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Benchmarking the I/O performance of the world's 5th largest CPU-based Supercomputer, ARCHER2

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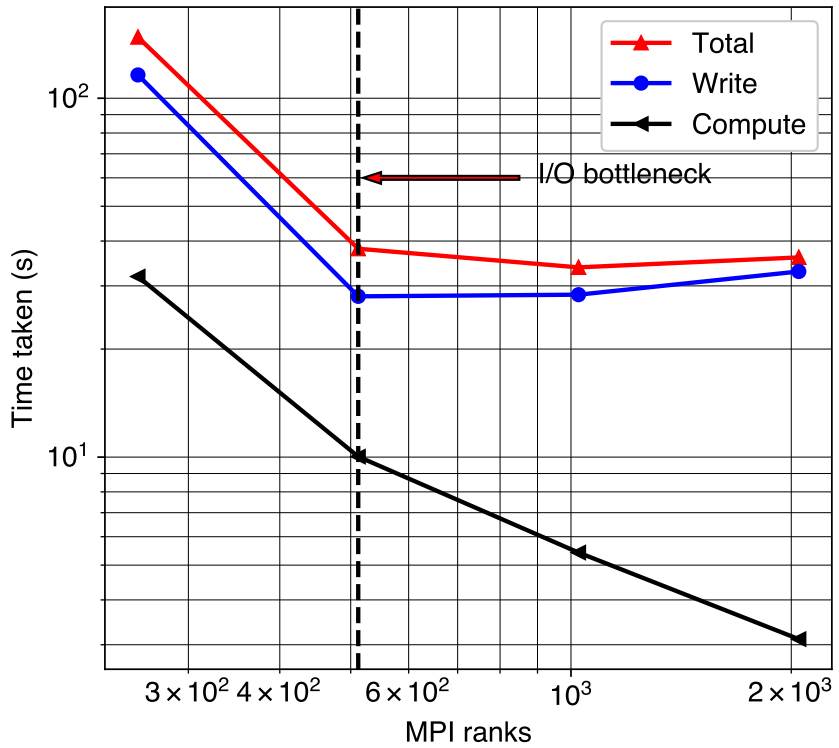
ASIMOV

archer2

Outline

- Addressing the I/O bottleneck is key for exascale computing.



XCompact3D benchmarking [1]

[1] Fulhame dataset `https://github.com/pbartholomew08/X3D-benchmarking.git`

Novel methods in I/O

- C based benchmark_c[1] derived from Fortran based benchio[2]
- Performs I/O benchmarking in different I/O backends; MPIIO, HDF5, ADIOS2
- Added features in bechmark_c include:
  - + ADIOS2 layer with runtime config file to use different backends
  - + Can read external datasets like CRESCENDO BDA datasets.
- ADIOS2[3]:
  - + Open source framework for scientific parallel I/O
  - + Low level support
  - + High level APIs and command line tools
  - + Abstractions provided for different I/O layers; HDF5,BP4, BP5
  - + Can initialise with config file to reduce need for re-compilation

[1] `https://github.com/sb15895/benchmark_c.git`

[2] `https://github.com/davidhenty/benchio.git`

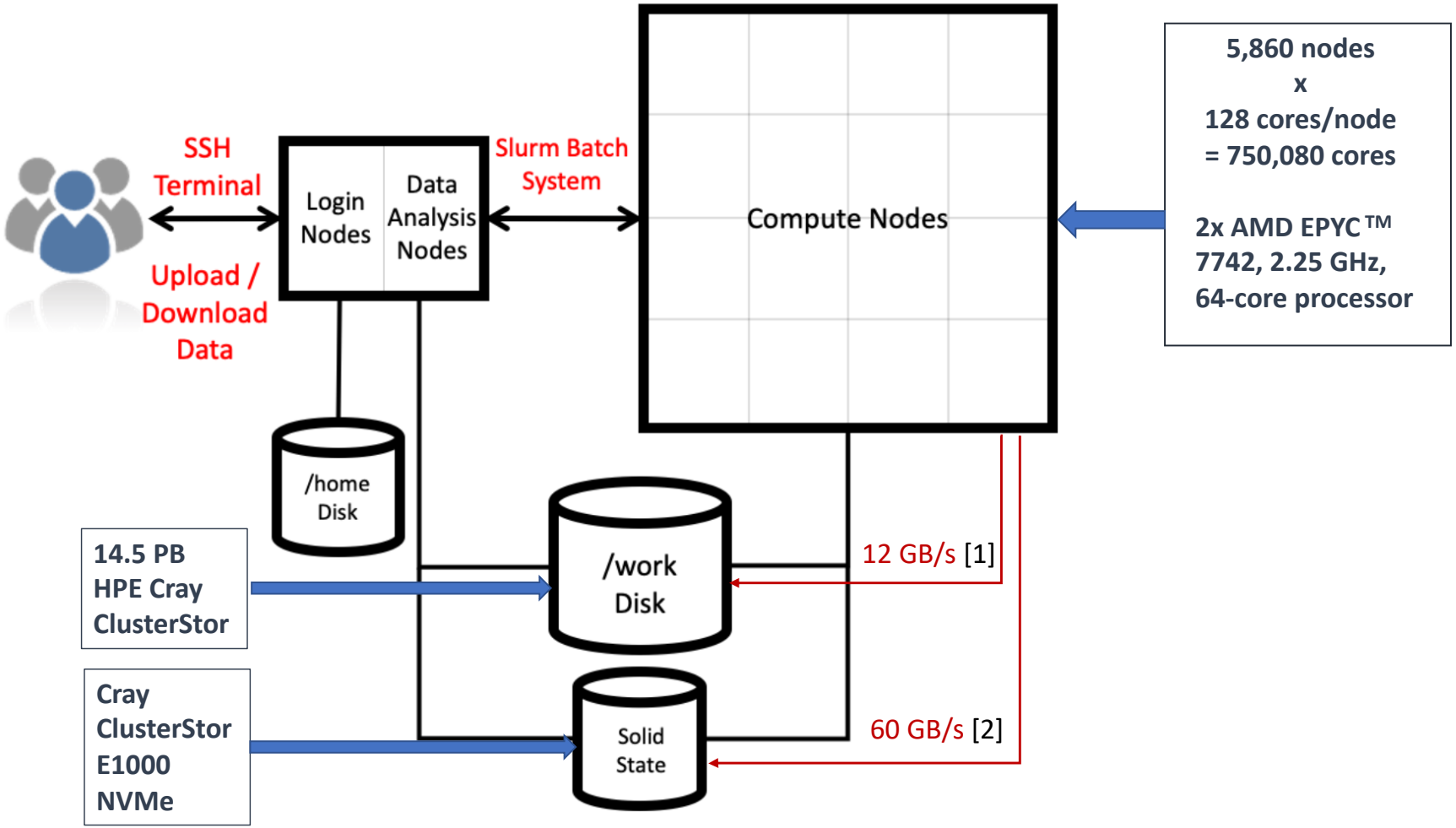
[3] `https://github.com/ornladios/ADIOS2.git`

- Next generation UK National Supercomputing Service
- Provided by UKRI, EPCC, Cray (an HPE company) and the University of Edinburgh[1].
- Estimated peak performance of 28 Pflop/s
- Average speedup compared to predecessor ARCHER were the following[2]:
  - 8.7x for CP2K
  - 9.5x for OpenSBLI
  - 11.3x for CASTEP
  - 12.9x for GROMACS
  - 18.0x for the HadGEM3 climate model
- Achieved 10th Position in IO500 in SC21 list,IO500 score of 10.68[3]

[1] `https://docs.archer2.ac.uk`

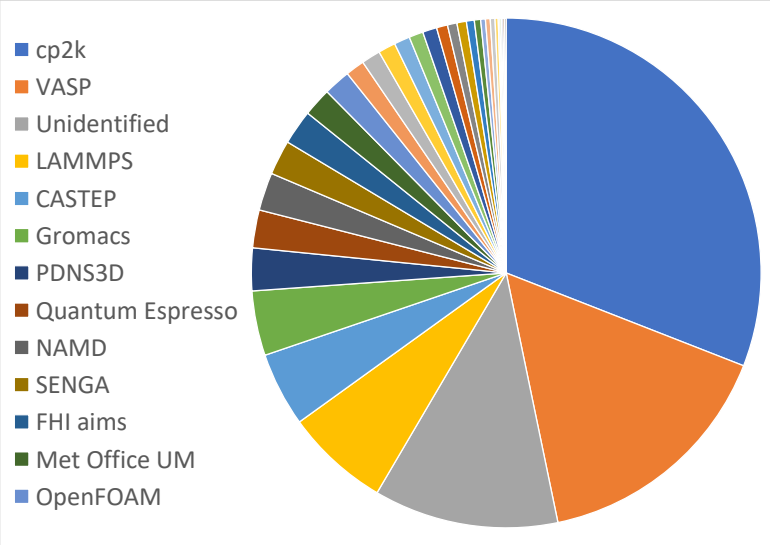
[2] `https://www.archer2.ac.uk/about/hardware.html`

[3] `https://io500.org/submissions/view/472`

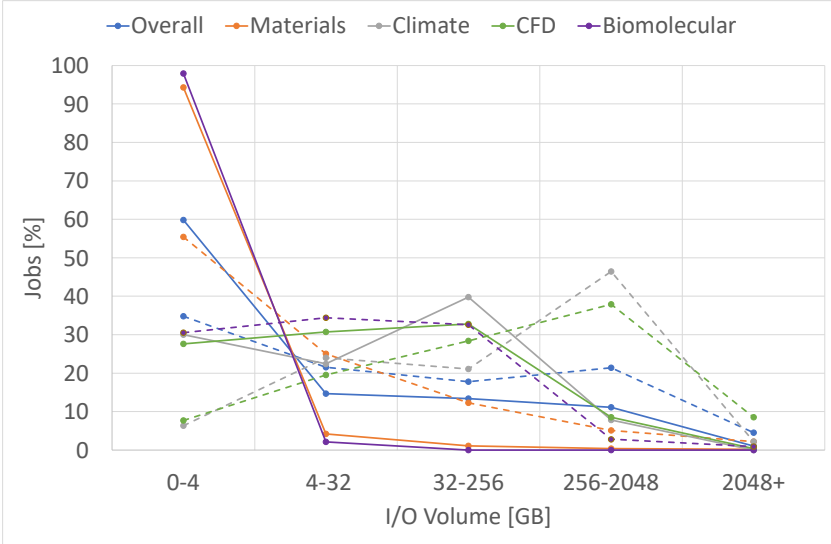


[1] https://docs.archer2.ac.uk/user-guide/hardware/

[2] https://www.hpe.com/psnow/doc/a00062172enw.pdf?jumpid=in_pdp-psnow-qs



ARCHER2 usage by CU [1]



ARCHER I/O usage statistics [2]

[1] https://www.archer2.ac.uk/news/2021/05/19/code-use.html

[2] https://cug.org/proceedings/cug2019_proceedings/includes/files/pap118s2-file1.pdf

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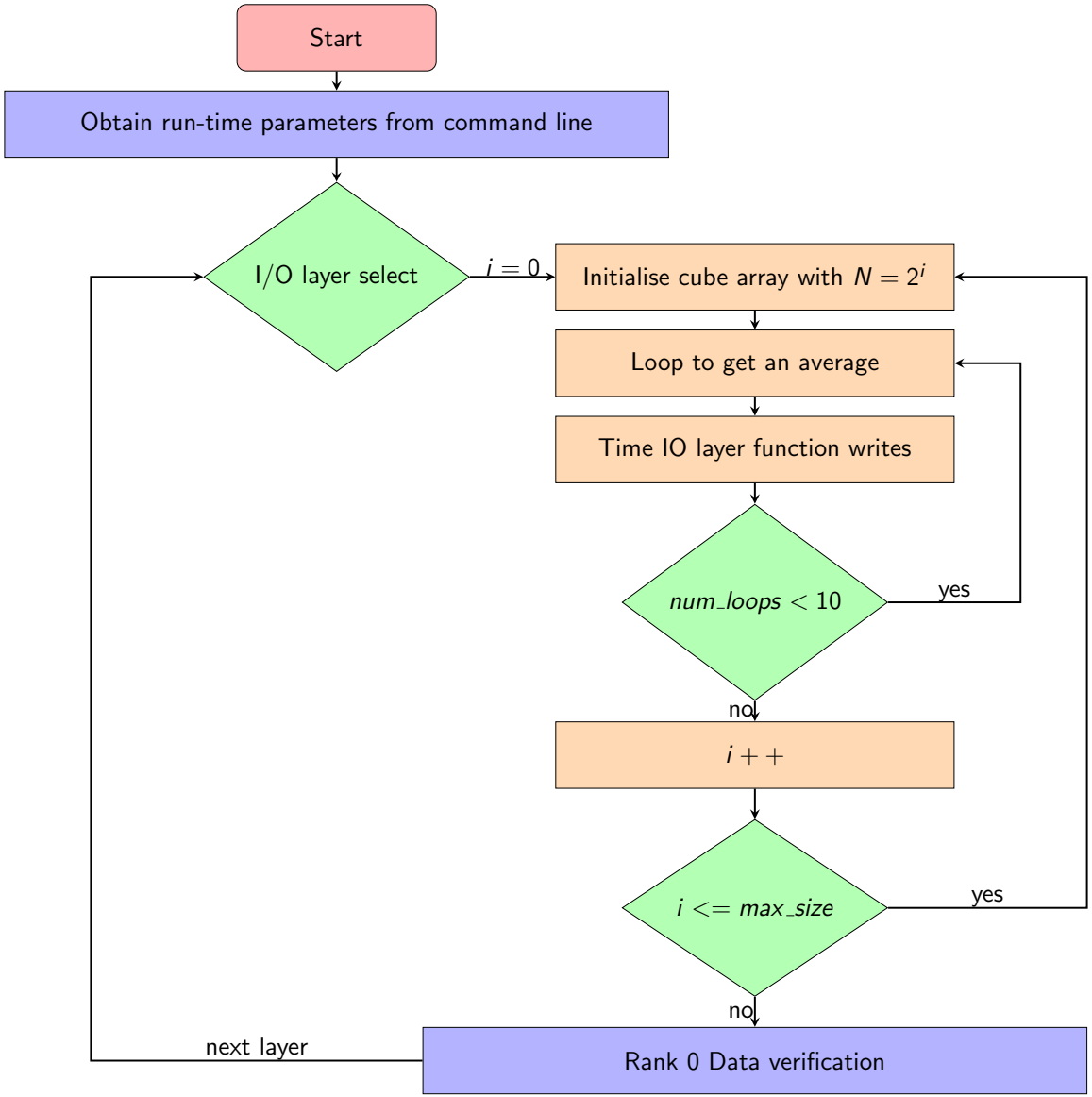
Start
Obtain run-time parameters from command line
I/O layer select
$i = 0$
Initialise cube array with $N = 2^i$
Loop to get an average
Time IO layer function writes
$num\_loops < 10$
yes
no
$i++$
$i <= max\_size$
yes
no
next layer
Rank 0 Data verification

```
// MPIIO write function
mpiiowrite(iodata, local_size, global_size, arraystart, NDIM, cartcomm,
           output_file[iolayer]);
// PHDF5 write function
phdf5write(iodata, local_size, global_size, arraystart, NDIM, cartcomm,
           output_file[iolayer]);
// ADIOS2 write function HDF5
adioswrite(iodata, local_size, global_size, arraystart, NDIM, cartcomm,
           "HDF5", output_file[iolayer]);
// ADIOS2 write function BP4
adioswrite(iodata, local_size, global_size, arraystart, NDIM, cartcomm,
           "BP4", output_file[iolayer]);
// ADIOS2 write function BP5
adioswrite(iodata, local_size, global_size, arraystart, NDIM, cartcomm,
           "BP5", output_file[iolayer]);
```

ADIOS2 runtime configuration

ADIOS2 runtime configuration

Variable passed IO_engine="BP4"

```
adios2_adios *adios = adios2_init_config(config_file, cartcomm, 1);
adios2_io *io = adios2_declare_io(adios, IO_ENGINE);
adios2_variable *var_iodata = adios2_define_variable(io, "iodata",
    adios2_type_double, NDIM, shape, start, count, adios2_constant_dims_true);
adios2_engine *engine = adios2_open(io, FILENAME, adios2_mode_write);
adios2_step_status status;
adios2_begin_step(engine, adios2_step_mode_update, 10.0, &status);
adios2_put(engine, var_iodata, iodata, adios2_mode_deferred);
adios2_end_step(engine);
adios2_close(engine);
adios2_finalize(adios);
```

ADIOS2 config file initialises BP4 engine

```
<?xml version="1.0"?>
<adios-config>
  <io name="BP4">
    <engine type="BP4">
    </engine>
  </io>
  <io name="HDF5">
    <engine type="HDF5">
    </engine>
  </io>
  <io name="BP5">
    <engine type="BP5">
    </engine>
  </io>
</adios-config>
```

- Modules and libraries loaded

I/O library	Version
Prg-Env-gnu	8.0.0
craype	2.7.6
GCC	10.2.0
Cray MPICH	8.1.4
Cray HDF5 parallel	1.12.0
ADIOS2	2.8.0
DARSHAN/Runtime	3.3.1

- Environment flags used; FI_OFI_RXM_SAR_LIMIT=64K [1]

[1] https://docs.archer2.ac.uk/user-guide/io/

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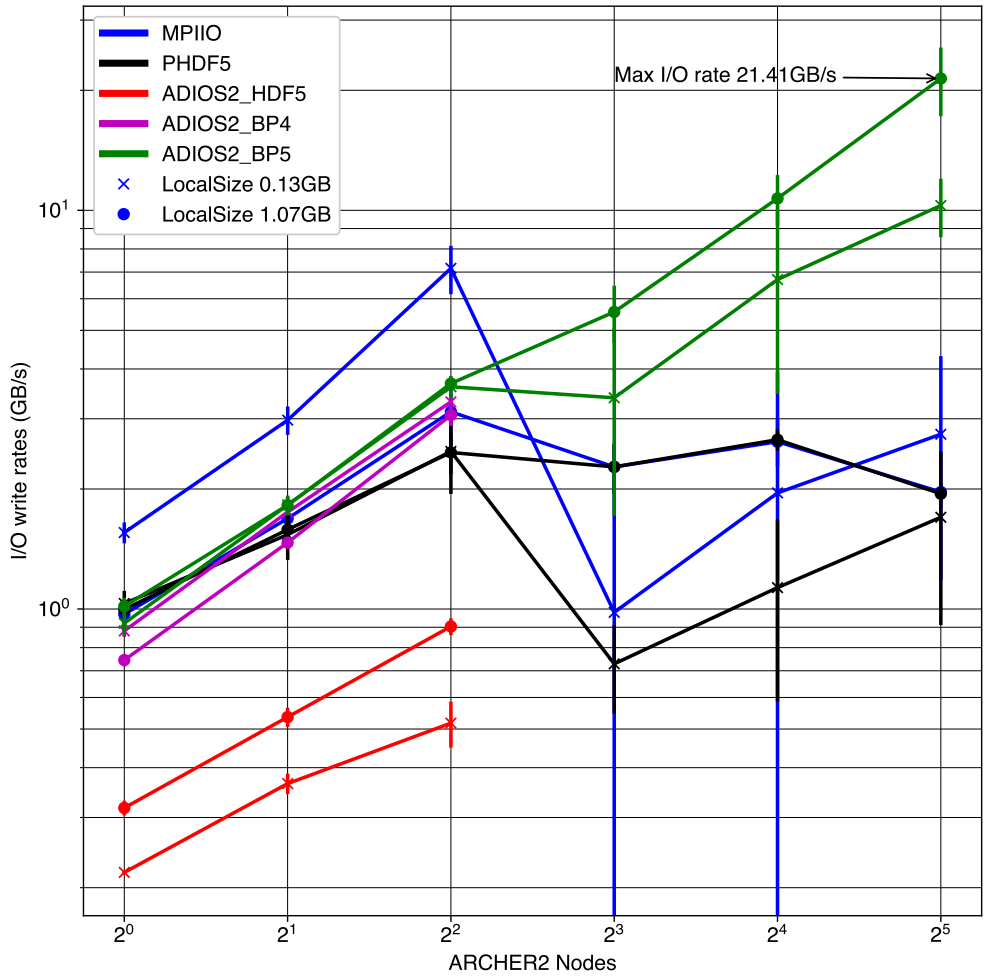
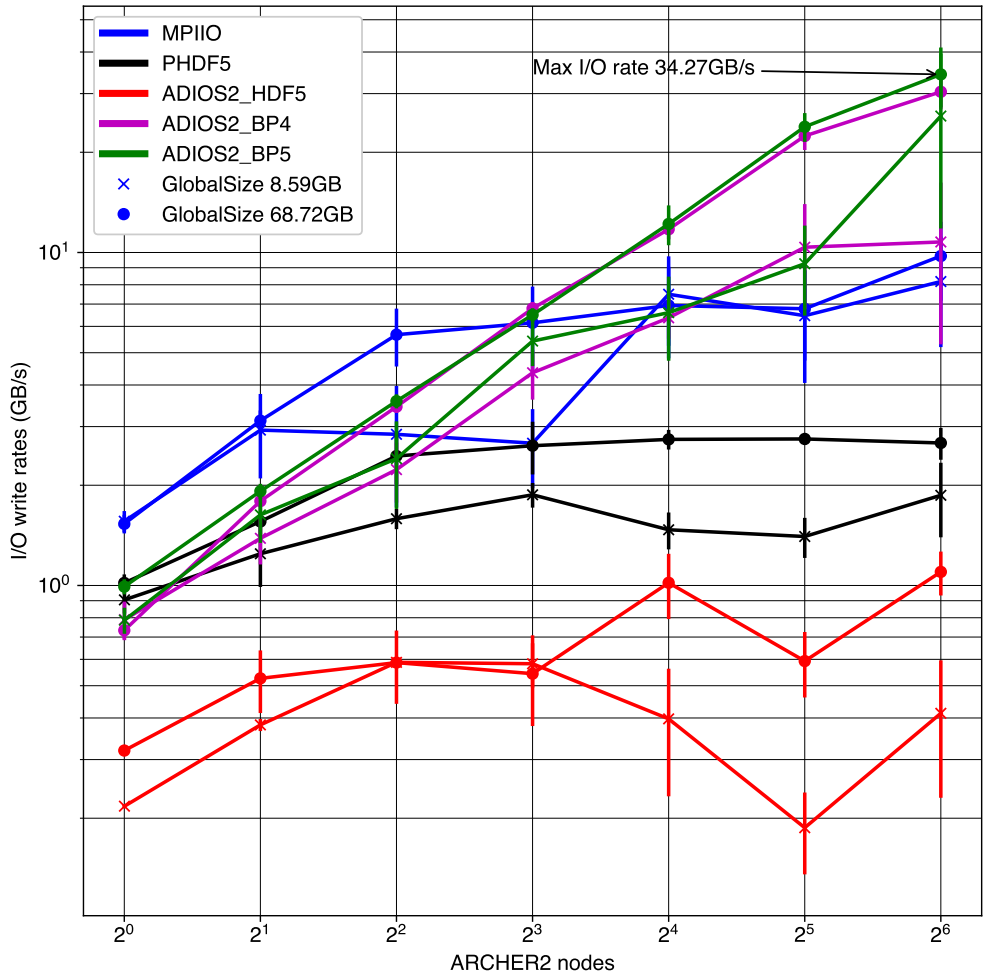
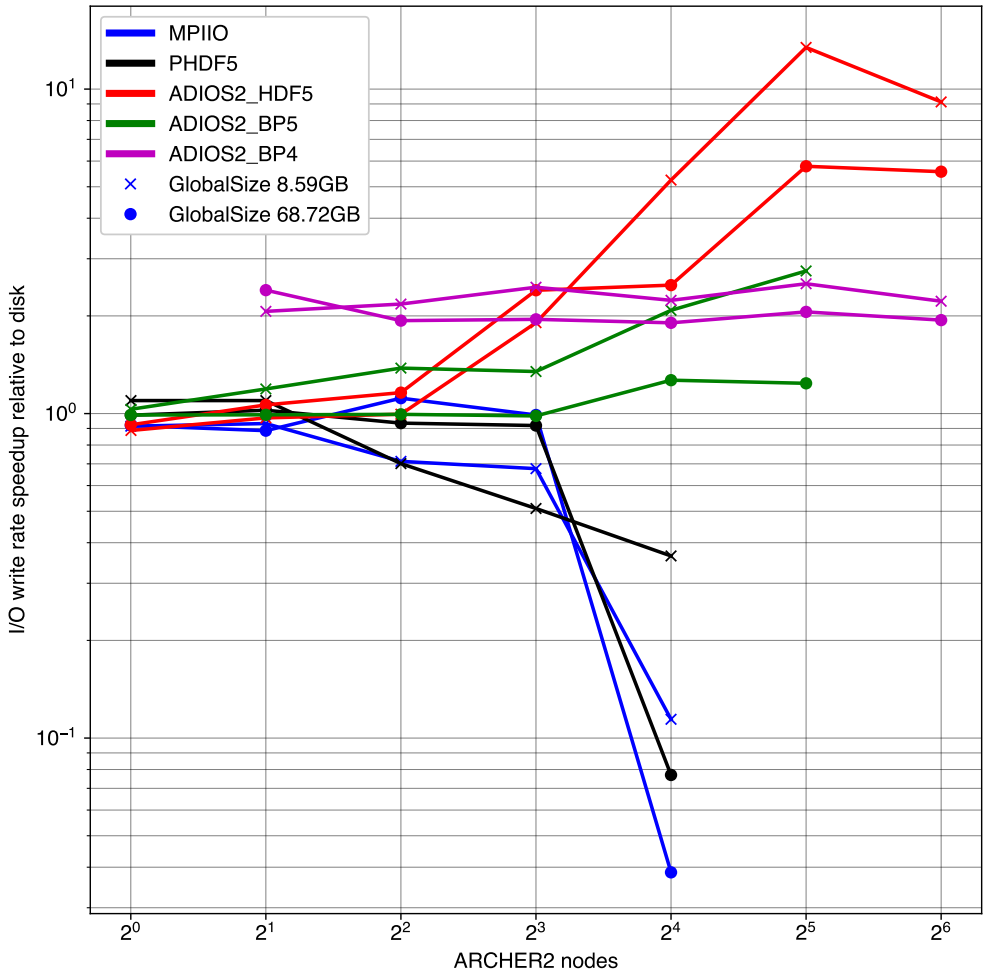


ARCHER2 weak scaling results upto local size 1.07GB

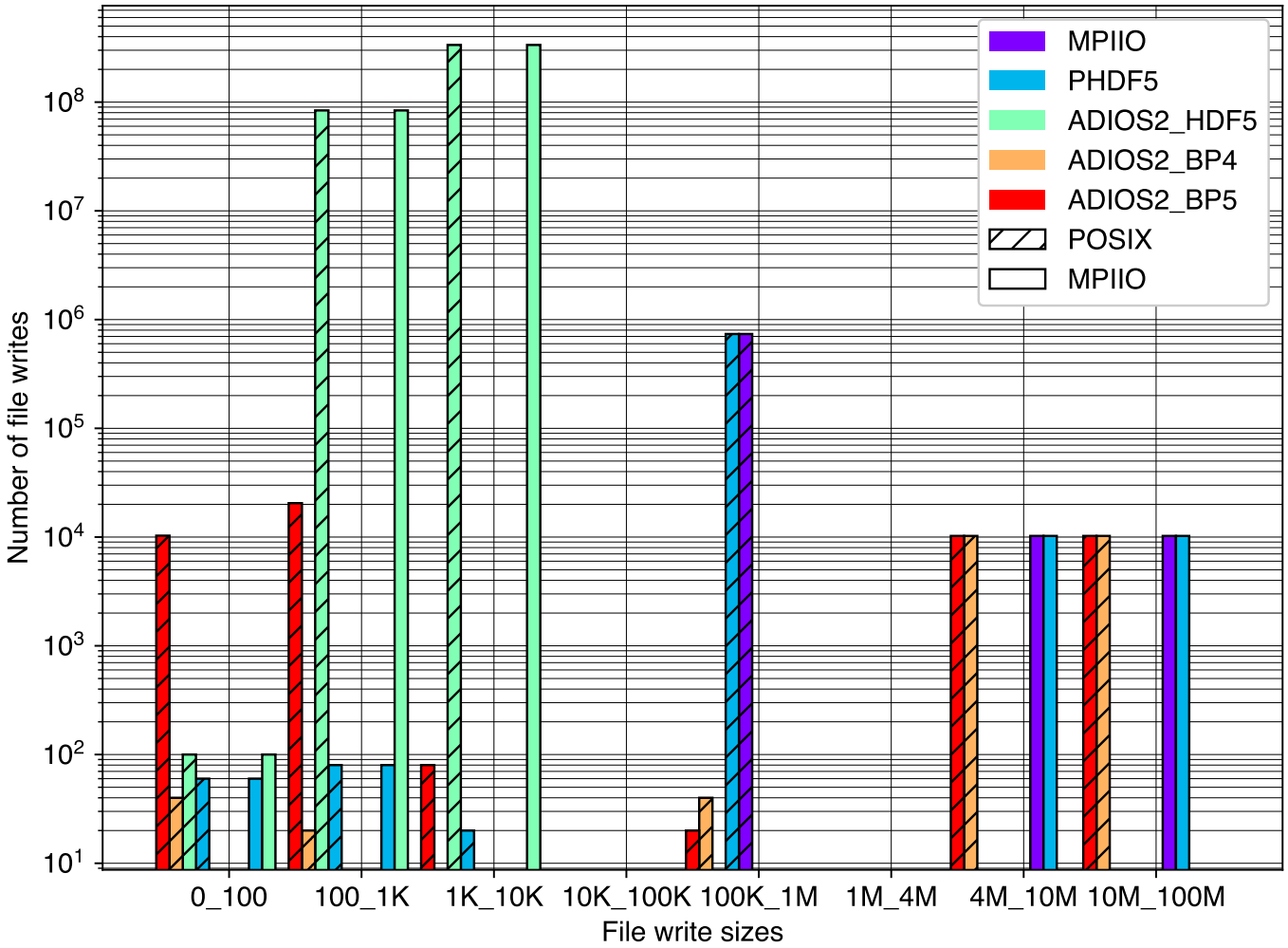


ARCHER2 strong scaling results upto global size 68.72GB

NVMe layer results speedup



ARCHER2 NVMe strong scaling speedup upto global size 68.72GB



DARSHAN I/O filesize distribution using 8 full nodes, 64GB global size

Conclusions

- ADIOS2 BP4 & BP5 scale more effectively v/s MPI, HDF5.
  - + DARSHAN profiler shows BP4 & BP5 layers create fewer file writes
  - + ADIOS2 BP4 & BP5 uses writers/node
  - + Improved performance can be due to less contention when writing
- ADIOS2 HDF5 performs slower than HDF5 as per results
  - + DARSHAN profiler shows larger no. of files generated v/s HDF5.
  - + The reason is yet to be explored.
- NVMe layer on ARCHER2 shows speedup in some layers
  - + Except MPI, PHDF5 which have negative performance
  - + Highest write rate achieved was 44GB/s from ADIOS2_BP4
  - + NVMe layer is not yet fully established, but needs more analysis.

Links

→ email: shrey.bhardwaj@epcc.ed.ac.uk

→ github: `https://github.com/sb15895/benchmark_c.git`

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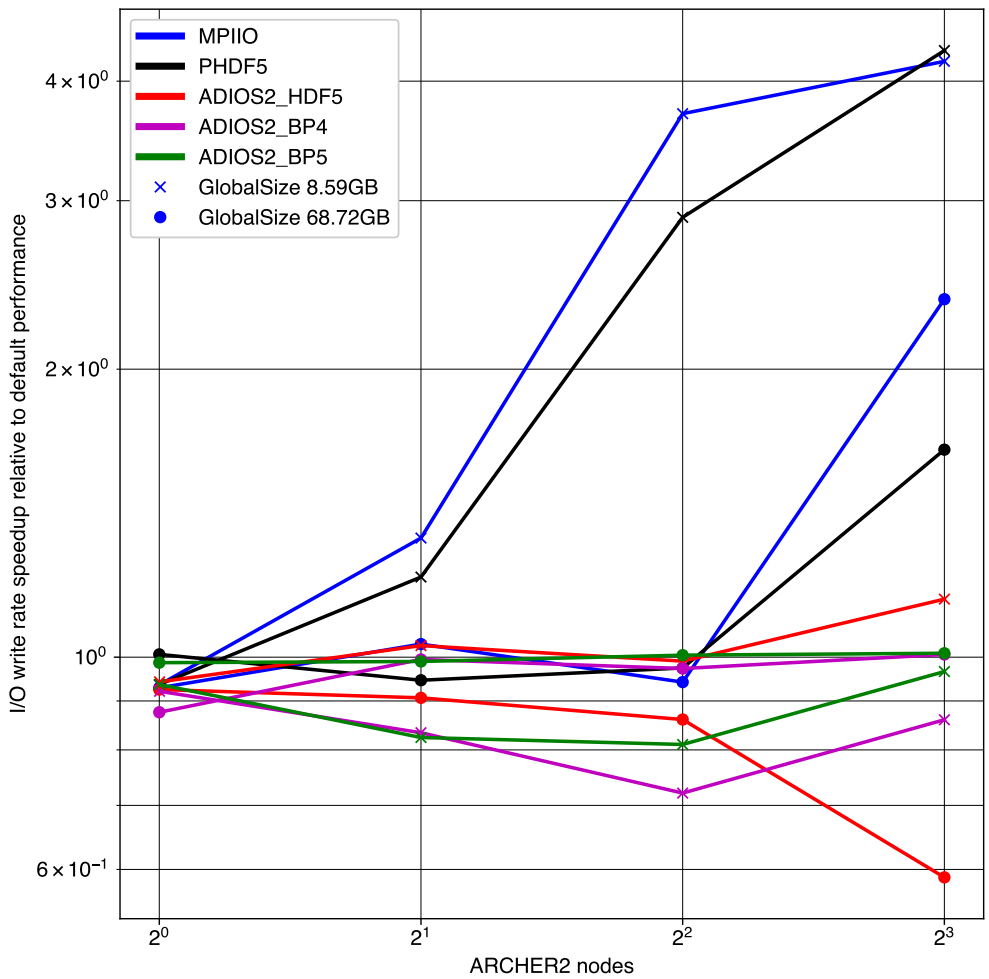
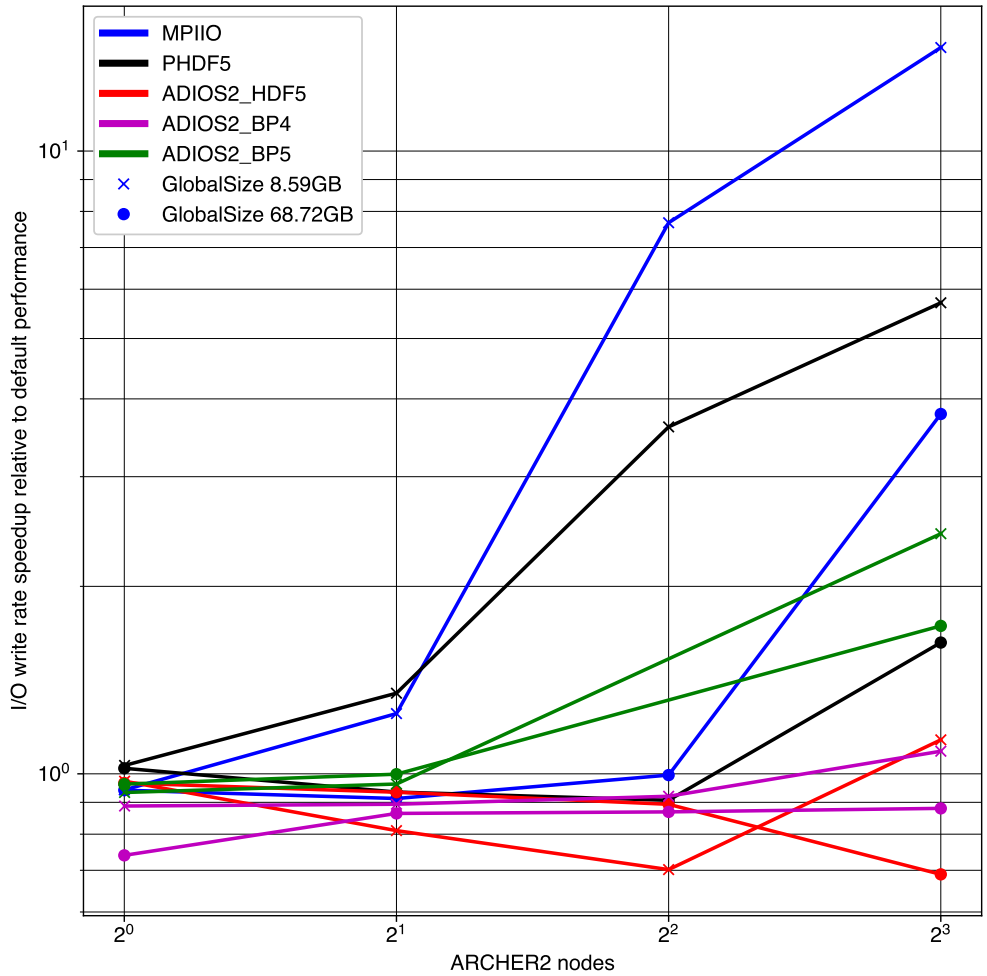


Impact on I/O performance from changing SAR LIM flag 8k to 64k



Impact on I/O performance from using non-default UCX MPI

Calls comparison