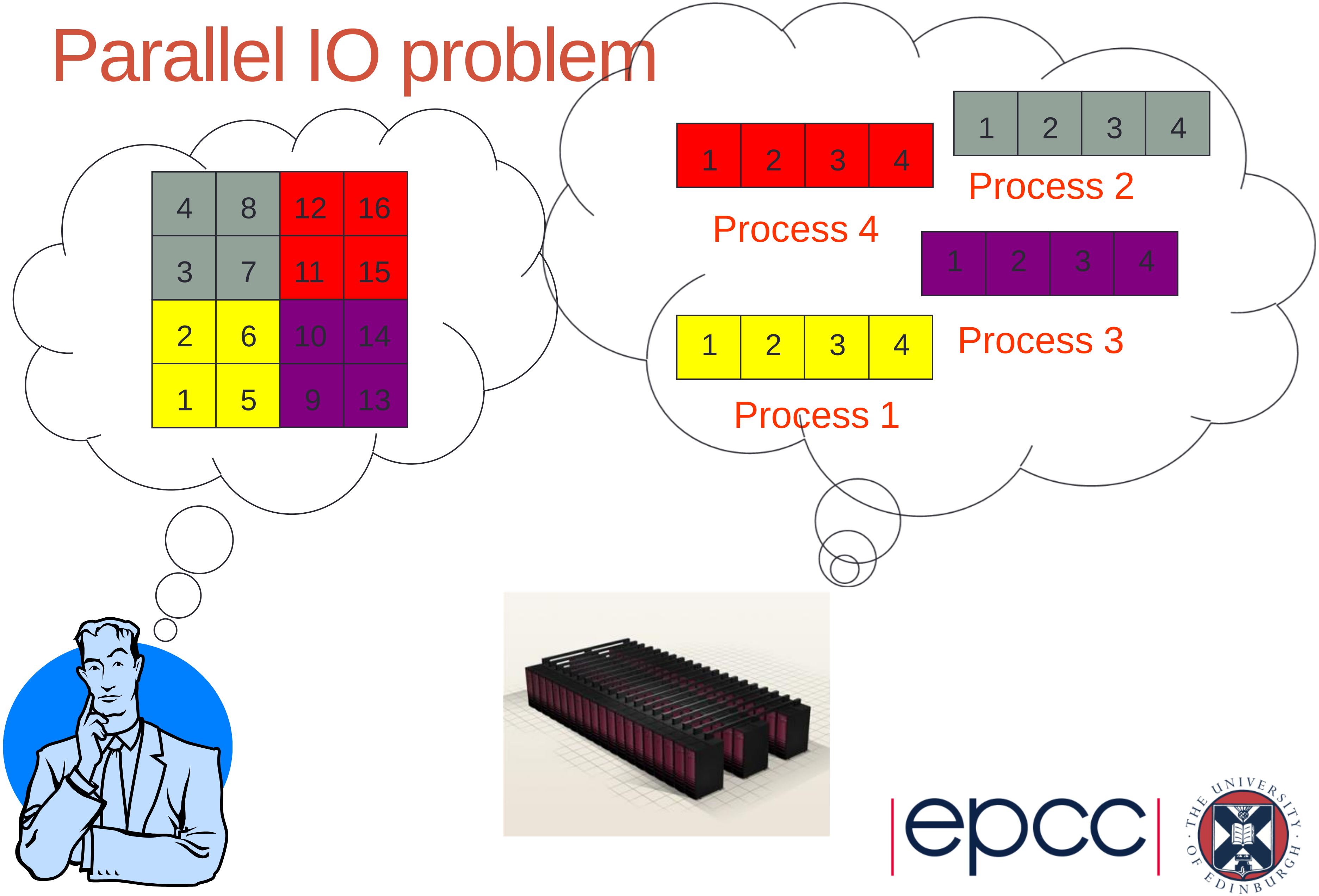
Outline

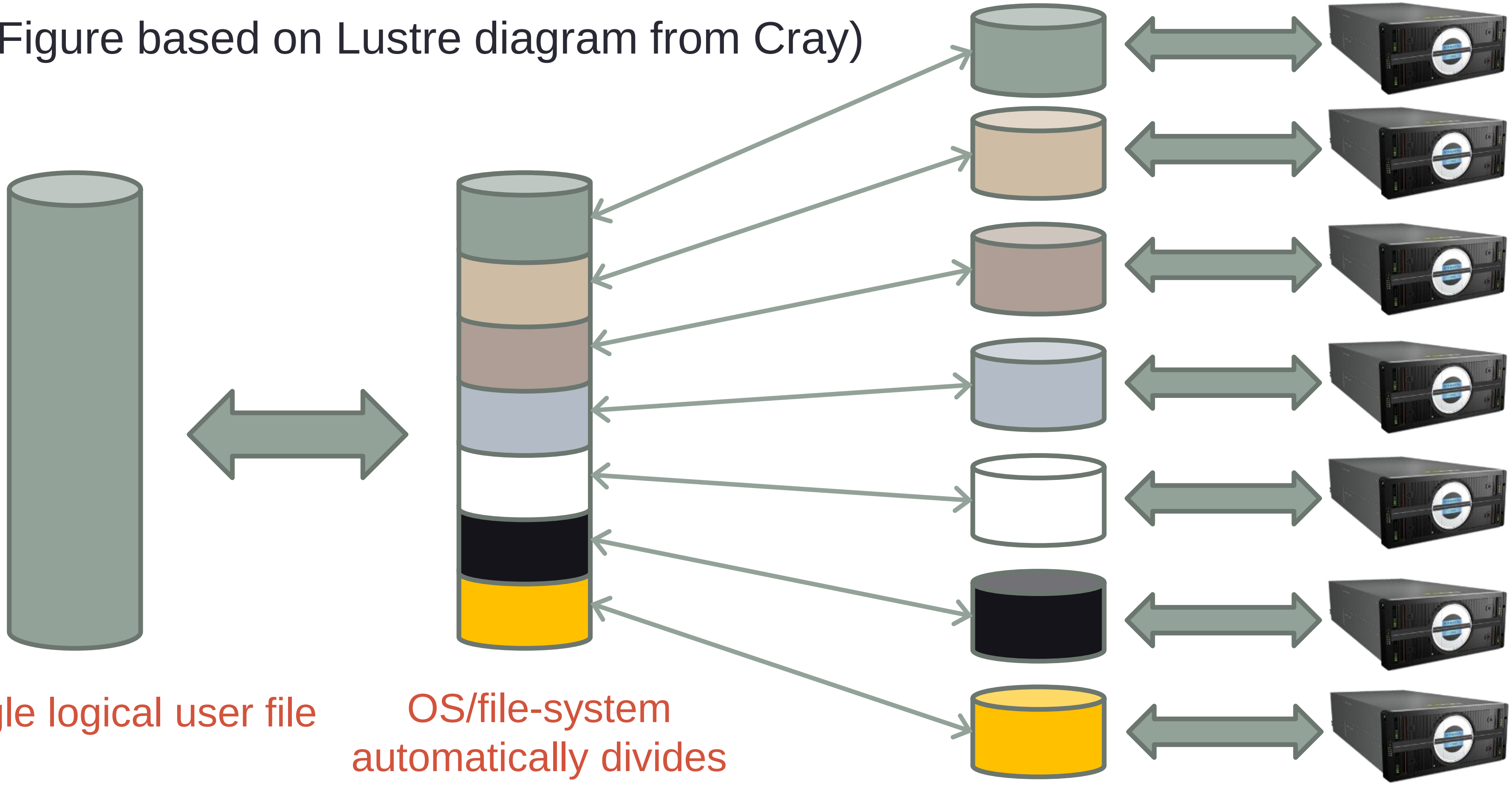
- Parallel IO problem
- Common IO patterns
- Parallel filesystems
- MPI-IO Benchmark results
- Filesystem tuning
- MPI-IO Application results
- HDF5 and NetCDF
- Conclusions

Parallel IO problem



Parallel Filesystems

(Figure based on Lustre diagram from Cray)



Single logical user file

OS/file-system automatically divides the file into stripes

Common IO patterns

- Multiple files, multiple writers
  - each process writes its own file
  - numerous usability and performance issues
- Single file, single writer (master IO)
  - high usability but poor performance
- Single file, multiple writers
  - all processes write to a single file; poor performance
- Single file, collective writers
  - aggregate data onto a subset of IO processes
  - hard to program and may require tuning
  - potential for scalable IO performance

Quantifying Performance

What is good performance on ARCHER?

- Generally see ~500MB/s per OST
- This is the serial limit. If getting that, not achieving parallel I/O

Always benchmark and quantify bandwidth

- Use the Cray performance tools

Contention is an issue – can see huge variance in results

- Do multiple runs at different times of day
- Look at best and worst case

Beware of caching effects on performance

Performance – Large Number of Files

“setting striping to 1 has reduced total read time for his 36000 small files from 2 hours to 6 minutes”

- comment on resolution of an ARCHER helpdesk query.

User was performing I/O on 36000 separate files of ~300KB with 10000 processes

Had set parallel striping to maximum possible (48 OSTs / -1) assuming this would give best performance

Overhead of querying every OST for every file dominated the access time

Moral: more stripes does not mean better performance

Performance – Large Number of Files 2

15GB consisting of 5500 1.5-4MB files

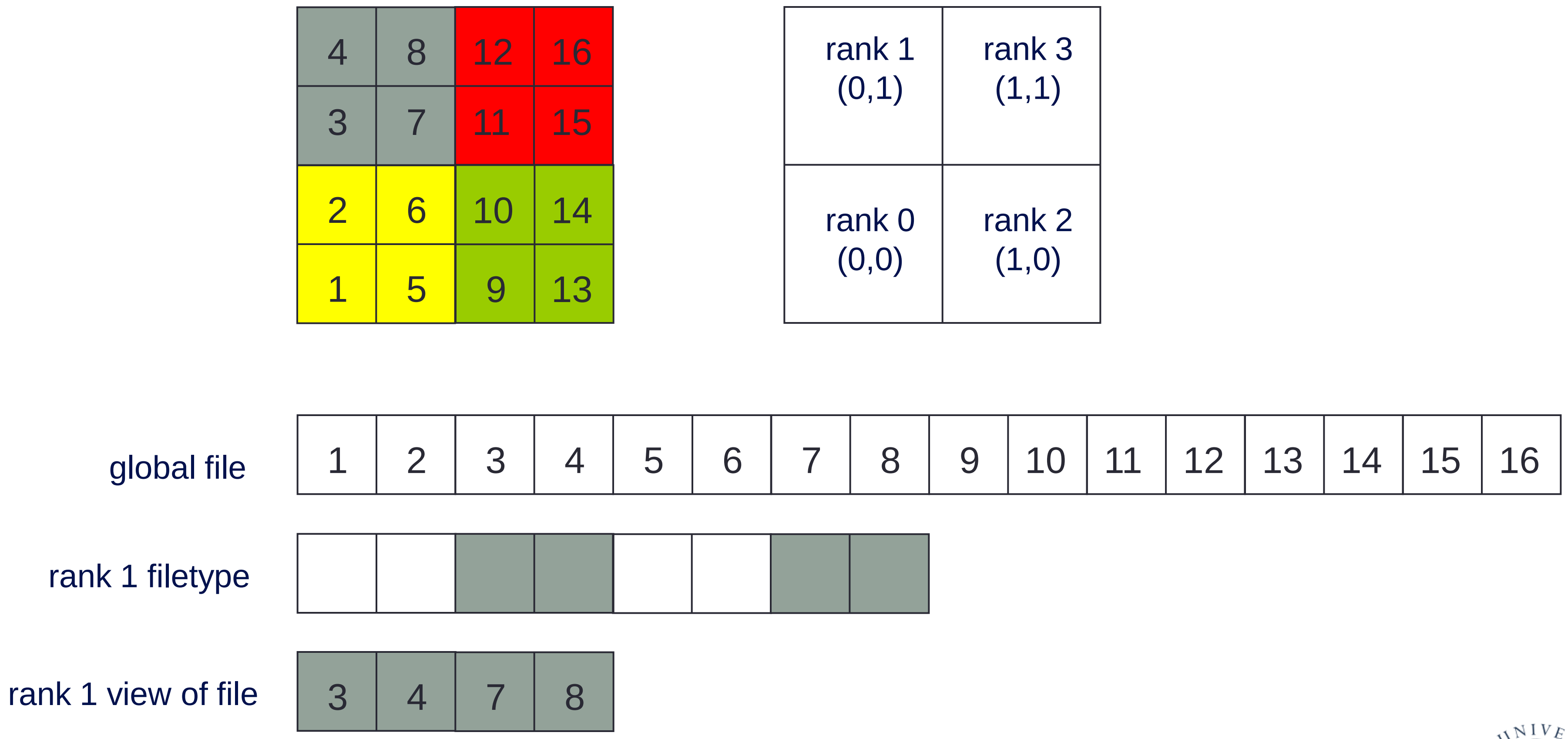
Effect of striping on serial "tar" operation:

```
$> time tar -cf stripe48.tar stripe48
real    31m19.438s
…

$> time tar -cf stripe4.tar stripe4
real    24m50.604s
…

$> time tar -cf stripe1.tar stripe1
real    18m34.475s
...
```

~40% reduction in operation time between 48 and 1 stripe

Still bottlenecks at MDS. This access pattern is not recommended, but it is common.

Global description: MPI-IO



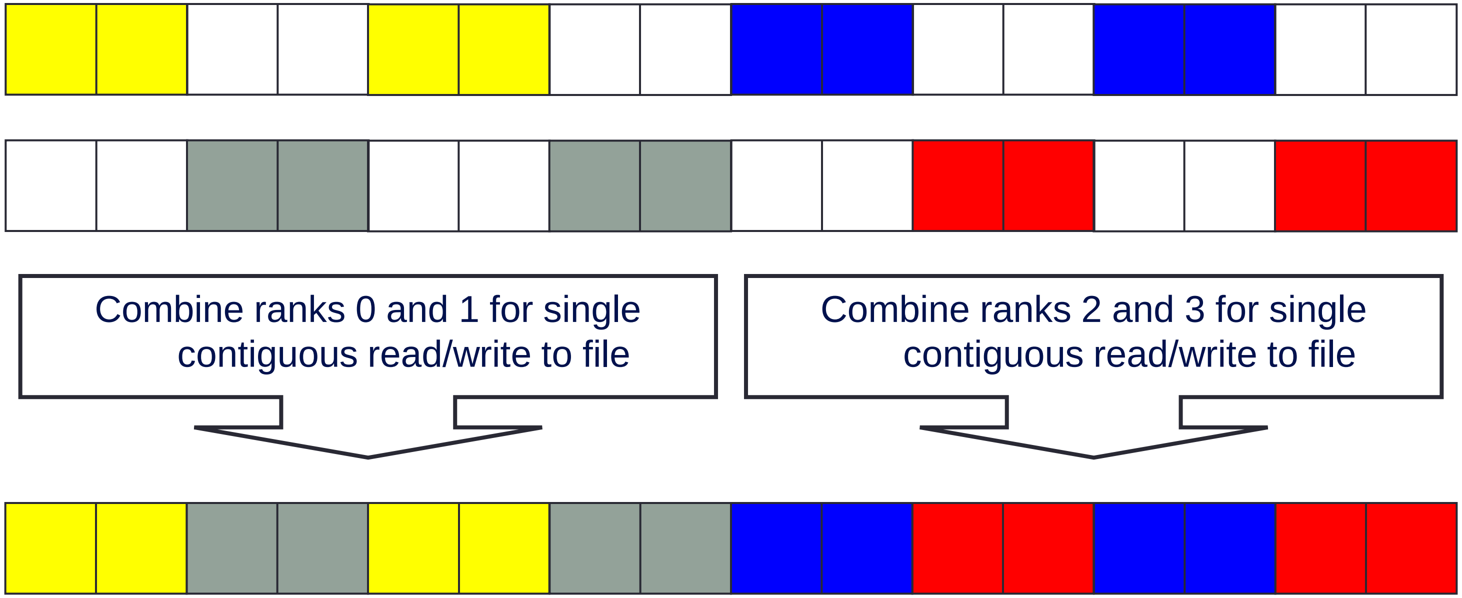
4	8	12	16
3	7	11	15
2	6	10	14
1	5	9	13

rank 1 (0,1)	rank 3 (1,1)
rank 0 (0,0)	rank 2 (1,0)

global file	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
rank 1 filetype	□	□	▨	▨	□	□	▨	▨								
rank 1 view of file	3	4	7	8												

Collective IO

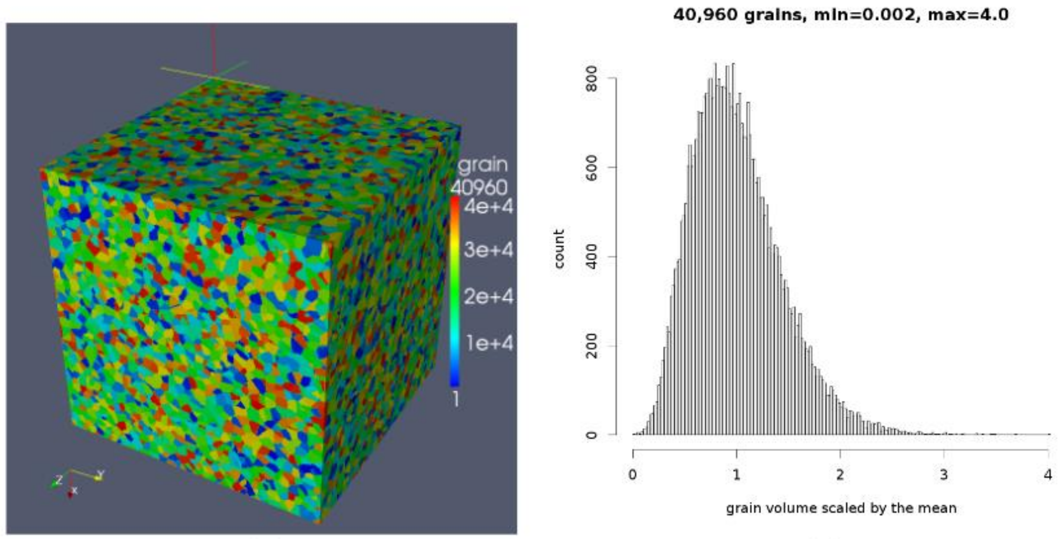
- Enables numerous optimisations in principle
  - requires global description and participation of all processes
  - does this help in practice?



Combine ranks 0 and 1 for single contiguous read/write to file

Combine ranks 2 and 3 for single contiguous read/write to file

Cellular Automaton Model



(a) (b)

Figure 1: A 4.1 × 10^9 cell, 40,960 grain equiaxed microstructure model, showing (a) grain arrangement with colour denoting orientation; (b) grain size size (volume) histogram.

- *Fortran coarray library for 3D cellular automata microstructure simulation*, Anton Shterenlikht, proceedings of 7th International Conference on PGAS Programming Models, 3-4 October 2013, Edinburgh, UK.

Benchmark

- Distributed regular 3D dataset across 3D process grid
  - local data has halos of depth 1; set up for weak scaling
  - implemented in Fortran and MPI-IO

```
! Define datatype describing global location of local data
call MPI_Type_create_subarray(ndim, arraygsize, arraysubsize, arraystart,
       MPI_ORDER_FORTRAN, MPI_DOUBLE_PRECISION, filetype, ierr)

! Define datatype describing where local data sits in local array
call MPI_Type_create_subarray(ndim, arraysize, arraysubsize, arraystart,
       MPI_ORDER_FORTRAN, MPI_DOUBLE_PRECISION, mpi_subarray, ierr)

! After opening file fh, define what portions of file this process owns
call MPI_File_set_view(fh, disp, MPI_DOUBLE_PRECISION, filetype,
                       'native', MPI_INFO_NULL, ierr)
! Write data collectively
call MPI_File_write_all(fh, iodata, 1, mpi_subarray, status, ierr)
```

ARCHER XC30

archer

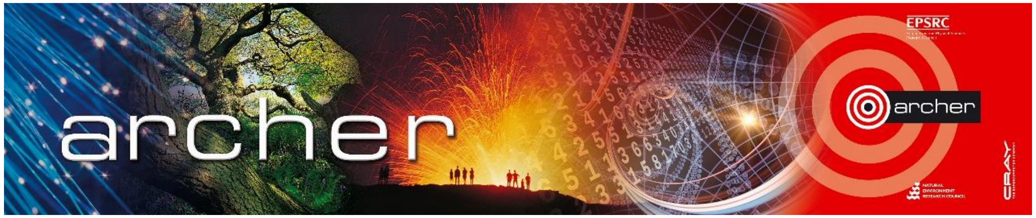
CRAY

THE SUPERCOMPUTER COMPANY

EPSRC

Engineering and Physical Sciences Research Council

NERC SCIENCE OF THE ENVIRONMENT



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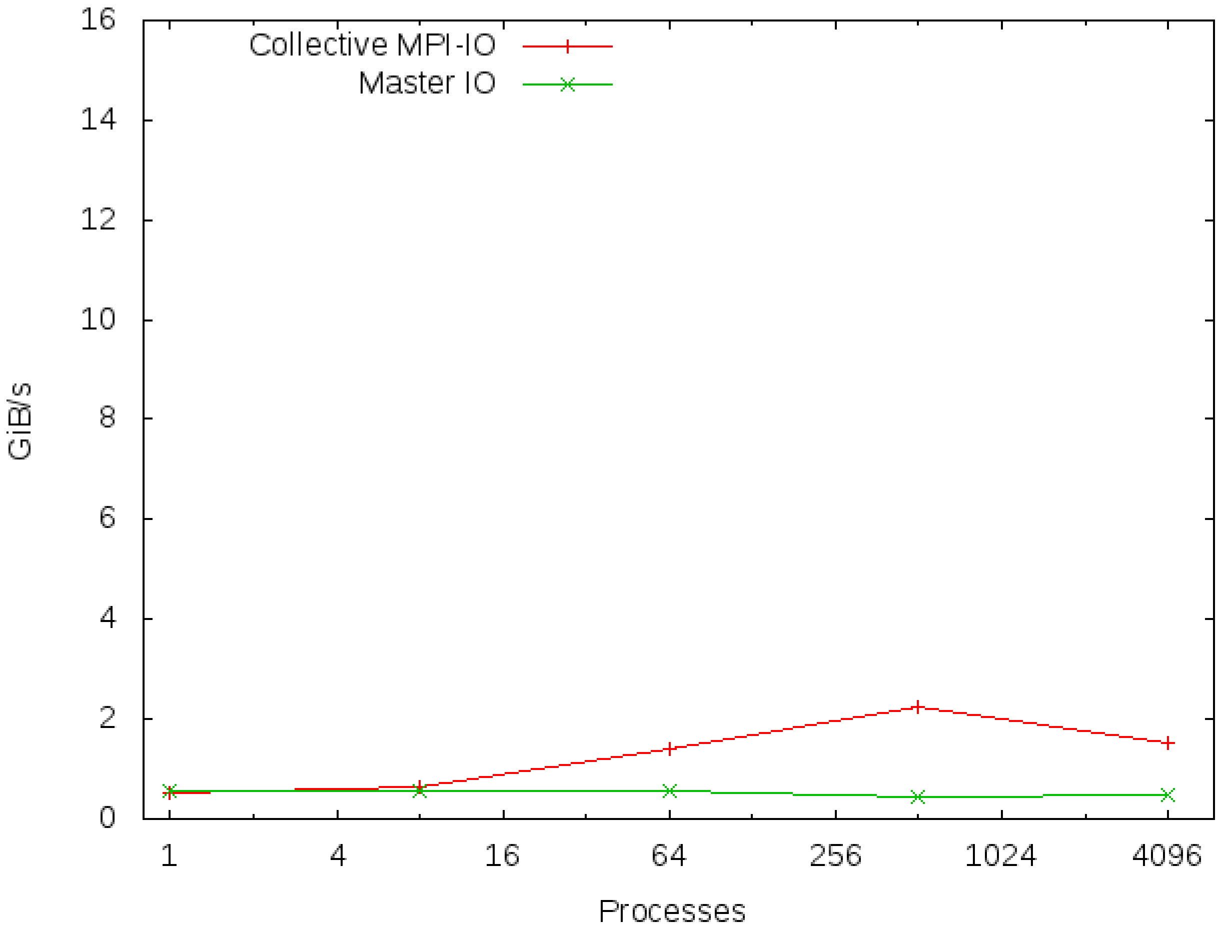
Single file, multiple writers

- Serial bandwidth on ARCHER around 400 to 500 MiB/s

- Use **`MPI_File_write`** not **`MPI_File_write_all`**
  - identical functionality
  - different performance

Processes	Bandwidth
1	49.5 MiB/s
8	5.9 MiB/s
64	2.4 MiB/s

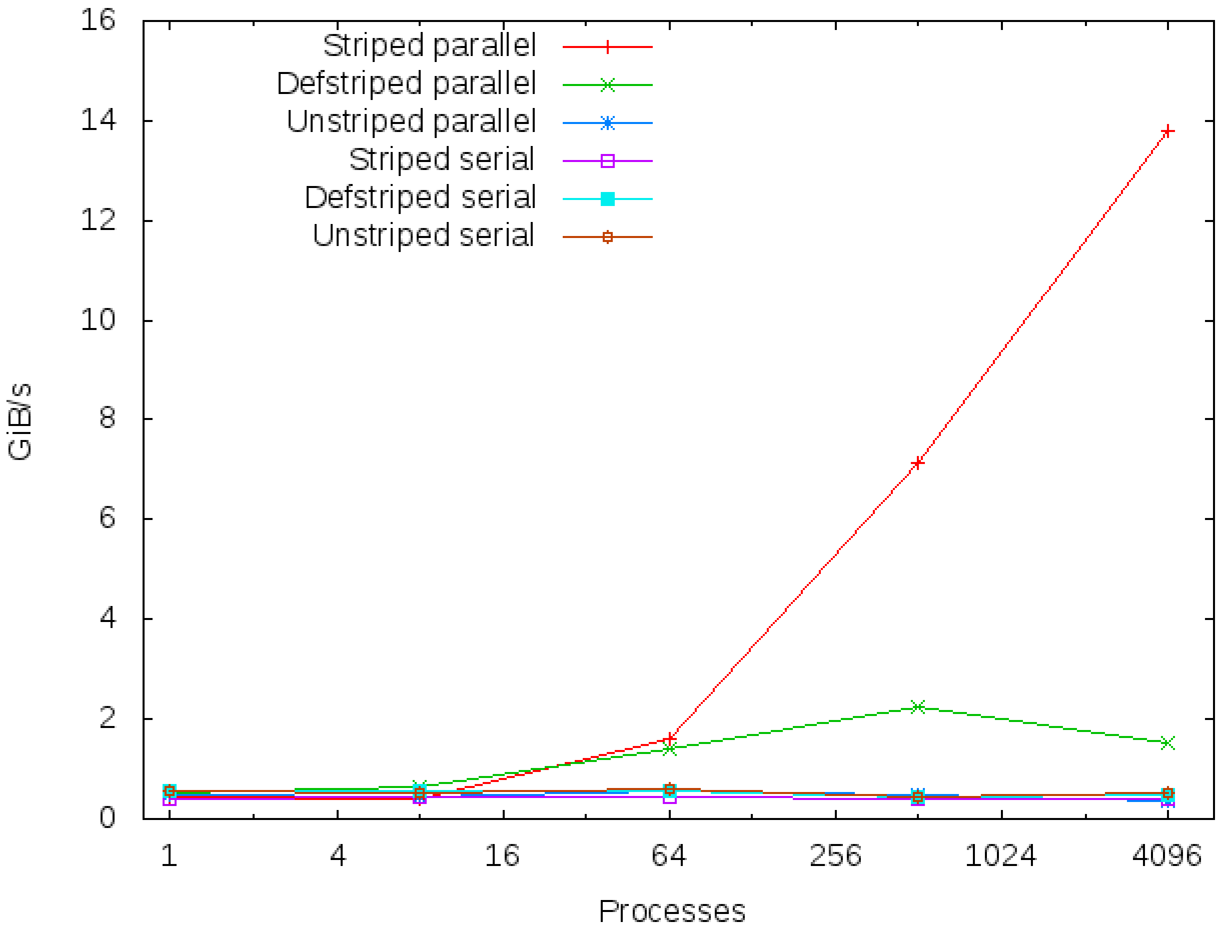
Single file, collective writers



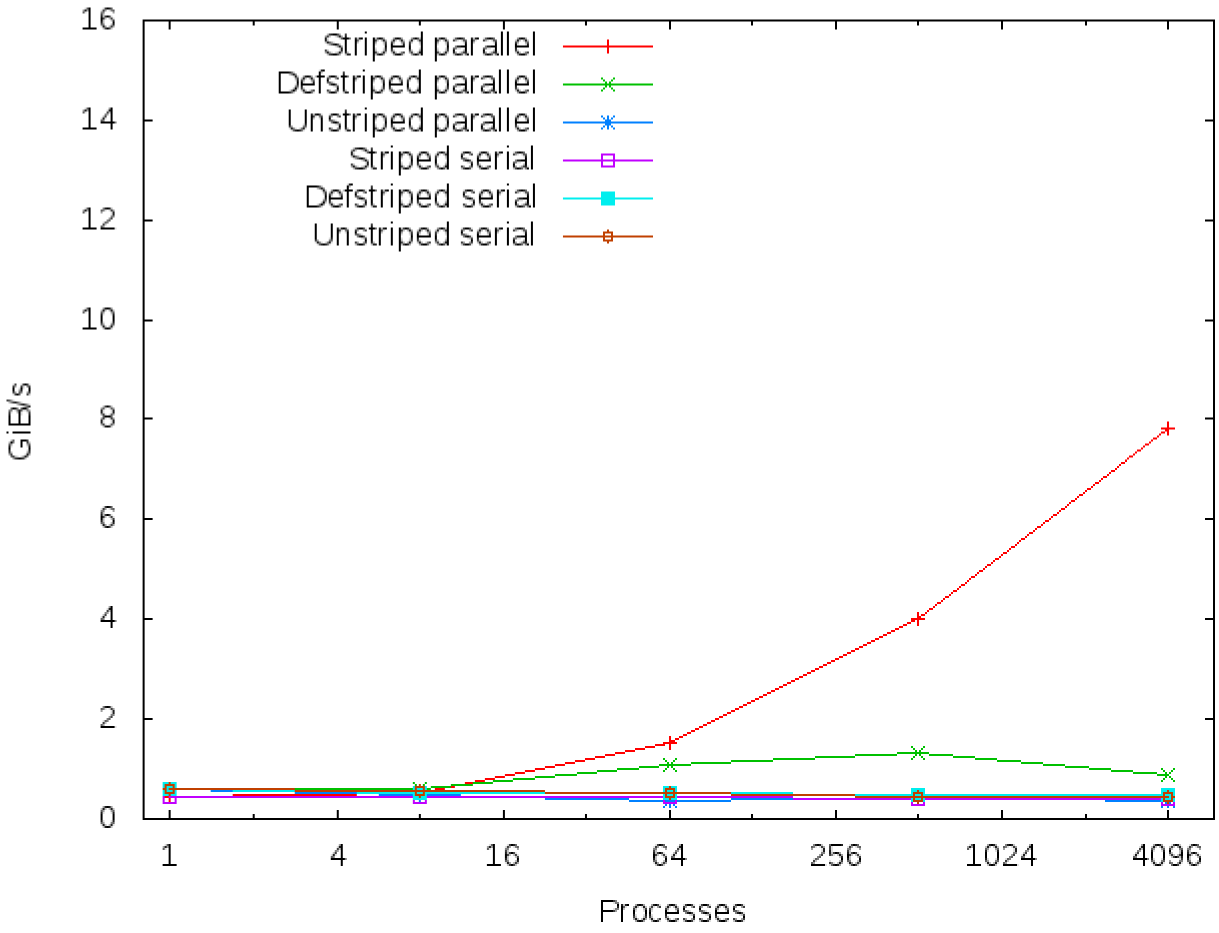
Lustre striping

- We’ve done a lot of work to enable (many) collective writers
  - learned MPI-IO and described data layout to MPI
  - enabled collective IO
  - MPI dynamically decided on number of writers
  - collected data and aggregates before writing
- ... for almost no benefit!
- Need many physical disks *as well as* many IO streams
  - in Lustre, controlled by the number of *stripes*
  - default number of stripes is 4; ARCHER has around 50 IO servers
- *User* needs to set striping count on a per-file/directory basis
  - **`lfs setstripe -c -1 <directory>`** # use maximal striping

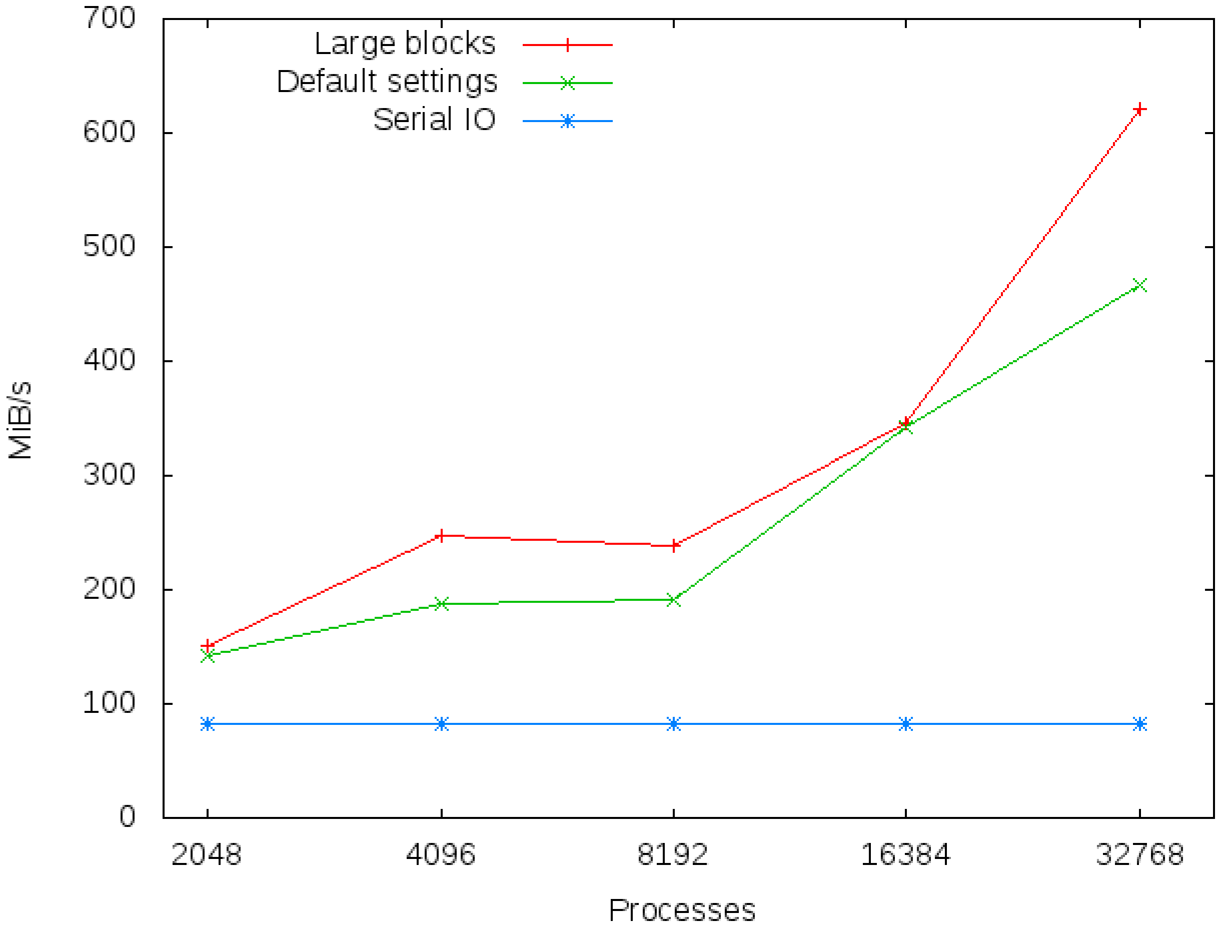
Cray XC30 with Lustre: 128^3 per proc



Cray XC30 with Lustre: 256^3 per proc



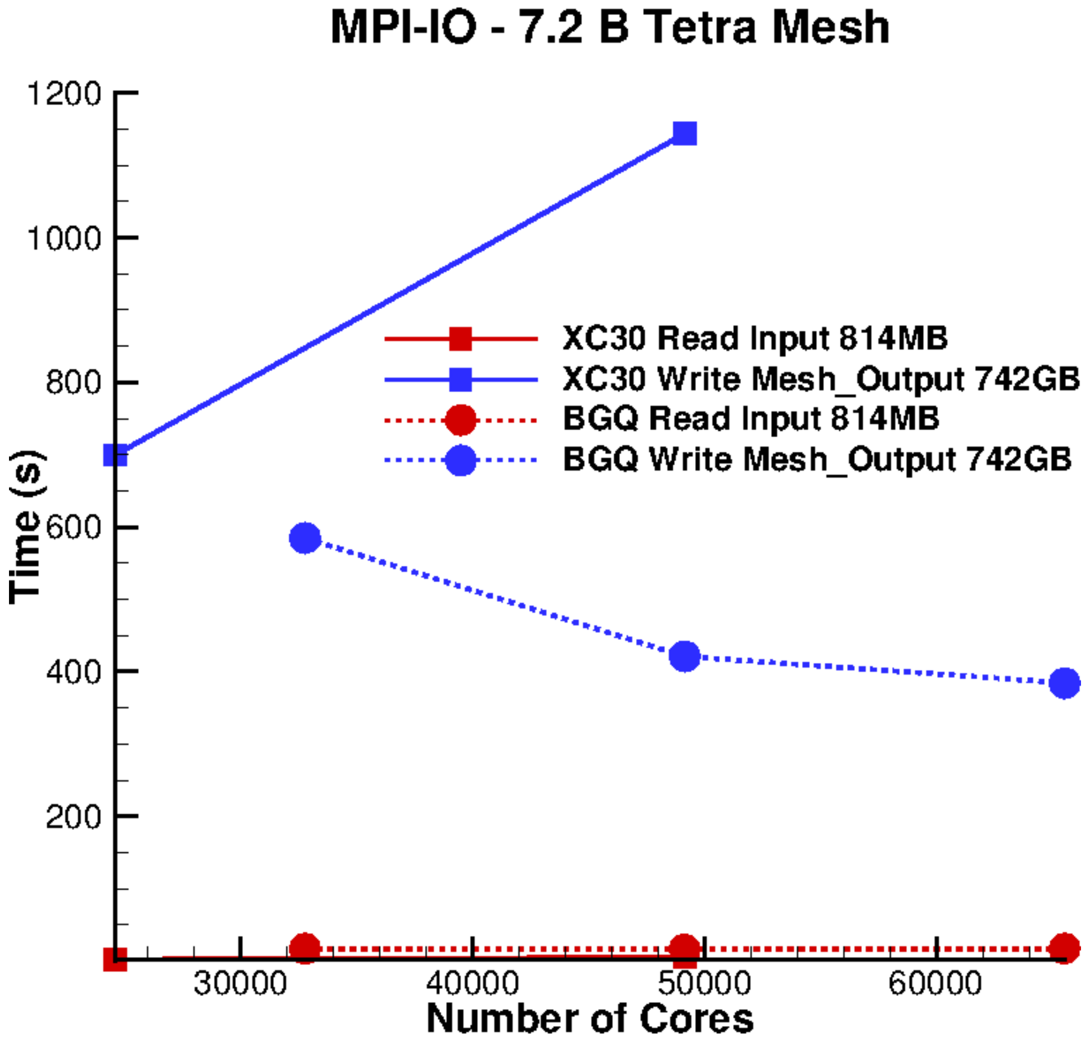
BG/Q: #IO servers scales with CPUs



Code_Saturne http://code-saturne.org

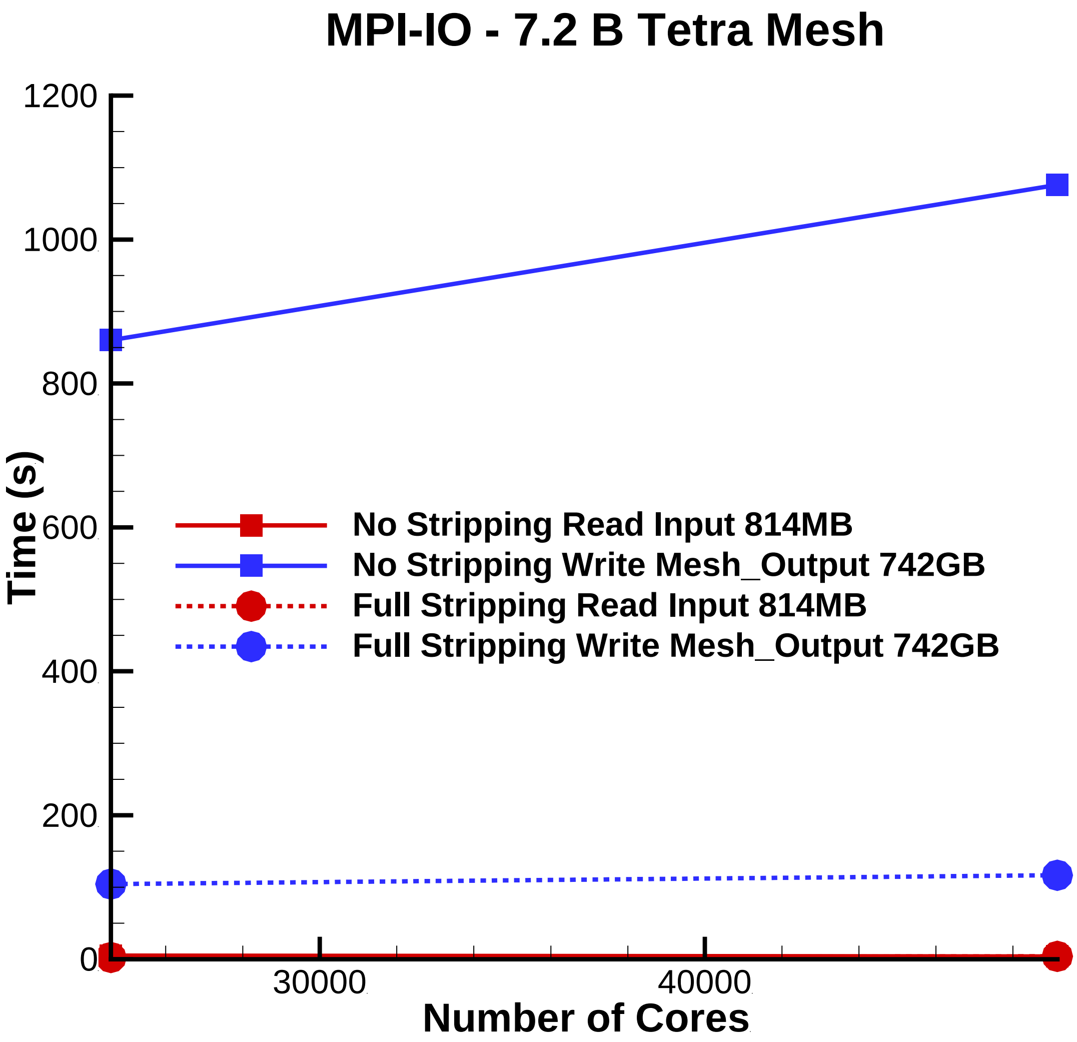
- CFD code developed by EDF (France)
- Co-located finite volume, arbitrary unstructured meshes, predictor-corrector
- 350 000 lines of code
  - 50% C
  - 37% Fortran
  - 13% Python
- MPI for distributed-memory (some OpenMP for shared-memory) **including MPI-IO**
- Laminar and turbulent flows: k-eps, k-omega, SST, v2f, RSM, LES models, ...

Code_SATURNE: default settings



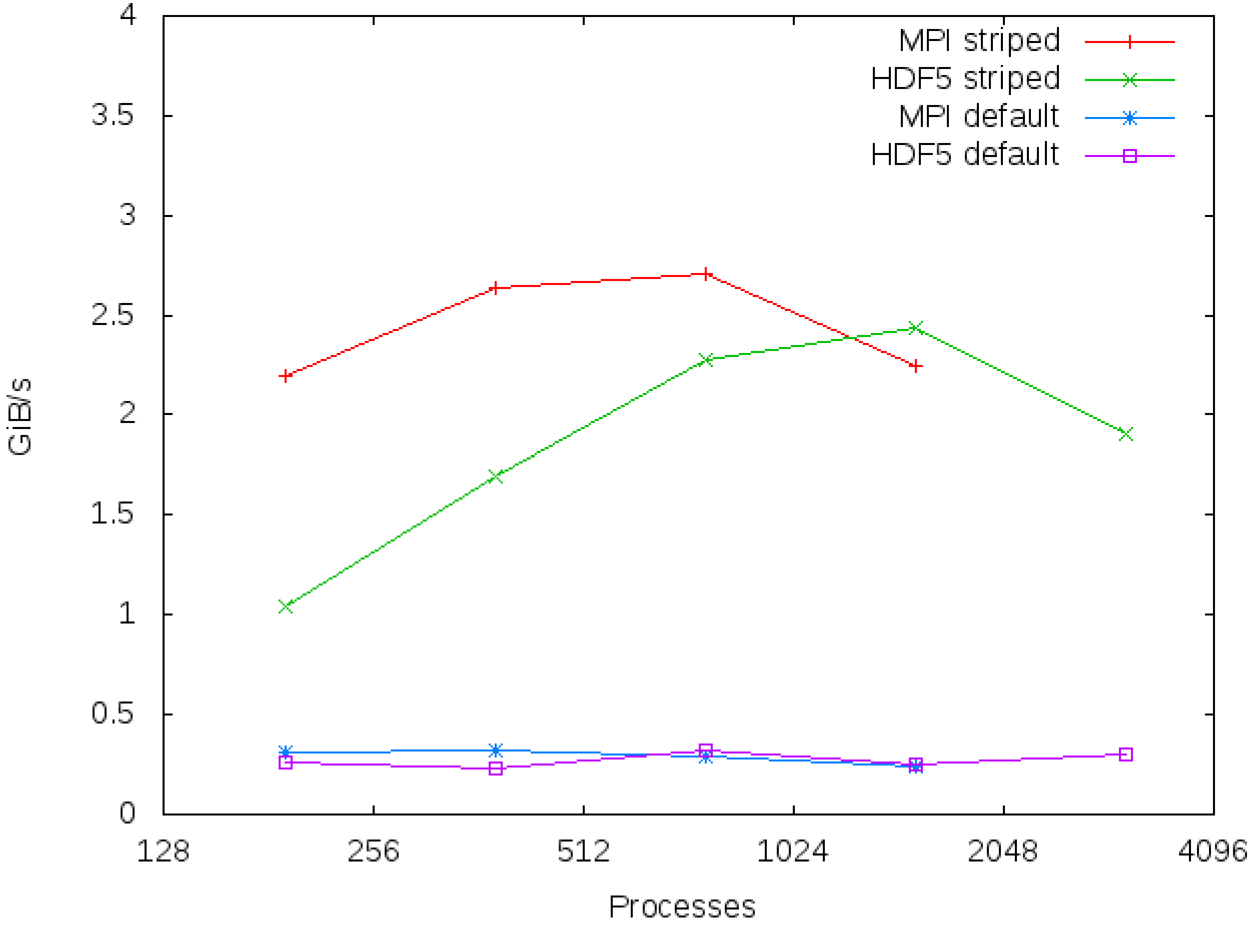
- Consistent with benchmark results
  - default striping Lustre similar to GPFS

Code_Saturne: Lustre striping



- Consistent with benchmark results
  - order of magnitude improvement from striping

Simple HDF5 benchmark: Lustre



Further Work

- Non-blocking parallel IO could hide much of writing time
    - or use more restricted split-collective functions
    - extend benchmark to overlap comms with calculation
- I don’t believe it is implemented in current MPI-IO libraries
    - blocking MPI collectives are used internally
- A subset of user MPI processes will be used by MPI-IO
    - would be nice to exclude them from calculation
    - extend **`MPI_Comm_split_type()`** to include something like **`MPI_COMM_TYPE_IONODE`** as well as **`MPI_COMM_TYPE_SHARED`** ?

Conclusions

- Efficient parallel IO requires **all** of the following
  - a global approach
  - coordination of multiple IO streams to the same file
  - collective writers
  - filesystem tuning

- MPI-IO Benchmark useful to inform real applications
  - NetCDF and HDF5 layered on top of MPI-IO
  - although real application IO behaviour is complicated

- Try a library before implementing bespoke solutions!
  - higher level view pays dividends