Parallel I/O Performance

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Reusing this material

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Acknowledgements

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Motivation

- I/O performance is becoming more critical for HPC application performance as applications scale up
  - Many applications now have an I/O-bound phase
- What is the maximum performance you can expect from the ARCHER parallel file systems in production?
  - Compared to other HPC parallel I/O setups?
- What are the best file layouts and Lustre striping settings for different scenarios?
- How do MPI-IO, NetCDF and HDF5 write performance compare?
  - …and how do they compare to naïve file-per-process?

Motivation (cont.)

- HPC users and application developers often poorly understand parallel I/O performance in terms of:
  - what “good” performance actually is on a particular file system;
  - what a particular application does;
  - what benchmarks illustrate.

Benchmarks: IOR

- Widely used for testing parallel file system performance from multiple processes
  - Supports: MPI-IO, HDF5, NetCDF
- Investigated as a benchmark but not chosen because:
  - the software is opaque with many different options; this hinders understanding on what I/O operations are actually being performed;
  - the naïve parallel I/O patterns implemented in IOR do not provide a good representation of user I/O so the results from the benchmark do not provide a useful measure of where the limits of performance are for users.

Benchmarks: benchio (SSF)

- Simple Fortran program:
  - Writes 3D distributed dataset to single shared file (SSF)
  - MPI-IO, HDF5, NetCDF
- Advantages:
  - Small number of options: dataset size, number of processes, simple to understand what program is doing
  - Data distribution closer to many I/O-bound user applications
- Disadvantages:
  - Write performance only (read added soon)
- https://github.com/EPCCed/benchio

Why not use IOR?

- IOR is like Linpack
  - data decomposition designed to measure maximum IO bandwidth
  - imagine 64 data elements on 8 processes
  - IOR file: 8 large blocks of 8 contiguous items:

Processor 0	Processor 1	Processor 2

- benchio uses more realistic (but still simple) decomposition
  - leads to surprisingly complicated IO patterns
- Imagine 4x4x4 grid split evenly across 8 processes (2x2x2)
  - benchio file contains multiple interleaved small blocks of 2 items

P0	P1	P0	P1	P2	P3	P2	P3	P0	P1	P0	P1	P2	P3	P2	P3
P4	P5	P4	P5	P6	P7	P6	P7	P4	P5	P4	P5	P6	P7	P6	P7

Benchmarks: benchio_fpp (FPP)

- FPP = File Per Process
- Derived from benchio:
  - Each process writes to own Fortran binary file
  - No HDF5, NetCDF support yet
- Need to be careful to ensure that buffering is not used by writing large amounts of data per process
  - MPI-IO bypasses buffering so not a problem for SSF version

Systems

- ARCHER
  - Cray Sonexion Lustre
  - Theoretical peak bandwidth: 30 GiB/s
- COSMA5
  - DDN GPFS
  - Theoretical peak bandwidth: 20 GiB/s
- Also small-scale systems (results not included here)
  - RDF – DDN GPFS, single node
  - JASMIN – PANASAS, small process counts

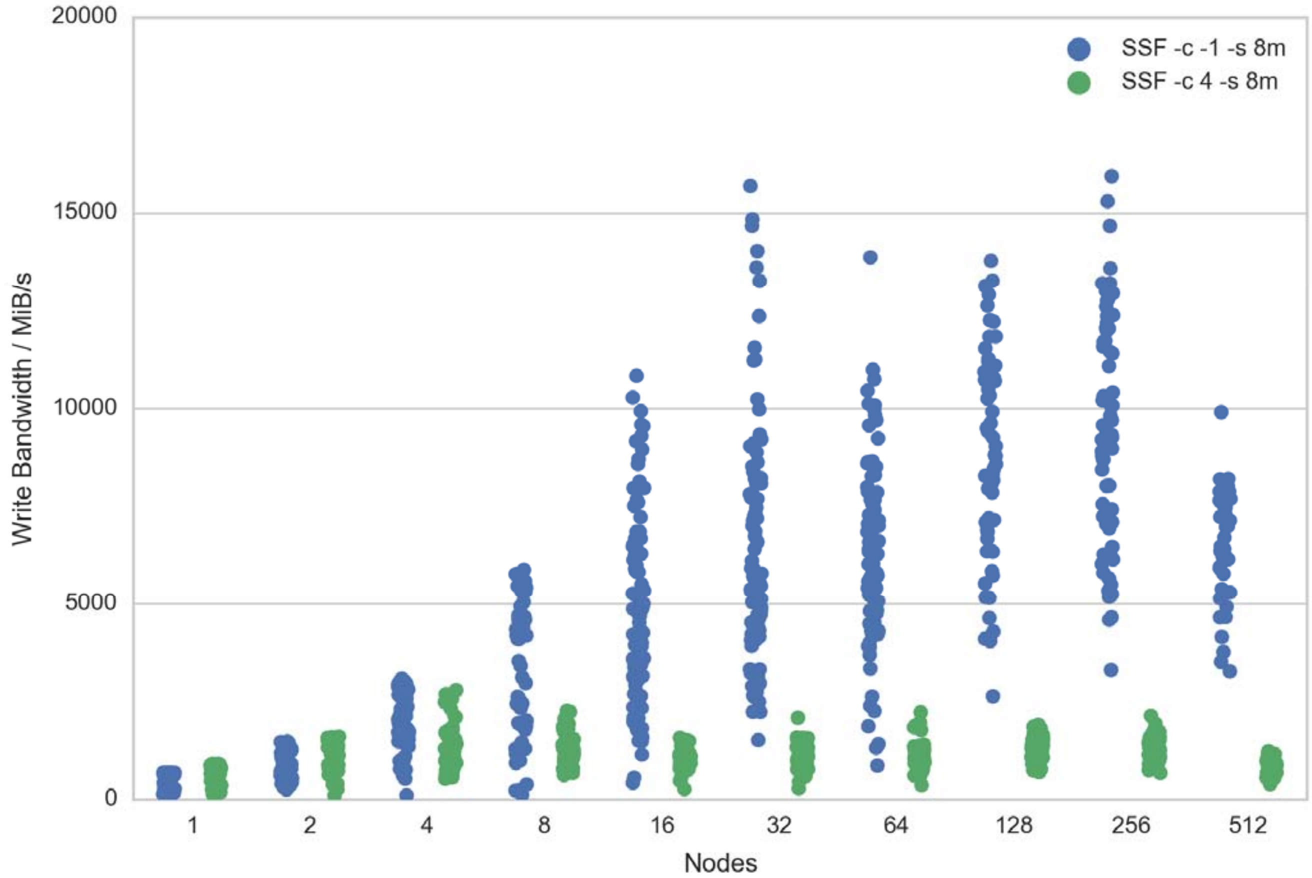
Setup

- MPI-IO collective operations used in all cases
  - Previous experience shows that this is required for performance
- All compute nodes fully populated
  - This is typically how users use the system
- All runs performed during production
  - Subject to same contention as all users
- Performance variation:
  - Run at approx. 3 day intervals to try and randomise across weekdays and times

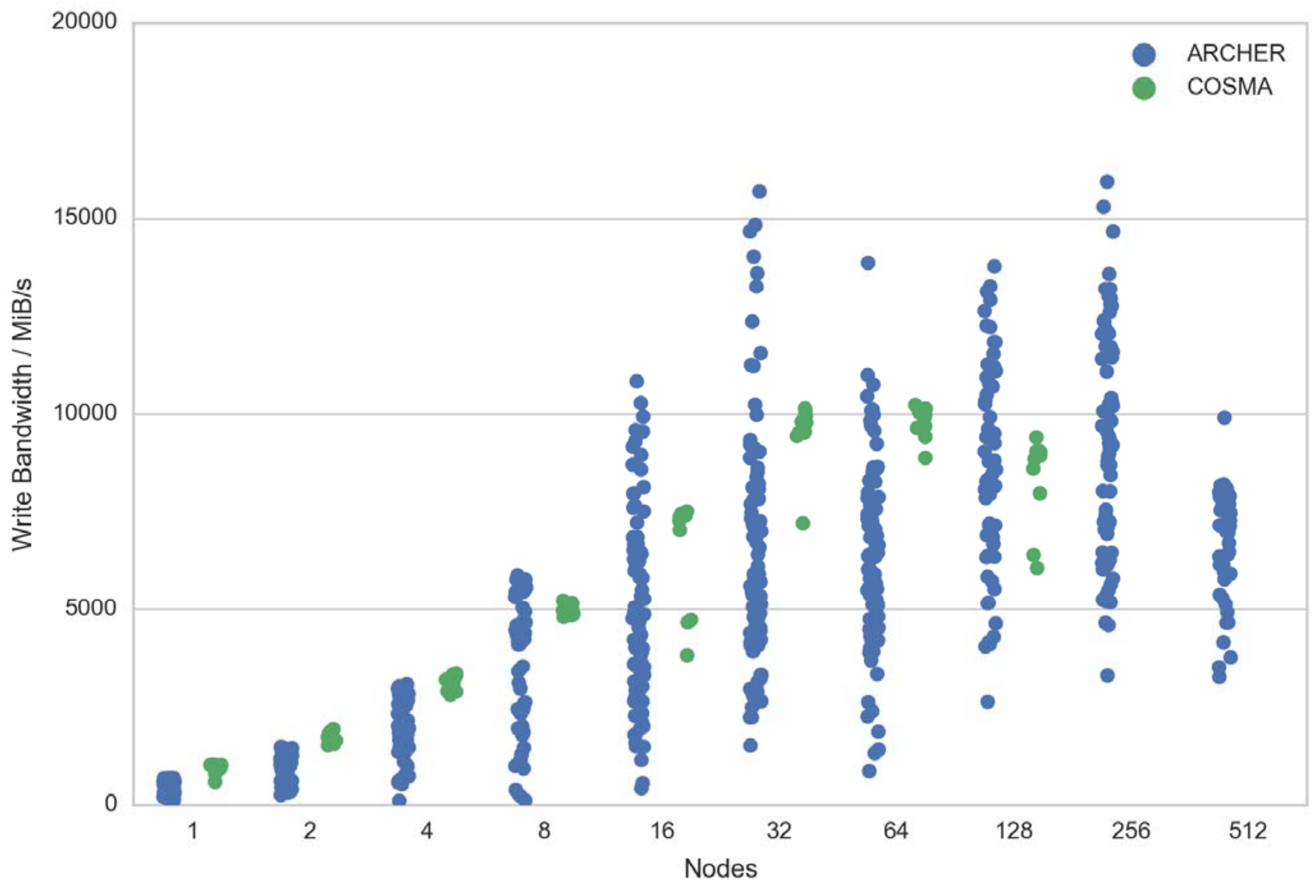
Single Shared File (SSF)

MPI-IO Comparisons

SSF: ARCHER Lustre



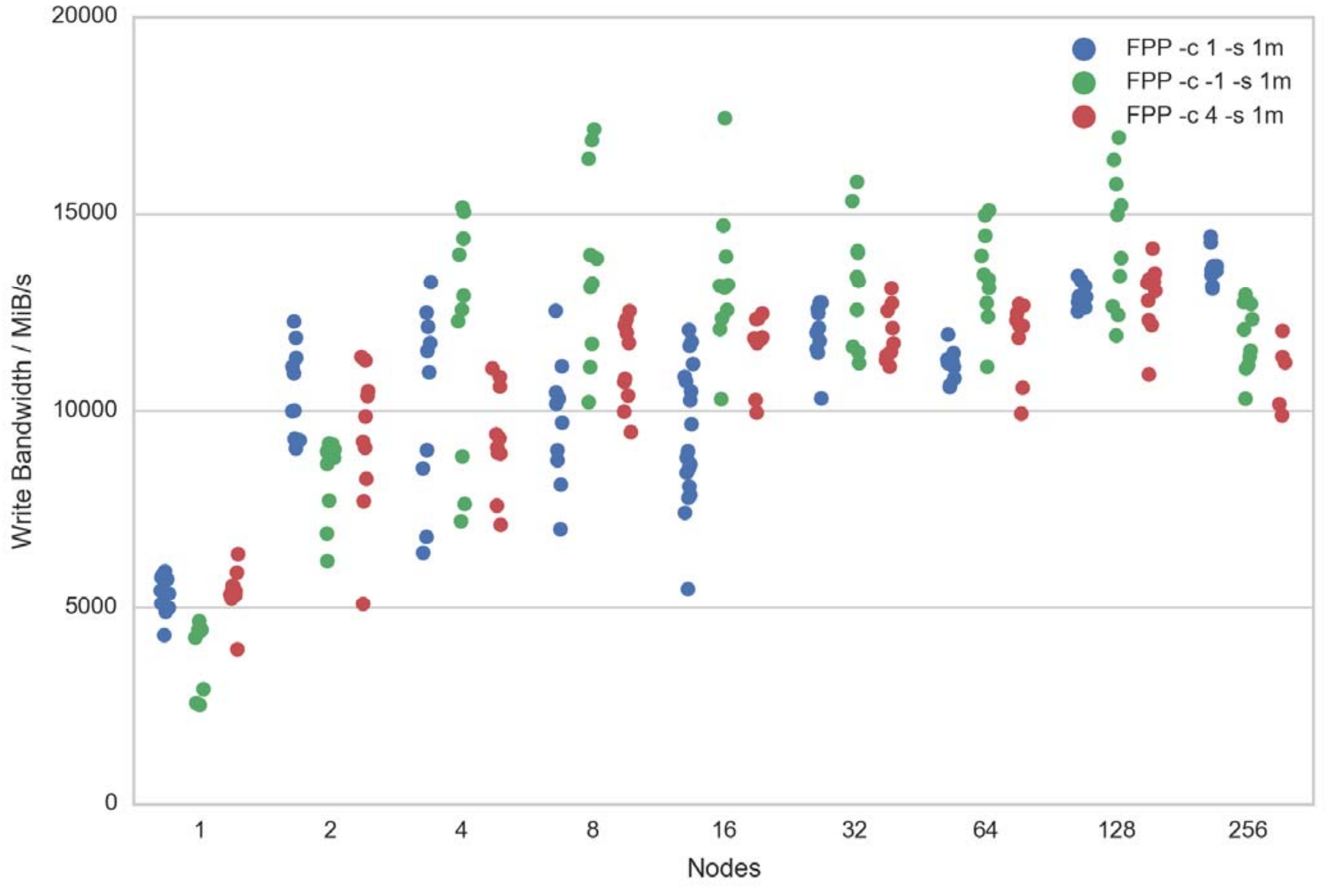
SSF: Lustre/GPFS Comparison



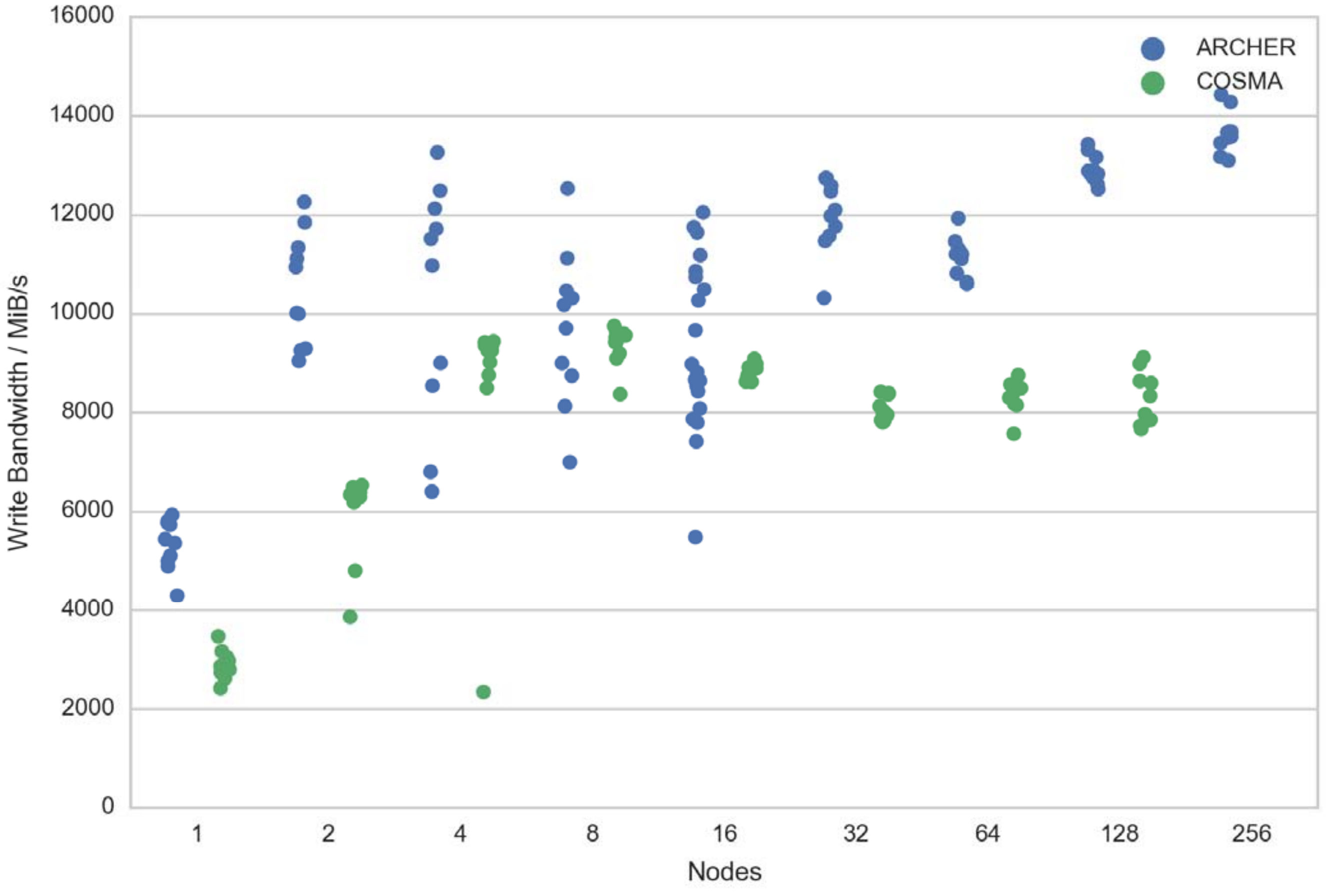
File Per Process (FPP)

Fortran Binary File Comparisons

FPP: ARCHER Lustre



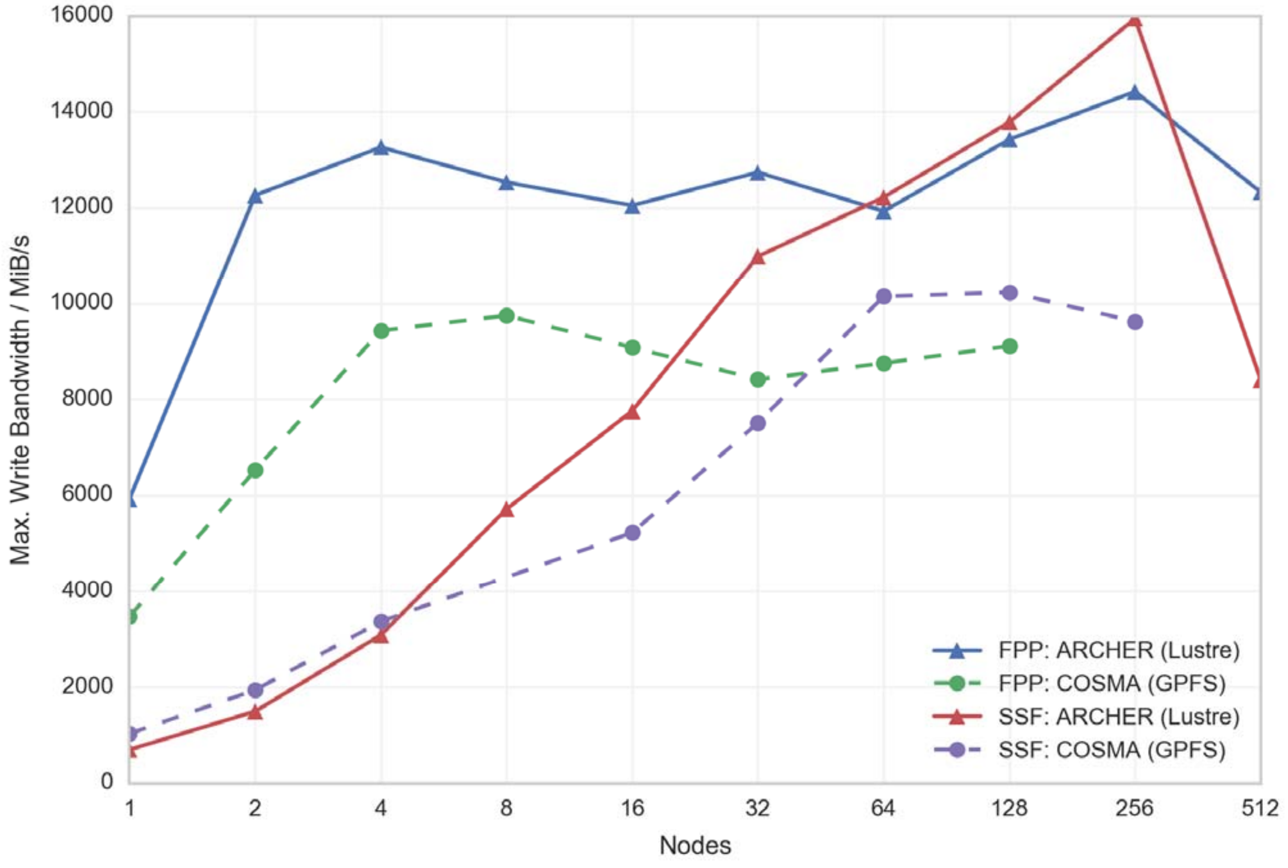
FPP: Lustre/GPFS Comparison



SSF vs. FPP

Comparisons

SSF vs. FPP



Max. Write Bandwidth / MiB/s
16000
14000
12000
10000
8000
6000
4000
2000
0
1
2
4
8
16
32
64
128
256
512
Nodes
FPP: ARCHER (Lustre)
FPP: COSMA (GPFS)
SSF: ARCHER (Lustre)
SSF: COSMA (GPFS)

SSF vs. FPP

- Simple file-per-process gives better performance at lower node counts…
  - …and is similar to shared file at higher node counts
- Should always use single striping for FPP on ARCHER:
  - Get random failures due to excessive metadata operations otherwise
- Disadvantages to FPP:
  - You will probably have to reconstruct the data for any analysis
  - For checkpoints, you must use identical decomposition
- FPP worth considering if you can live with constraints
- Both schemes achieve a maximum of ~50% of peak for both GPFS and Lustre in production

SSF vs. FPP (cont.)

- SSF can give excellent performance:
  - Each I/O client (node) writes a single block of data
  - Usually requires significant internal communication to reorganise data layout
  - Contingent on using well written parallel I/O libraries to perform this reorganisation…
  - …and this requires parallel collective I/O (without this the performance can be orders of magnitude less)
  - Advantage that data is often in a format that can be analysed or reused at the end of the simulation

Summary and Further Work

Summary

- File-per-process is simple and performs well up to high node counts
  - Probable cost in data reconstruction
  - May be useful for pure checkpointing
- Shared file competitive at high node counts
  - Must use MPI-IO collectives
  - Must use maximum stripe count on Lustre
  - Stripe size has small effect
- Maximum of ~50% peak file system performance

Further Work

- Understand where ~50% maximum performance limit comes from
- Analyse results for HDF5 and NetCDF
- Extend benchio to benchmark read performance
- Run I/O-bound application benchmarks
- Analyse automatically-gathered Lustre performance statistics

Useful Tools

- Pandas:
  - Python statistical analysis library
  - Invaluable for exploring data with multiple classification characteristics
- Seaborn:
  - Python statistical plotting library
  - Visual exploration of data
  - Simple plotting of complex data visualisations

Efficient Parallel I/O Course

- ARCHER Training
- 29-30 March 2017
- University of Durham
- Free for all attendees

- http://www.archer.ac.uk/training/
- Provide access to ARCHER during the course but lessons are generic for all parallel file systems