# Evaluation of Intel Optane DCPMM for memory and I/O intensive HPC applications

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# About EPCC

- Supercomputing centre at the University of Edinburgh
- 30 years old in 2020, 110 staff
- UK HPC National Service provider
- Wide range of work from HPC to Data Analytics
- Two MSc programmes
  - “HPC” and “HPC with Data Science”
  - 75 students this year

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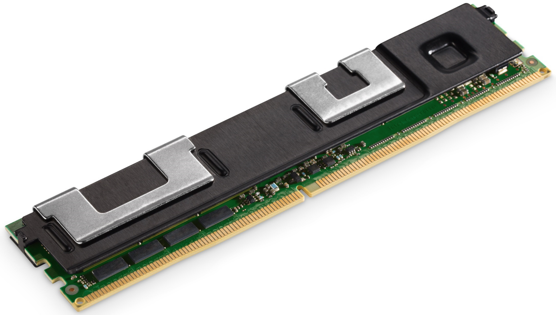
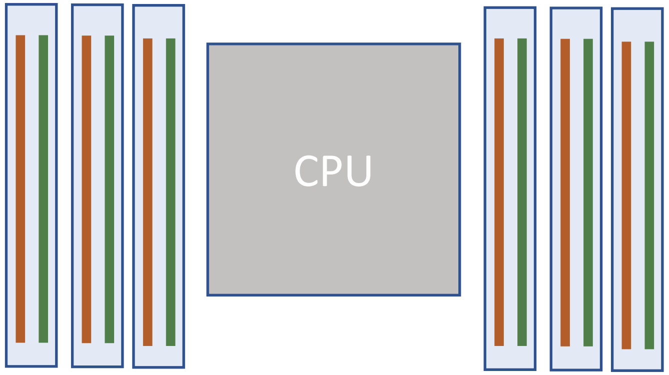
# Optane DCPMM

- Intel Optane DC Persistent Memory, based on 3D XPoint device technology
  - Hosted in the DIMM slots, additional memory controller
- Byte addressable connected to the memory bus like normal DRAM
  - Cache Coherent, Load /Store Accesses
  - Ability to do DMA & RDMA
- 128/256/512GB per module, 2 socket system up to 6TB
- High Endurance with 5 years lifetime assuming maximum write bandwidth
  - ~500 Petabyte written per module (flash devices  ~500-700 Terabyte)
- **Storage I/O** operations **become fast persistent memory** operations
  - No Paging for storage I/O
  - No Context Switching for storage I/O
  - No Interrupts for storage I/O
  - No Kernel Code Running for storage I/O



- System built by Fujitsu using bespoke motherboard
- 34 compute nodes
- Node configuration
  - Dual socket, 2 x 24-core Intel Xeon Platinum 8260M CPUs
  - 192GB DDR4 DRAM (12 x 16GB)
  - 3TB DCPMM (12 x 256GB)
- Omni-Path interconnect
  - Dual rail
- 270TB Lustre file system



- Total memory capacity
  - 6.5TB DRAM
  - 100TB NVRAM

# Basic throughput & latency

**DDR4 DRAM**

- ~70ns idle latency
- ~18.7GB/s read
- ~8.9GB/s write

**DCPMM NVRAM**

- ~176ns idle latency (2.5x)
- ~8.0GB/s read (2.4x)
- ~1.5GB/s write (6x)

- Values are *per device*
- Bandwidth between sockets (UPI) ~83,2 GB/s bidirectional

The measured idle latencies (in ns) reported by Intel Memory Latency Checker

# Platform modes

**2LM**

- NVRAM is transparent and **not** persistent
- All DRAM is used as L4 cache for the memory mode space
- Use application as normal, no changes required

**1LM**

- NVRAM needs to be addressed directly
- Persistent
- Various namespaces options
  - e.g. fsdax, devdax

**Memory mode:**
Size of all memory mode space in all DCPMMs == the size of the OS main memory
→ can only be used in 2LM platform mode

**App Direct mode:**
App Direct space can be accessed via memory mapped operations
→ can be used in both 1LM and 2LM platform mode

# System setup

- DCPMM devices are socket local
- Memory space has 192GB Level 4 cache
  - OS main memory is 3TB per node
- App Direct space configured as fsdax (ext4) namespace
  - fsdax == filesystem dax
  - `/mnt/pmem_fsdax{0,1}`

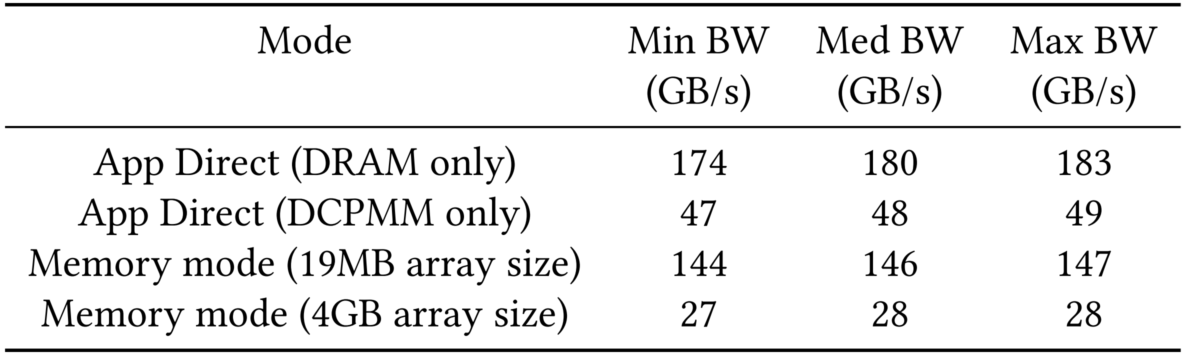
# STREAM benchmark

https://github.com/NGIOproject/benchmarks

- Synthetic application designed to measure the achievable memory bandwidth
- Standard STREAM for DRAM and Memory mode
- Modified STREAM for App Direct
  - Initial memory allocation replaced with a call to `pmem_map_file` & memory offset calculations
  - Add "data persist" instructions to ensure data is fully stored on the DCPMM
- Configuration
  - DRAM and App Direct: array size 19MB per process (2.7GB total)
  - Memory mode: array sizes 19MB and 4GB per process (768GB total)

# STREAM Triad

- Theoretical peak (DRAM only) is 210GB/s
- Configuration: 48 MPI processes per node, 10 nodes
- App Direct DCPMM bandwidth is ~5x less than DRAM
- Memory mode bandwidth for small size is roughly same as DRAM
  - This does not fulfil the “*array size should be at least 4x the size of the sum of all the last-level caches used in the run*” rule



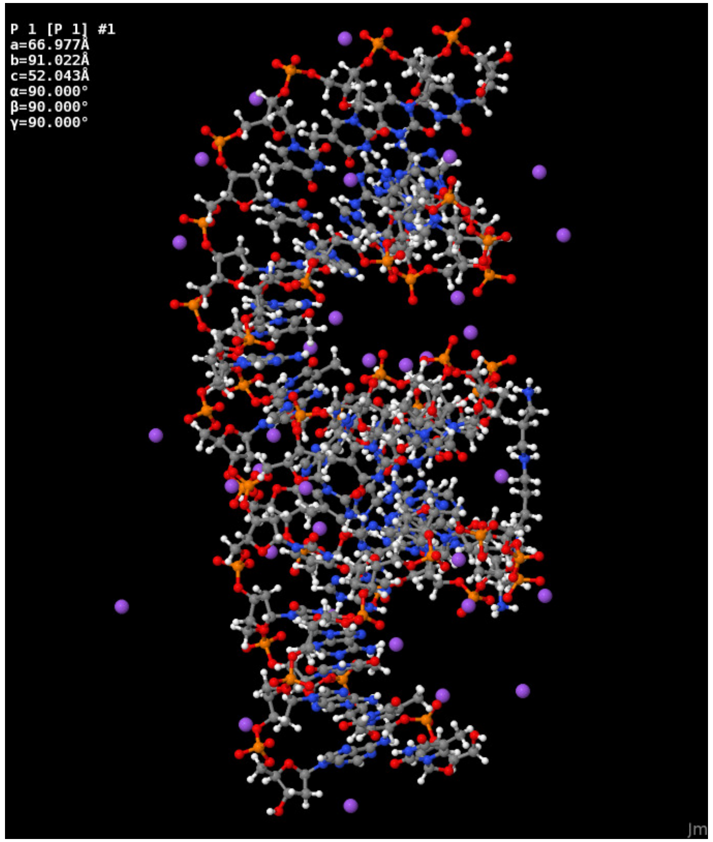
| Mode | Min BW (GB/s) | Med BW (GB/s) | Max BW (GB/s) |
|---|---|---|---|
| App Direct (DRAM only) | 174 | 180 | 183 |
| App Direct (DCPMM only) | 47 | 48 | 49 |
| Memory mode (19MB array size) | 144 | 146 | 147 |
| Memory mode (4GB array size) | 27 | 28 | 28 |

# Memory intensive application

# CASTEP

- Materials modelling application
- Needs scale to satisfy memory demands
- BUT poor scaling behaviour due to high volume of all-to-all communications
  - Poor parallel efficiency – CPUs underutilised

| Number of nodes | MPI procs | Average mem per node (GBs) | Total mem (TBs) |
|---|---|---|---|
| 20 | 720 (36 MPI per node) | 103.21 | 2.01 |



# CASTEP baseline, no DCPMM

- DNA test case
  - Application’s own estimates of memory requirements and parallel efficiency
  - Measurement of wallclock time for 3 SCF loop iterations

| Nodes | MPI x OpenMP | Active cores | Memory estimate per process | Runtime | Overall parallel efficiency |
|---|---|---|---|---|---|
| 34 | 48x1 | 1632 | 5,486.6 MB | OOM | N/A |
| 24 | 36x1 | 864 | 6,476.0 MB | 3,959.01s | 23% |
| 24 | 24x2 | 1152 | 7,491.2 MB | 4,598.74s | 28% |
| 20 | 36x1 | 720 | 7,034.9 MB | 3,311.88s | 33% |
| 20 | 24x2 | 960 | 8,320.0 MB | 4,377.15s | 36% |
| 18 | 36x1 | 648 | 7,355.5 MB | 3,587.94s | 34% |
| 18 | 24x2 | 864 | 8,843.5 MB | 4,814.94s | 36% |

# More memory capacity

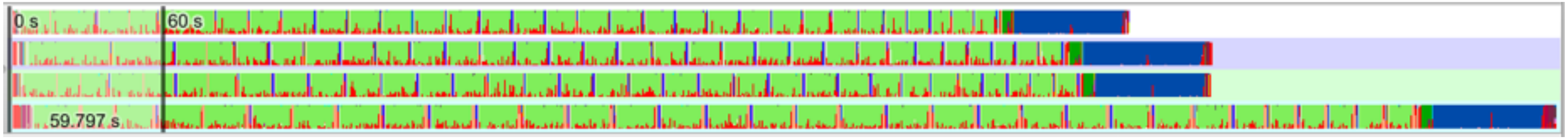
- DCPMM can provide more memory per core in two ways
  - 2LM Memory mode - transparent
  - 1LM App Direct mode using *libvmmalloc* (PMDK library)

- *libvmmalloc* intercepts calls to dynamic memory allocations (e.g. malloc, memalign or free) and replaces them with persistent memory allocations

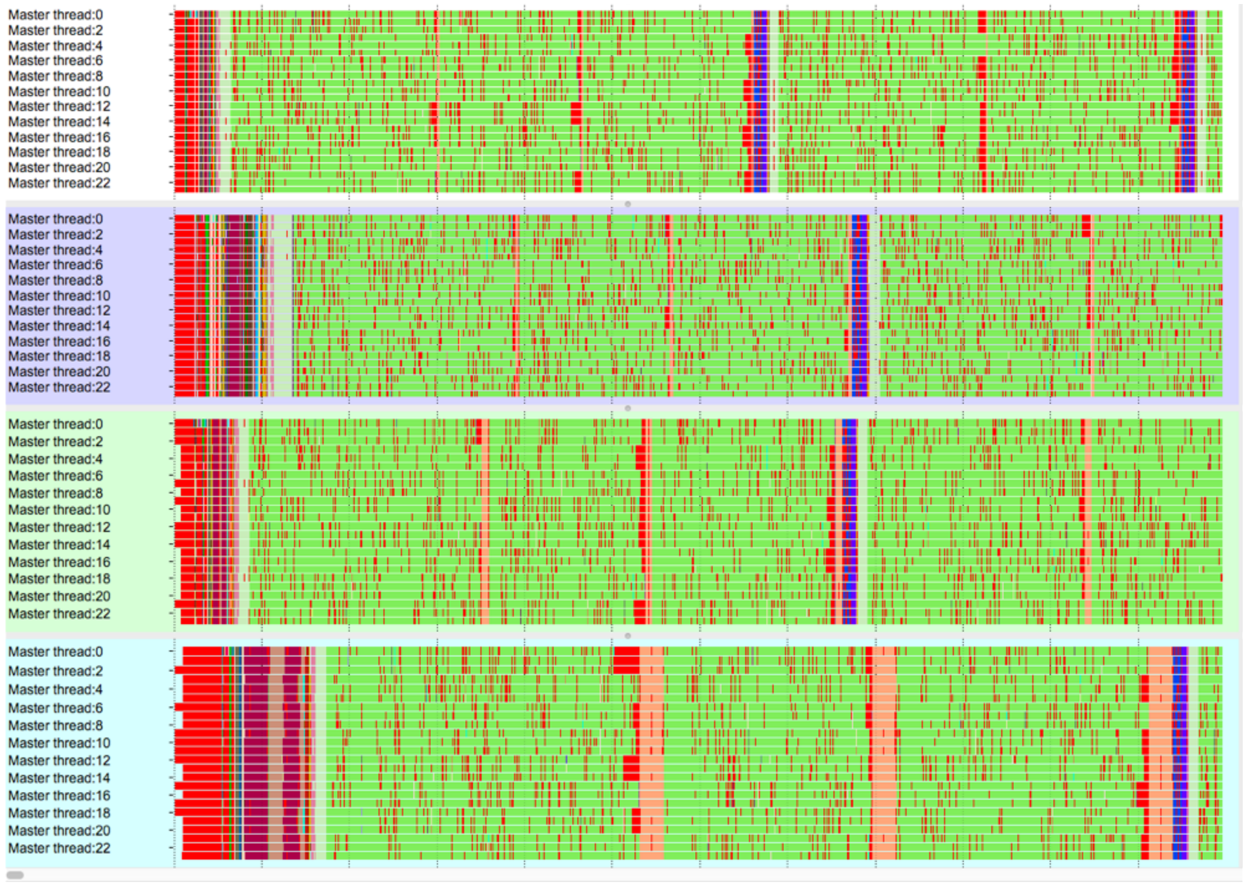
1. Set the size of the non-volatile memory pool (`VMMALLOC_POOL_SIZE`) and the location of the pool (`VMMALLOC_POOL_DIR`)
2. The path to the non-volatile memory pool points to a directory that is created in `/mnt/pmem_fsdax{0,1}`
3. Preload *libvmmalloc* using `LD_PRELOAD` and launch the application as normal

# Tracing with a smaller test case

- TiN test case – fits on single node, memory high watermark ~19GB
- 4 scenarios (top to bottom)
  1. DRAM only
  2. Memory mode
  3. App Direct + *libvmmalloc*, compute and DCPMM on socket 0
  4. App Direct + *libvmmalloc*, compute on socket 0 and DCPMM on socket 1



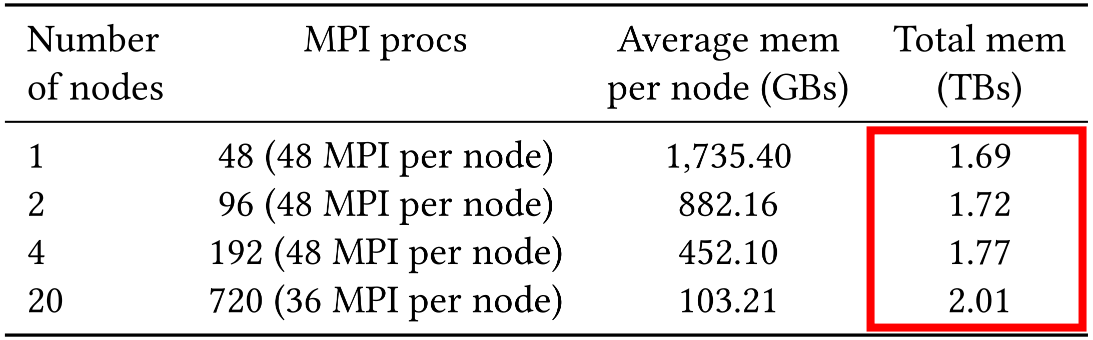
# Tracing with a smaller test case (2)



| Mode | Runtime (s) | Slowdown |
|---|---|---|
| App Direct (DRAM only) | 442.30 | - |
| Memory mode | 484.90 | 1.10x |
| App Direct + libvmmalloc local | 468.89 | 1.06x |
| App Direct + libvmmalloc remote | 599.70 | 1.36x |

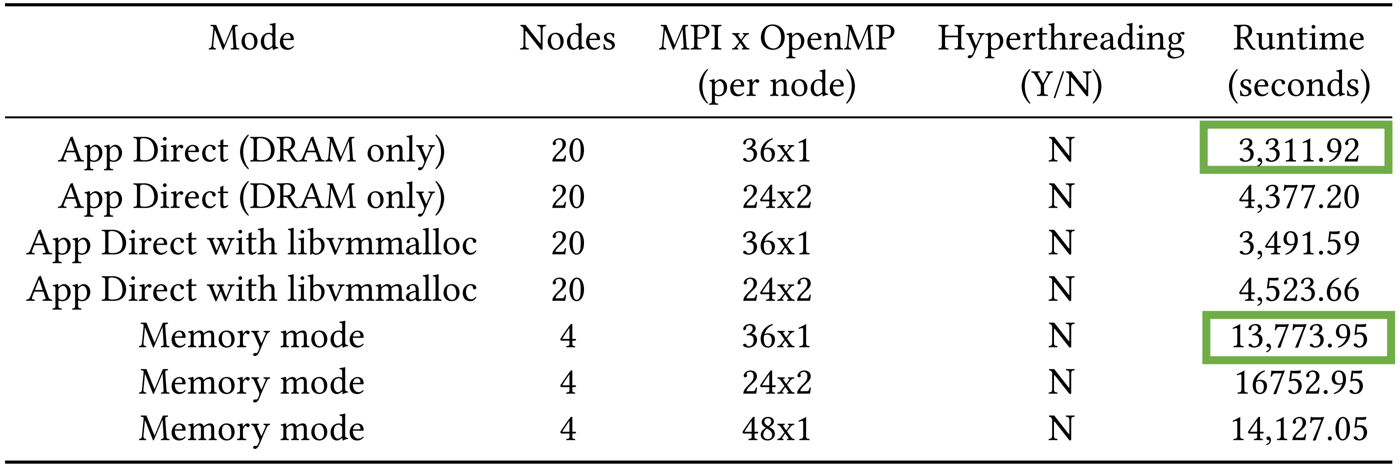
| Mode | CPI | Stall cycles | Load instructions from DCPMM |
|---|---|---|---|
| App Direct (DRAM only) | 1.17 | 1.62E+13 | 0 |
| Memory mode | 1.25 | 1.87E+13 | 3.81E+08 |
| App Direct + libvmmalloc local | 1.25 | 1.84E+13 | 6.87E+08 |
| App Direct + libvmmalloc remote | 1.57 | 2.45E+13 | 5.66E+08 |

# DNA test case



| Number of nodes | MPI procs | Average mem per node (GBs) | Total mem (TBs) |
|---|---|---|---|
| 1 | 48 (48 MPI per node) | 1,735.40 | 1.69 |
| 2 | 96 (48 MPI per node) | 882.16 | 1.72 |
| 4 | 192 (48 MPI per node) | 452.10 | 1.77 |
| 20 | 720 (36 MPI per node) | 103.21 | 2.01 |

DNA test case now fits on a single node



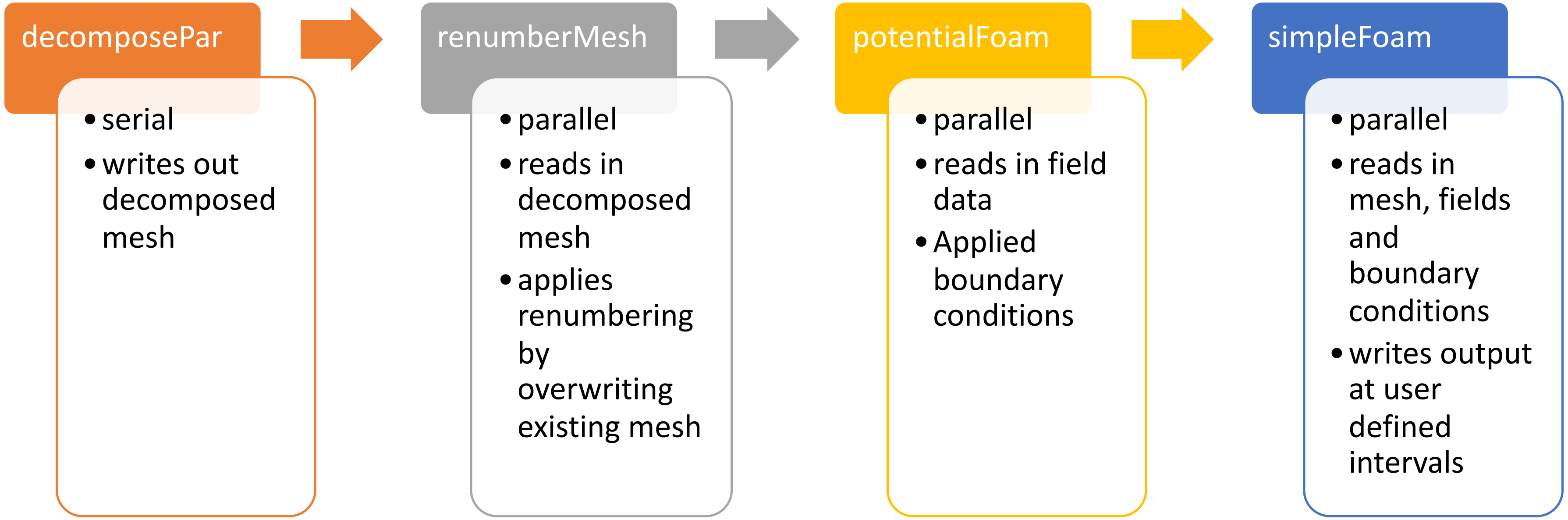
| Mode | Nodes | MPI x OpenMP (per node) | Hyperthreading (Y/N) | Runtime (seconds) |
|---|---|---|---|---|
| App Direct (DRAM only) | 20 | 36x1 | N | 3,311.92 |
| App Direct (DRAM only) | 20 | 24x2 | N | 4,377.20 |
| App Direct with libvmmalloc | 20 | 36x1 | N | 3,491.59 |
| App Direct with libvmmalloc | 20 | 24x2 | N | 4,523.66 |
| Memory mode | 4 | 36x1 | N | 13,773.95 |
| Memory mode | 4 | 24x2 | N | 16752.95 |
| Memory mode | 4 | 48x1 | N | 14,127.05 |

20% throughput improvement

# I/O intensive application

# OpenFOAM

- v1812 built with Intel 19.0.3.199 compilers & MPI library
- Test case: open wheel race car geometry – 90 million cells



decomposePar

- serial
- writes out decomposed mesh

renumberMesh

- parallel
- reads in decomposed mesh
- applies renumbering by overwriting existing mesh

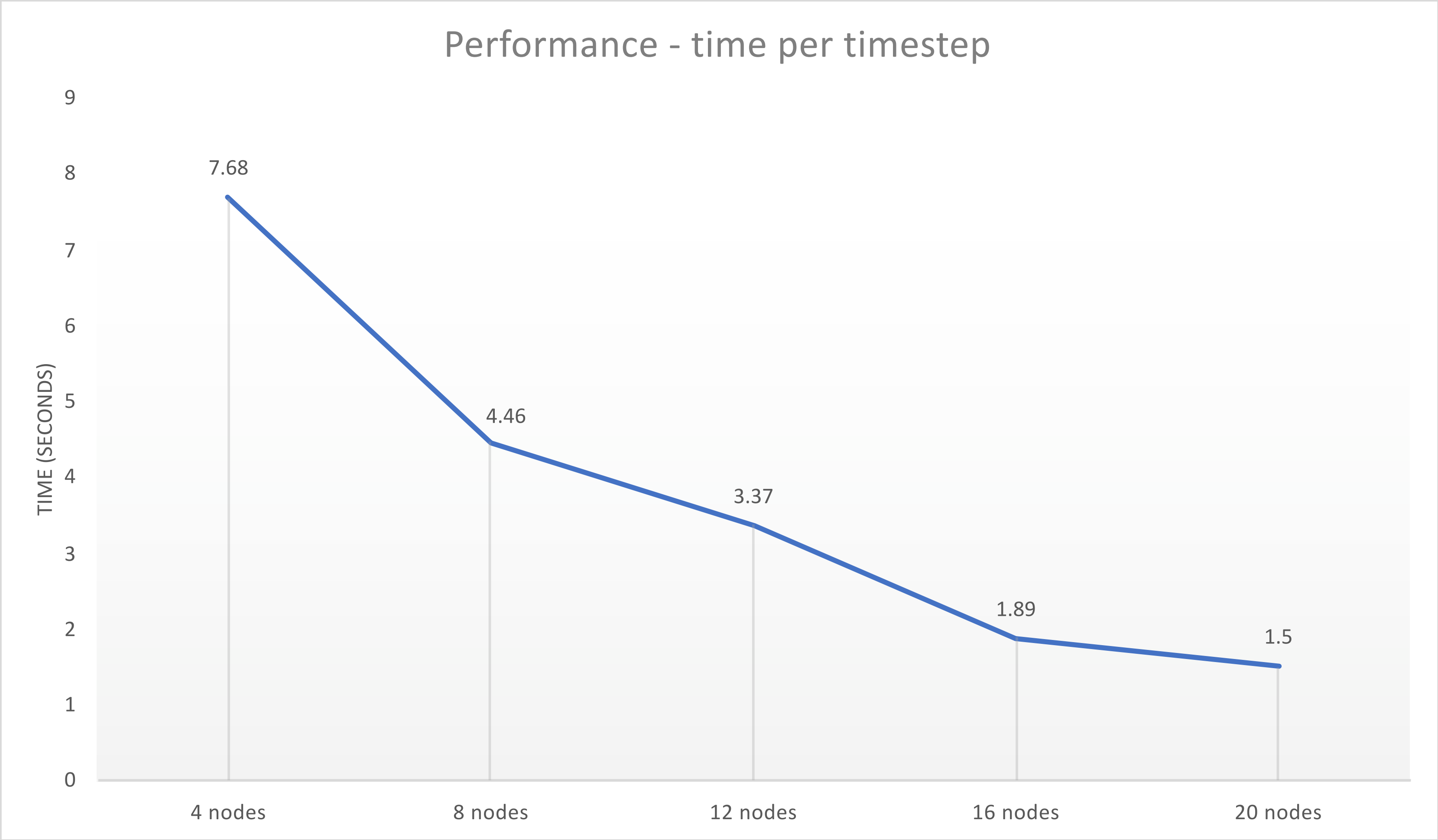
potentialFoam

- parallel
- reads in field data
- Applied boundary conditions

simpleFoam

- parallel
- reads in mesh, fields and boundary conditions
- writes output at user defined intervals

# Performance of default setup



# I/O characteristics for this case

```
-- processorN
  |-- constant
  |-- 0
  |-- timestepT
     |-- k
     |-- nut
     |-- omega
     |-- p
     |-- phi
     |-- U
     |-- uniform
        |-- time
        |-- functionObjects
           |-- functionObjectProperties
```

“constant” and “0” are input – 31GB

timestep folder and its contents are output

Data volume for 192 processes:
~40MB per timestep on each process
→ total: 7.5GB per timestep

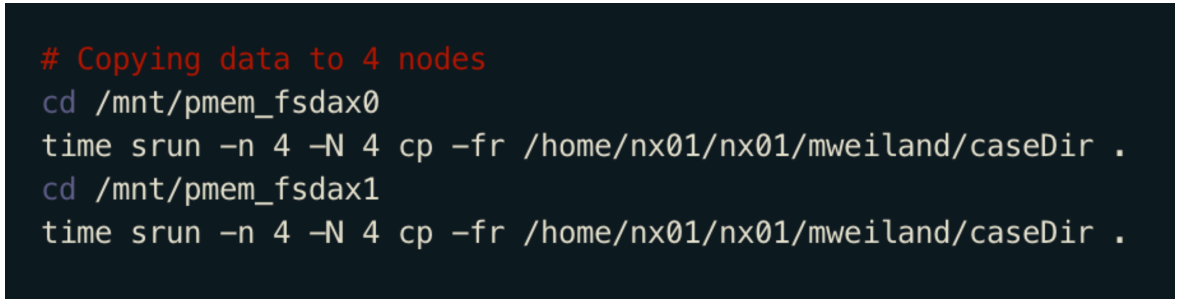
→ writing every step for 500 steps
7.5GB * 500 = ~3.7TB

Total number of files created: N * T * 8
Total number of directories created: N * T * 3

Example: 960 processors, 100 iterations, write interval 1
→ 960 * 100 * 8 = 768,000 files
→ 960 * 100 * 3 = 288,00 directories

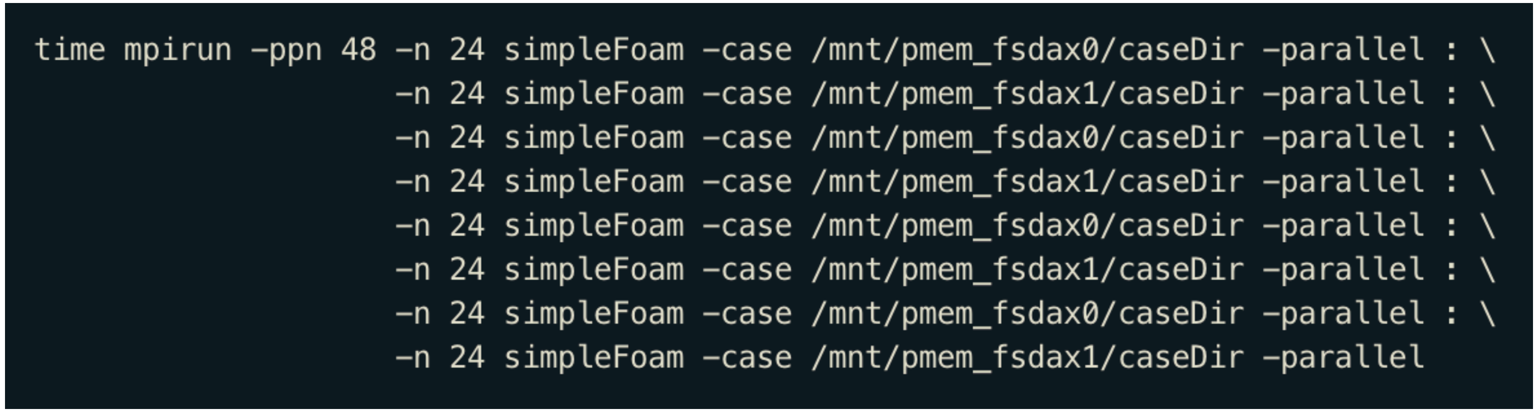
# Using fsdax directly

- Taking advantage of OpenFOAM's I/O strategy – use `fsdax` namespace
  - Write once, read never
  - Write locally



```
# Copying data to 4 nodes
cd /mnt/pmem_fsdax0
time srun -n 4 -N 4 cp -fr /home/nx01/nx01/mweiland/caseDir .
cd /mnt/pmem_fsdax1
time srun -n 4 -N 4 cp -fr /home/nx01/nx01/mweiland/caseDir .
```

- Copy test case data to DCPMM
  - *Use fsdax on both sockets!*



```
time mpirun -ppn 48 -n 24 simpleFoam -case /mnt/pmem_fsdax0/caseDir -parallel : \
                    -n 24 simpleFoam -case /mnt/pmem_fsdax1/caseDir -parallel : \
                    -n 24 simpleFoam -case /mnt/pmem_fsdax0/caseDir -parallel : \
                    -n 24 simpleFoam -case /mnt/pmem_fsdax1/caseDir -parallel : \
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                    -n 24 simpleFoam -case /mnt/pmem_fsdax0/caseDir -parallel : \
                    -n 24 simpleFoam -case /mnt/pmem_fsdax1/caseDir -parallel
```
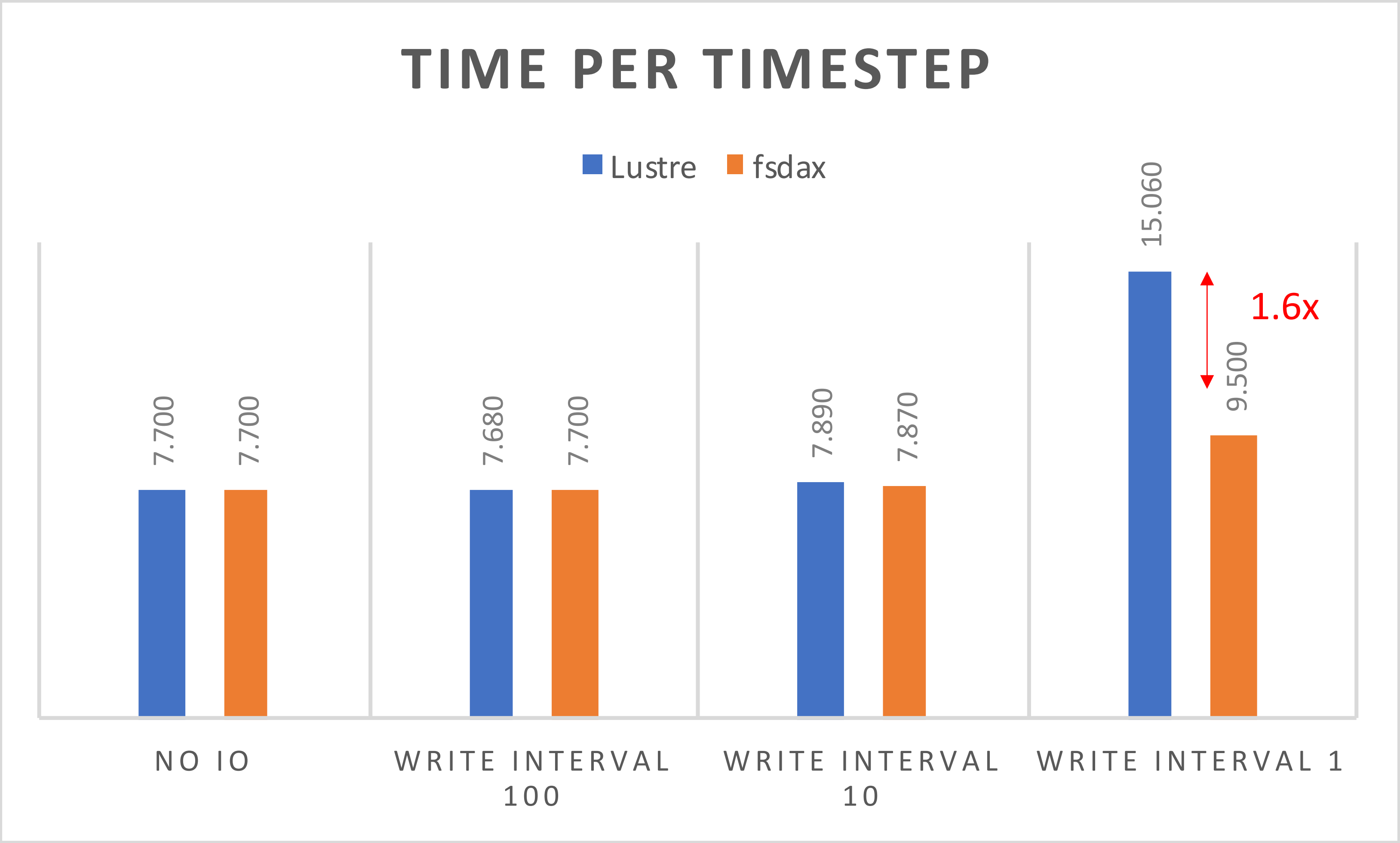

- Exploit MPMD for good data locality

Total number of files created:
Write interval 1: 192 * 100 * 8 = 153,600

Total number of directories created: N * T * 3
Write interval 1: 192 * 100 * 3 = 57,600

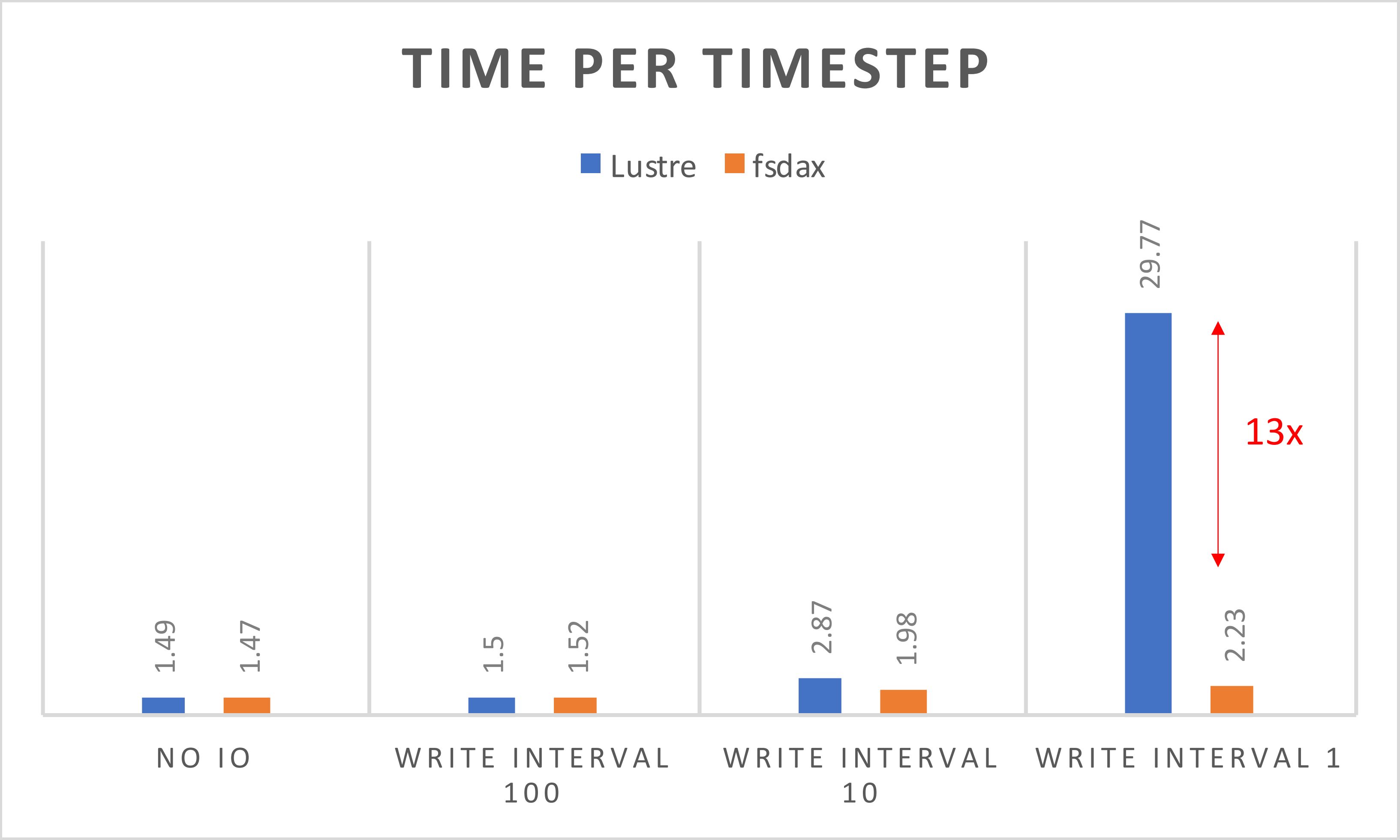
# 4 node experiment



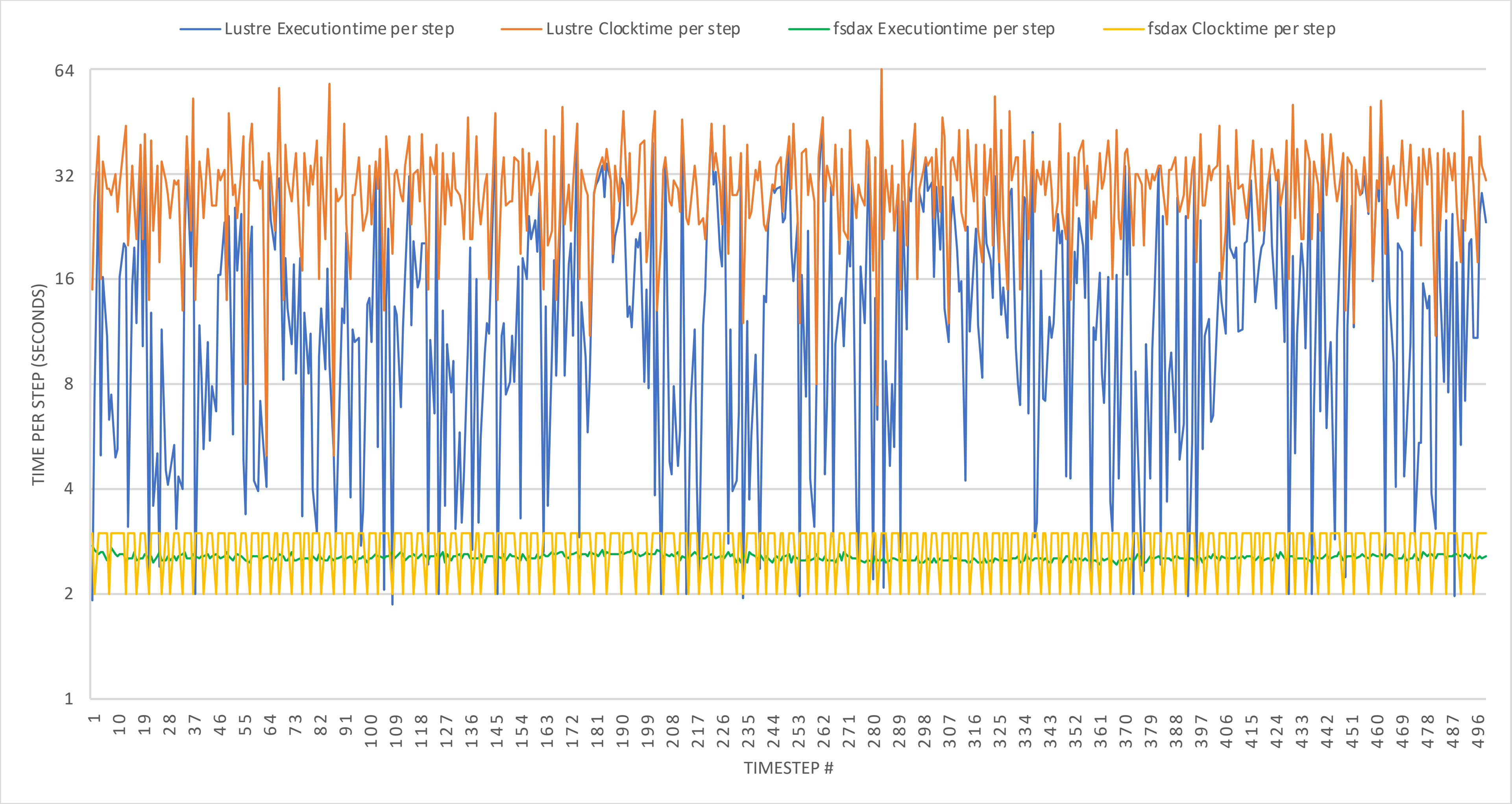
Total number of files created:
Write interval 1: 960 * 100 * 8 = 768,000

Total number of directories created: N * T * 3
Write interval 1: 960 * 100 * 3 = 256,000

# 20 node experiment



# Performance stability



# Achieved I/O performance

- Difference in time per timestep between “no IO” and “write interval X” can be entirely attributed to data writes and associated metadata operations

- On 20 nodes – for “write interval 1”:

Lustre *29.77s - 1.47s = 28.28s*
*7.5GB / 28.28s = 0.256GB/s*

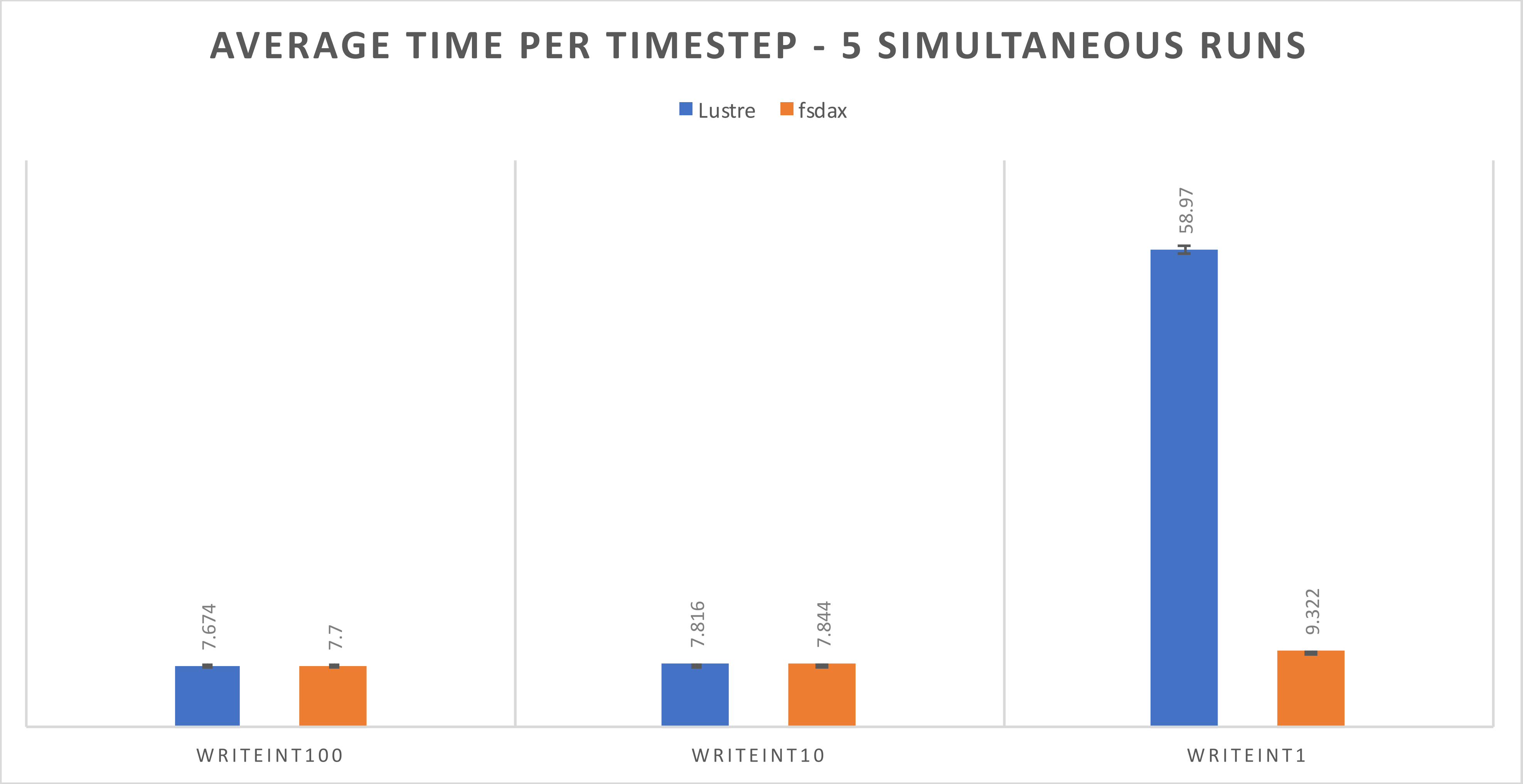
fsdax *2.23s – 1.47s = 0.76s*
*7.5GB / 0.76s = 9.87GB/s*

# Ensemble experiments

- Nobody runs on empty systems
- Single isolated experiments are also rare

- For a more realistic view, we compare performance of five 4-node experiments running concurrently
  - Using a total of 20 nodes, but independent simulations
  - More representative of real, busy environments
  - Plus: same number of metadata operations, but 5 times the amount of data written
    - 7.5GB per timestep *per simulation*

# Ensemble performance



# Time per timestep: single run vs ensemble

| | **Lustre** | | **fsdax** | |
|---|---|---|---|---|
| | Single run<br>(4 nodes) | Ensemble average<br>(5 x 4 nodes) | Single run<br>(4 nodes) | Ensemble average<br>(5 x 4 nodes) |
| write interval 100 | 7.680 | 7.674 | 7.700 | 7.700 |
| write interval 10 | 7.890 | 7.816 | 7.870 | 7.844 |
| write interval 1 | 15.060 | **58.97** | 9.500 | 9.322 |

7.5GB per step

37.5GB per step

Lustre *7.5GB / (15.06-7.68) = 1.01GB/s*
*37.5GB / (58.97-7.67) = 0.73GB/s*

fsdax *7.5GB / (9.5-7.7) = 4.17GB/s*
*37.5GB/ (9.3-7.7) = 23.12GB/s*

# Conclusions

- DCPMM is a new memory technology that offers unprecedented opportunities both as memory & storage device
    - Through byte-addressability, high capacity, low latency (and persistence)

- CASTEP in Memory mode → increased throughput
- OpenFOAM in App Direct mode → performance hit of I/O negated

- Many avenues for research still left to be explored

Michèle Weiland, Holger Brunst, Tiago Quintino, Nick Johnson, Olivier Iffrig, Simon Smart, Christian Herold, Antonino Bonanni, Adrian Jackson, and Mark Parsons. 2019. **An Early Evaluation of Intel's Optane DC Persistent Memory Module and its Impact on High-Performance Scientific Applications**. In The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC'19), November 17–22, 2019, Denver, CO, USA. https://doi.org/10. 1145/3295500.3356159

# Questions?

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