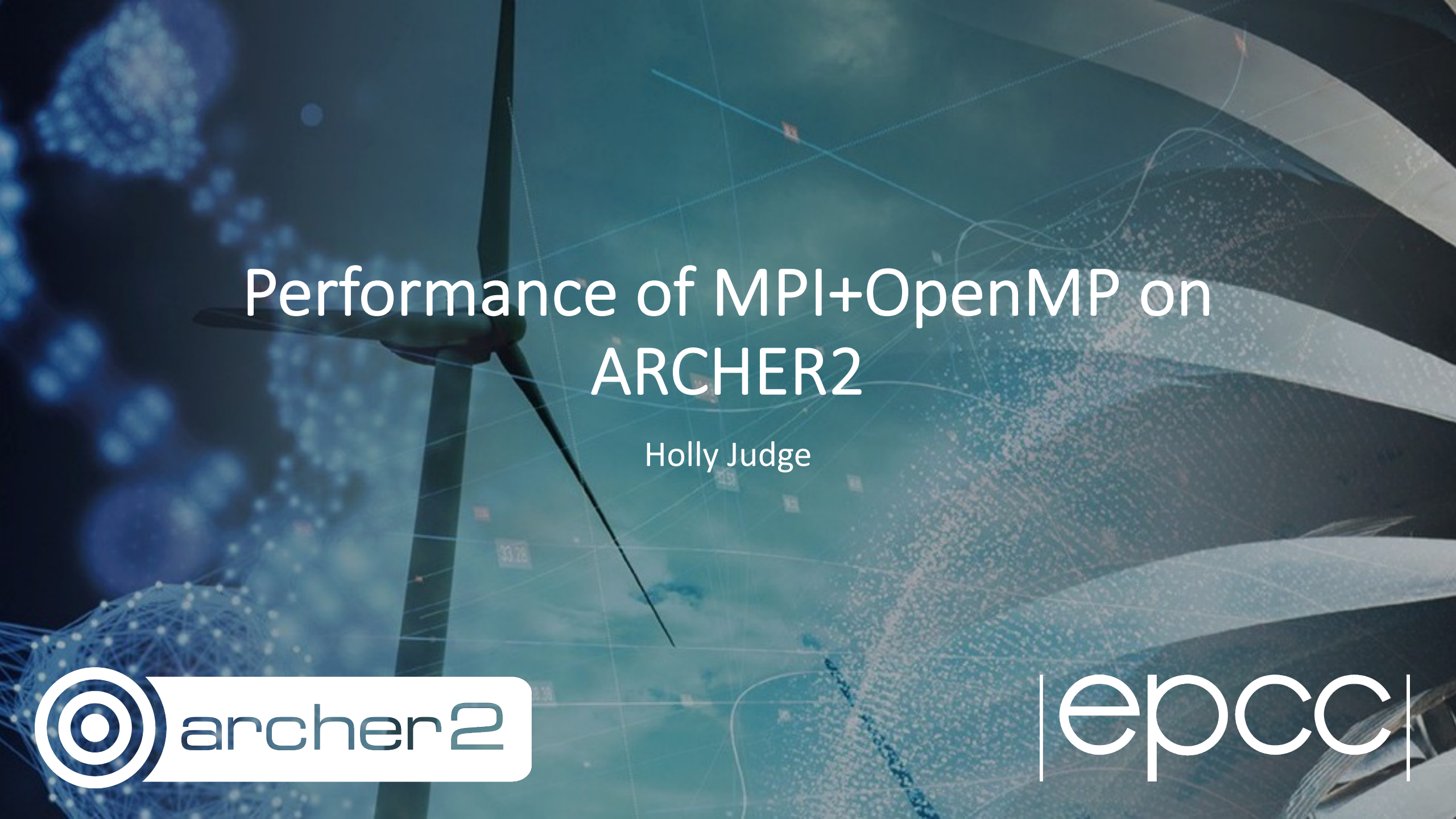

Performance of MPI+OpenMP on ARCHER2

Holly Judge

archer2

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Introduction

- HPC applications are typically run with MPI
  - For some applications MPI+OpenMP can be used as an alternative to MPI
  - This may achieve better performance than MPI – but this depends
- Using MPI+OpenMP may be good for taking advantage of the resources on ARCHER2 nodes
  - 128 cores per node
  - Different to ARCHER – 24 cores per node
- When can we get good performance with MPI+OpenMP?
  - Which applications?
  - What sort of systems/test cases?
  - How many threads?

Outline

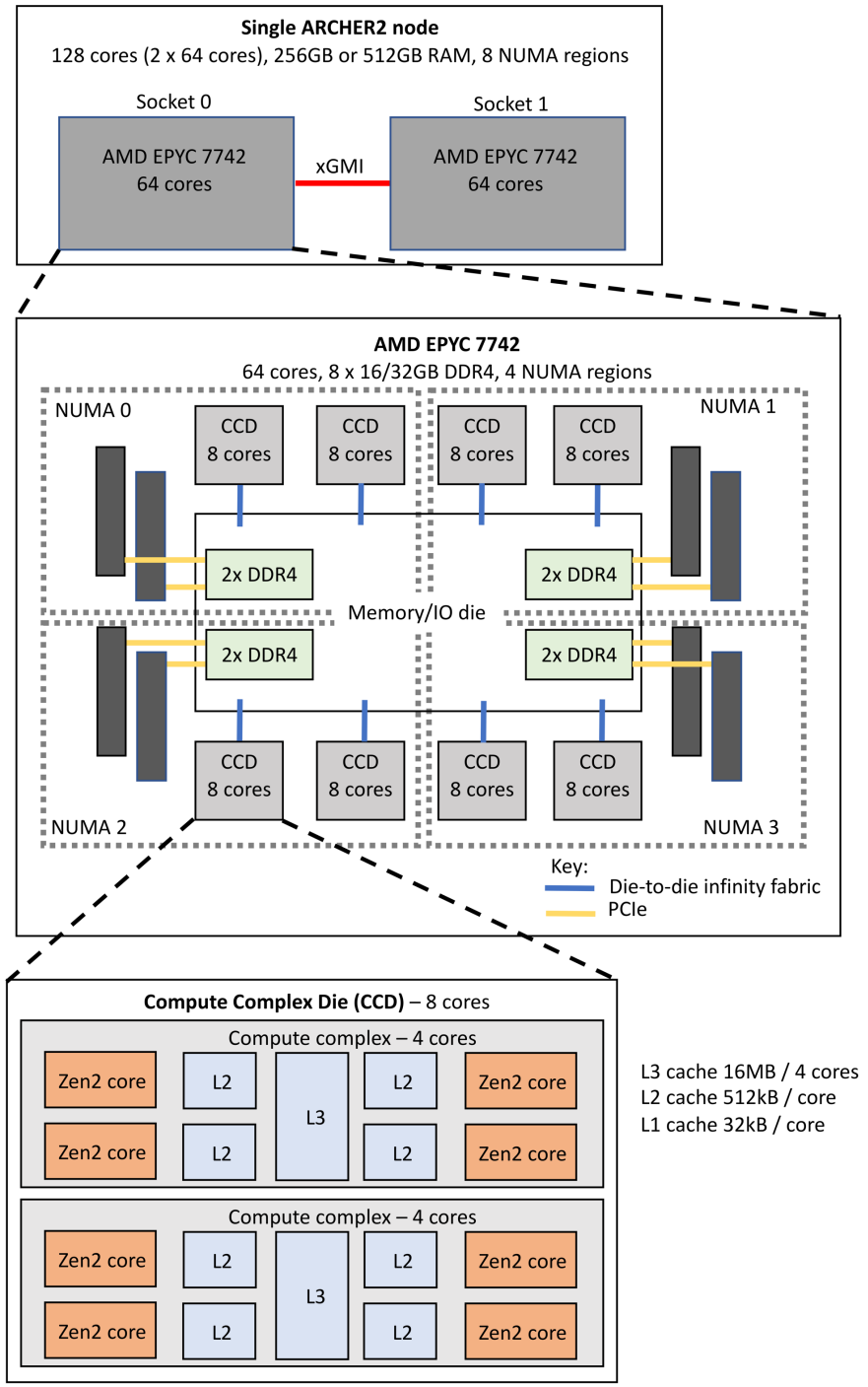
- ARCHER2
- MPI+OpenMP overview
  - How is it different to MPI?
  - How can it be used on ARCHER2?
- MPI+OpenMP performance investigation on ARCHER2
  - Applications investigated
  - Test cases
  - Results
- How can users benefit from MPI+OpenMP on ARCHER2?

ARCHER2

- UK national service used for scientific research
- HPE EX system
- 5,860 nodes (750,080 cores)
- AMD EPYC processors
- HPE Slingshot interconnect

Node-level architecture

- Two 64 core AMD EPYC 7742 processors – 128 cores
- 256 GB of memory per standard node
- 8 non-uniform memory access (NUMA) regions of 16 cores
- Groups of 4 cores which share L3 cache



ARCHER2 node usage

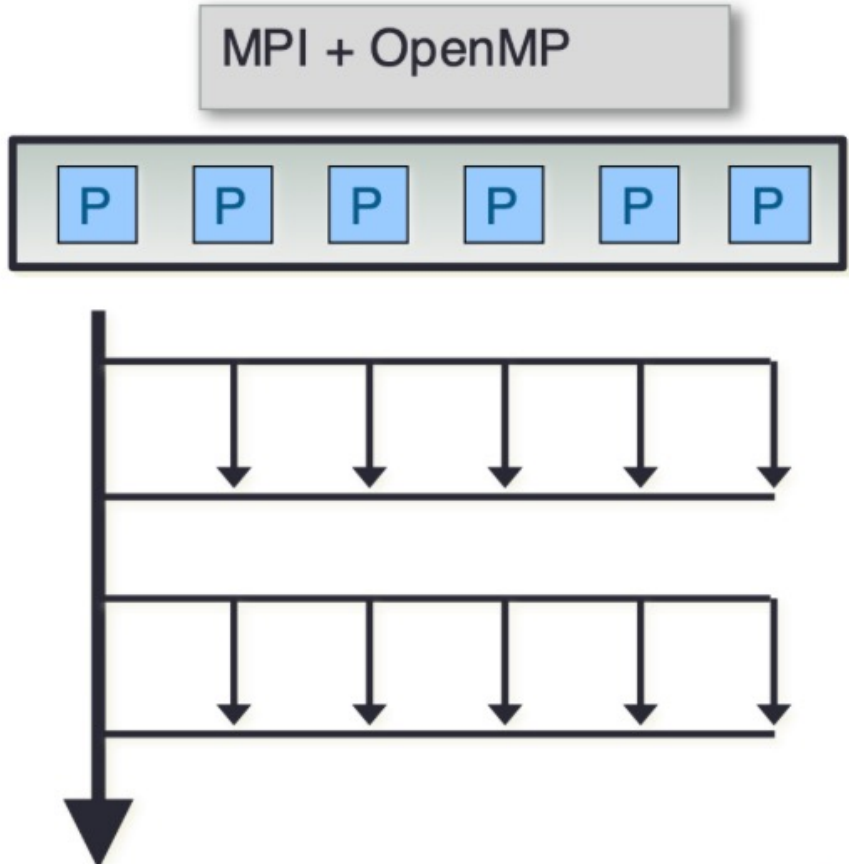
- ARCHER2 nodes have 256 GB of memory and 128 cores
- Using one MPI process per core gives 2 GB of memory per process
  - Less than ARCHER - roughly 2.6 GB per process
- This can be not enough for memory intensive applications – OOM errors – underpopulation sometimes necessary
- Using one process per core can affect the MPI communication performance
- Using MPI+OpenMP (less processes with multiple threads per process) can maybe help here

MPI and MPI+OpenMP in practice

- MPI
  - each core has one process (task) spawned on it
    - Own distinct memory space for each process
  - Communication between processes takes place via messages
  - 128 cores per node on ARCHER2 --tasks-per-node=128
    - OMP_NUM_THREADS = 1
    - 2 GB of memory per task
- MPI+OpenMP
  - Using a mixture of threads and processes spawned onto the cores
    - Groups of multiple threads within a memory region
    - At least one process per memory region
    - Messages between processes
  - Less processes mean more memory per process (shared between threads)
    - Less copies of data on a node
  - Less processes can mean less internode messages

MPI+OpenMP Usage

- Implemented in many HPC applications
- However not always more performant than using a single thread (e.g. pure MPI)
- Good OpenMP coverage within the code required
- Number of threads per process to use needs to be tuned to the use case and the machine
- Need to be aware of the underlying node structure when running e.g. regions when memory is shared



MPI+OpenMP ARCHER2 usage

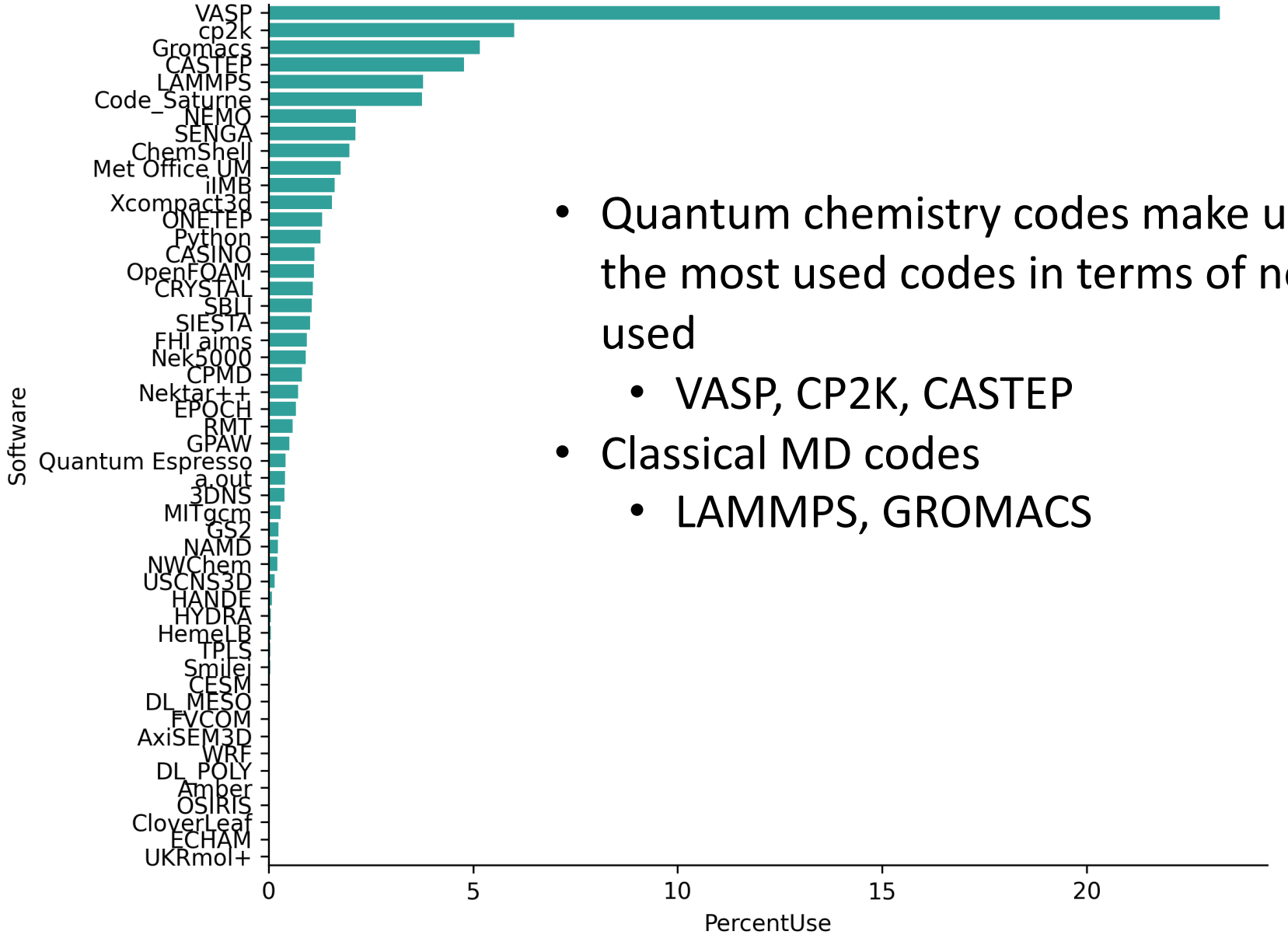
- Using multiple OpenMP threads per process
  - Less processes (or tasks) than 128
- Need to ensure `tasks-per-process` x threads = 128
  - Fully occupied nodes
  - Threads not greater than 16 (size of NUMA region on ARCHER2)
- `cpus-per-task` should equal `OMP_NUM_THREADS`
- 1, 2, 4, 8, 16 good values for threads on ARCHER2

```
#!/bin/bash

# Slurm job options (job-name, compute nodes, job time)
#SBATCH --job-name=Example_MPI_Job
#SBATCH --time=0:20:0
#SBATCH --nodes=4
#SBATCH --tasks-per-node=8
#SBATCH --cpus-per-task=16

# Replace [budget code] below with your project code (e.g. t01)
#SBATCH --account=[budget code]
#SBATCH --partition=standard
#SBATCH --qos=standard



# Set the number of threads to 16 and specify placement
#   There are 16 OpenMP threads per MPI process
#   We want one thread per physical core
export OMP_NUM_THREADS=16
export OMP_PLACES=cores

# Launch the parallel job
#   Using 32 MPI processes
#   8 MPI processes per node
#   16 OpenMP threads per MPI process
#   Additional srun options to pin one thread per physical core
srun --hint=nomultithread --distribution=block:block ./my_mixed_executable.x
```

ARCHER2 PERFORMANCE INVESTIGATION

MPI+OpenMP performance of ARCHER2 applications

ARCHER2 applications usage – June 2022



- Quantum chemistry codes make up the bulk of the most used codes in terms of node hours used
  - VASP, CP2K, CASTEP
- Classical MD codes
  - LAMMPS, GROMACS

ARCHER2 applications investigated

- Well used applications
- Centrally supported by the ARCHER2 team
- MPI+OpenMP enabled
- Different test cases for each application for different scales
- Full results: https://github.com/holly-t/ARCHER2_hybrid_benchmarking
- Compare performance of using 1, 2, 4, 8 and 16 threads per MPI process

Applications

- CASTEP - density functional theory software package for electronic structure calculations using plane waves
  - Version 20.11 - GCC version 10.2, Intel MKL 19, Cray-mpich 8.1.4, Cray-fftw 3.3.8.11
  - OpenMP usage – FFTW, linear algebra libraries
- CP2K - quantum chemistry and solid state physics package – mixed plane wave/Gaussian
  - Version 8.1 - GCC version 11.2, Intel MKL 19, Cray-mpich 8.1.9, Cray-fftw 3.3.8.11
  - OpenMP usage - realspace to planewave transfer, collocate and integrate, FFTW, linear algebra libraries, + more
- GROMACS – classical MD of biological systems
  - Version 2021.3 - GCC version 11.2, Cray-mpich 8.1.9
  - OpenMP usage – PME calculations
- LAMMPS – classical MD for materials modelling
  - Jan 2022 version - GCC version 10.2, Cray-mpich 8.1.4, Cray-fftw 3.3.8.11
  - OpenMP usage – pair interactions, FFTW
- Quantum ESPRESSO - electronic-structure calculations with plane waves
  - Version 6.8 - GCC version 11.2, Cray-libsci 21.08.1.2, Cray-mpich 8.1.9, Cray-fftw 3.3.8.11
  - OpenMP usage - space integrals, point function evaluations, 3D FFTW, linear algebra libraries

Application test cases

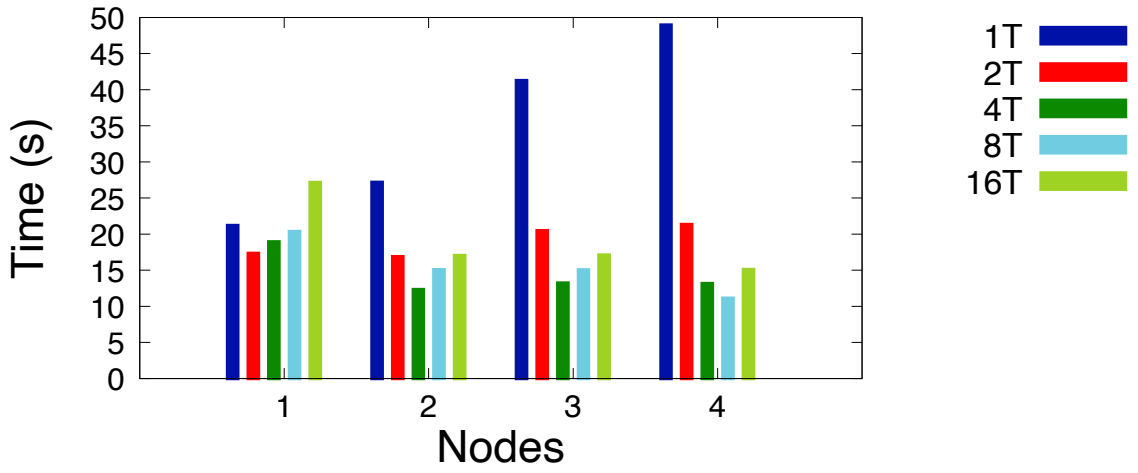
- CASTEP
  - DNA (large memory intensive system)
  - Al3x3 (smaller system)
- CP2K
  - H2O-64 (small water system, LDA)
  - H2O-512 (larger water)
  - LiH-HFX (Hartree Fock exchange, memory intensive)
- GROMACS
  - 1400k and 3000k atom MD simulations
  - BenchPEP – 12m atom MD simulation
- LAMMPS
  - 3000k atom MD simulation
- Quantum ESPRESSO
  - GRIR (scf calculation, 4 k-points)
  - CNT (single k-point, large and memory intensive system)

RESULTS

Application MPI+OpenMP results

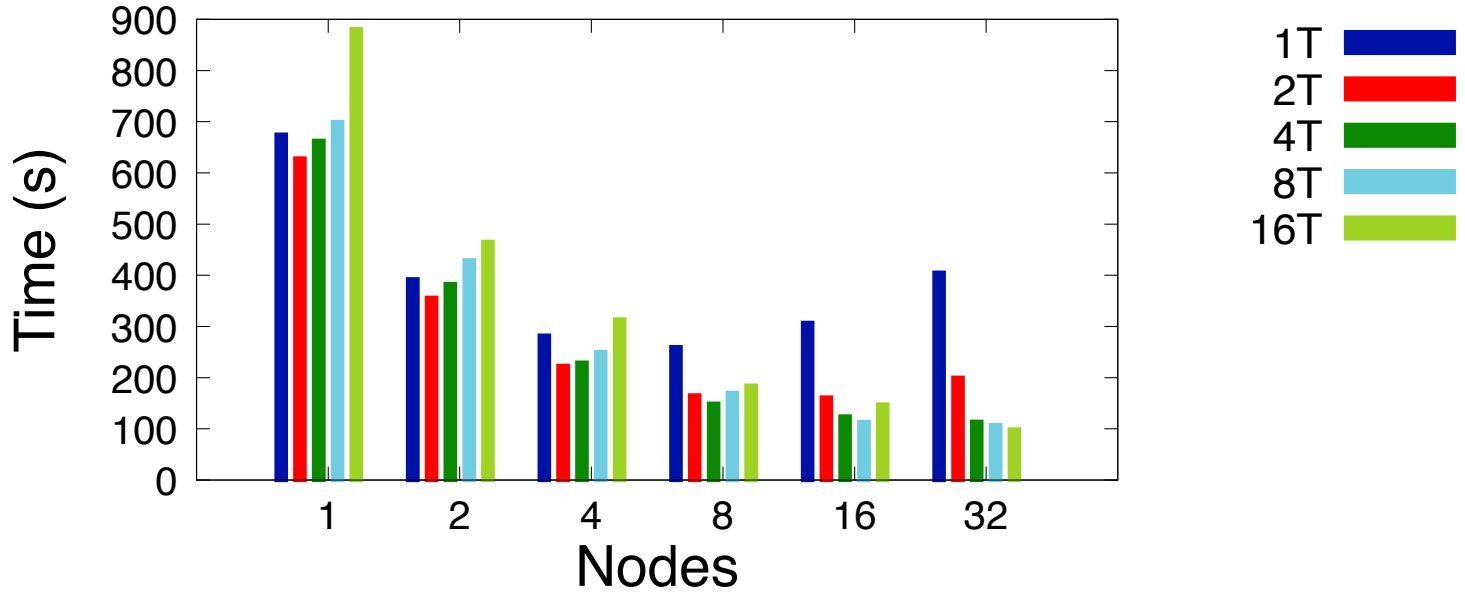
CP2K - H2O-64 benchmark

- Small system that does not scale beyond a couple of nodes
- Clear benefit from using multiple threads per process
- Run time dominated by MPI_Alltoall, which contributes more on multiple nodes
- Using MPI+OpenMP reduces the run time of these communications – message aggregation



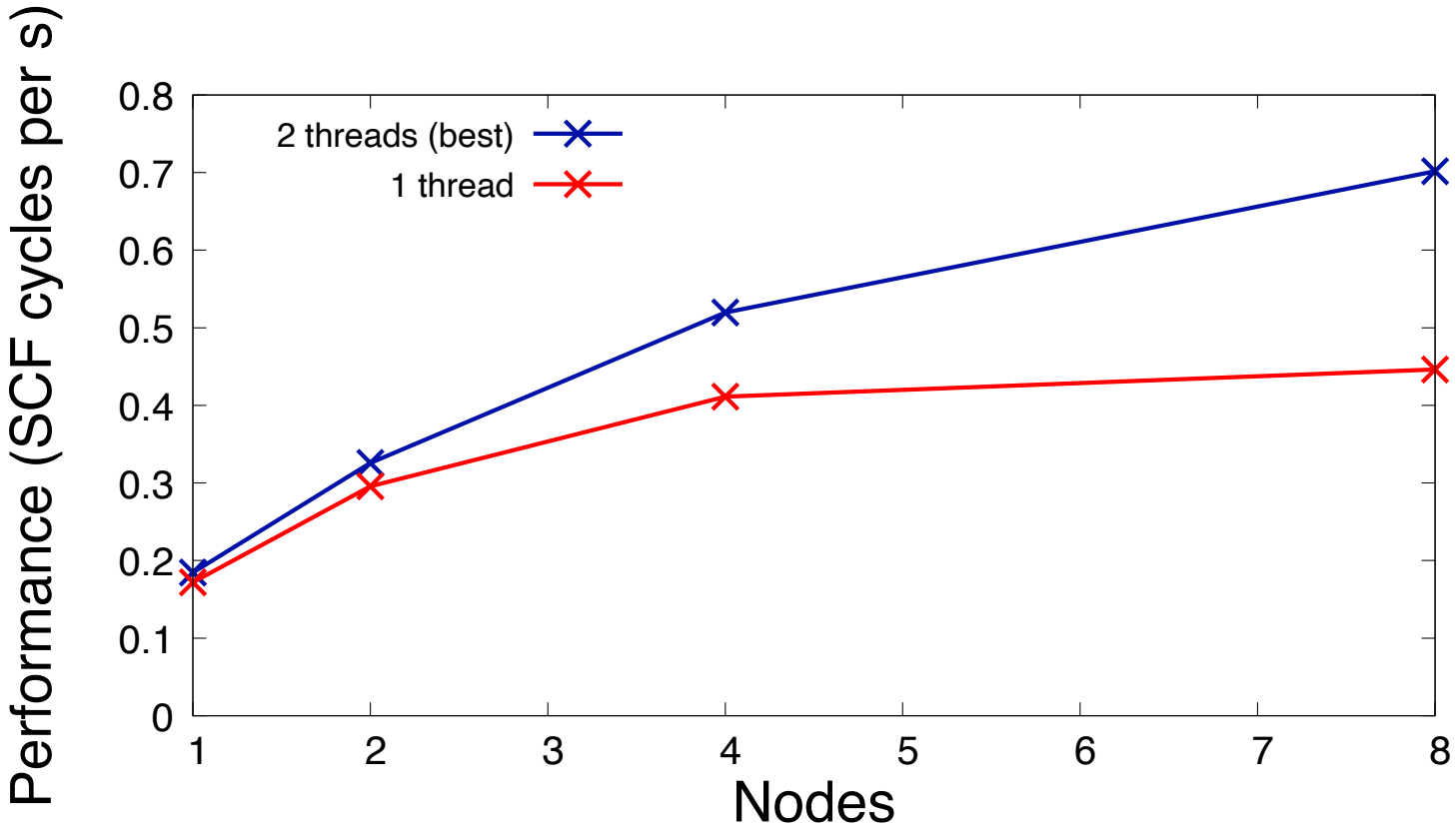
Nodes	mp_alltoall time (s)	
	1 thread	4 threads
1	2.12	1.22
2	10.844	1.599
3	18.918	2.138
4	23.612	3.273

CP2K - H2O-512 benchmark



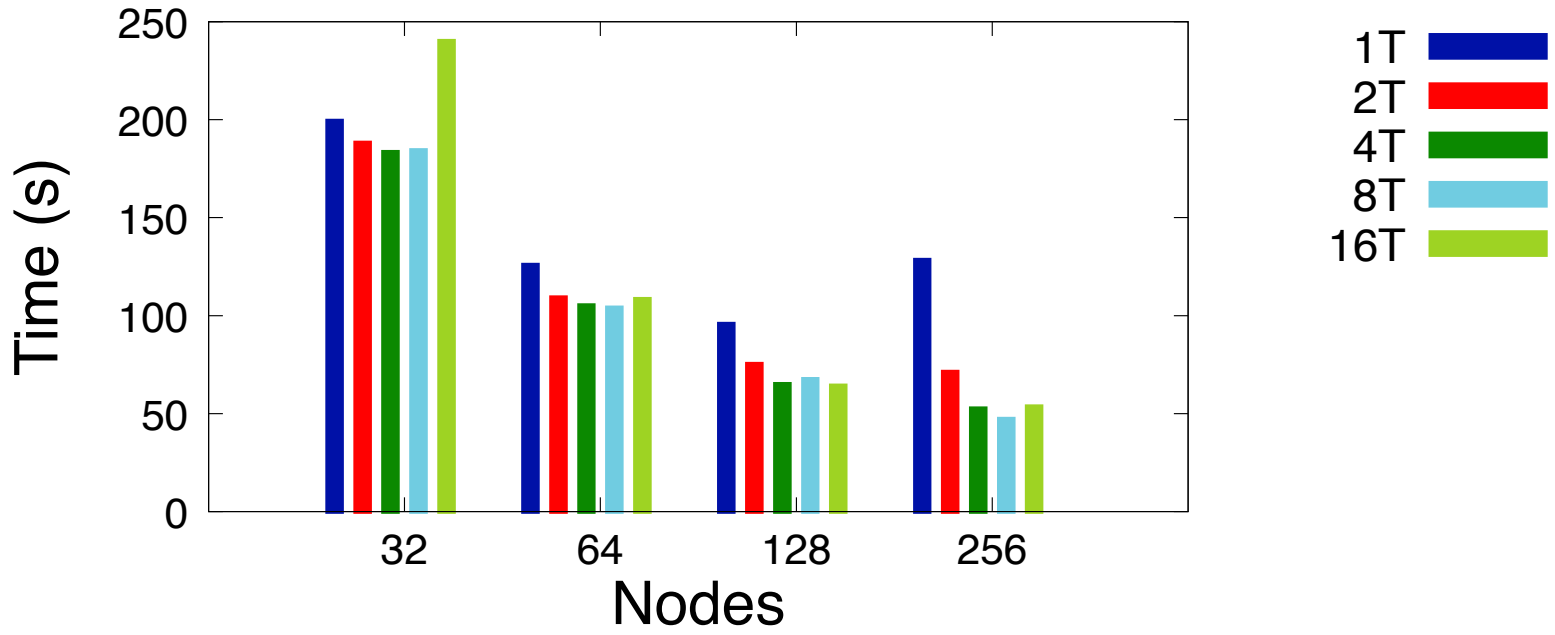
- Larger version of H2O-64 benchmark
- Using multiple threads per process allows for further scaling beyond the single threaded version
- Using 2 or 4 threads per process gives best performance due to reduction in communications overhead

CP2K - H2O-512 benchmark



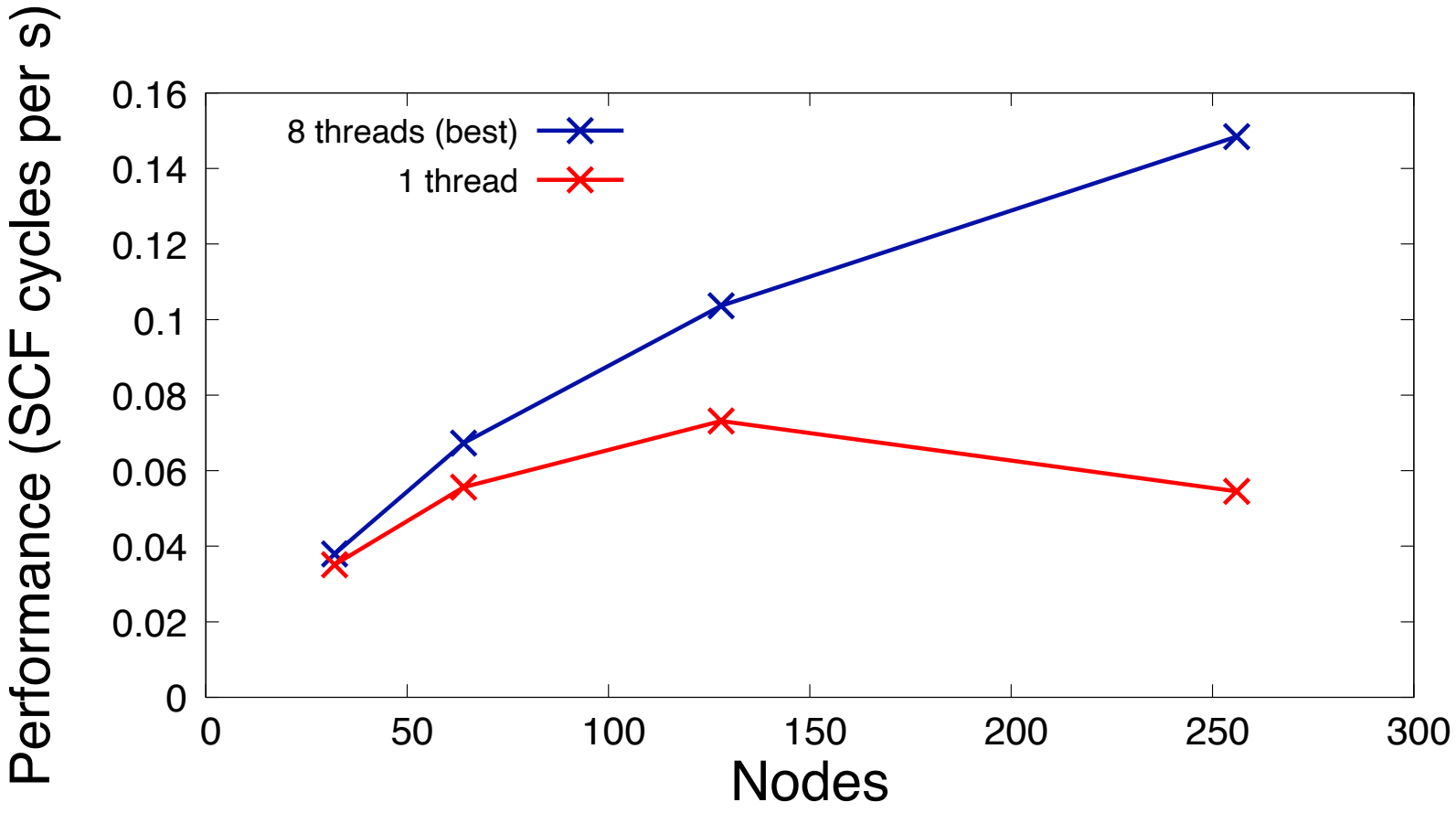
Parallel efficiency	4 nodes
1 thread per process	60%
2 threads per process	70%

CP2K – LiH-HFX benchmark



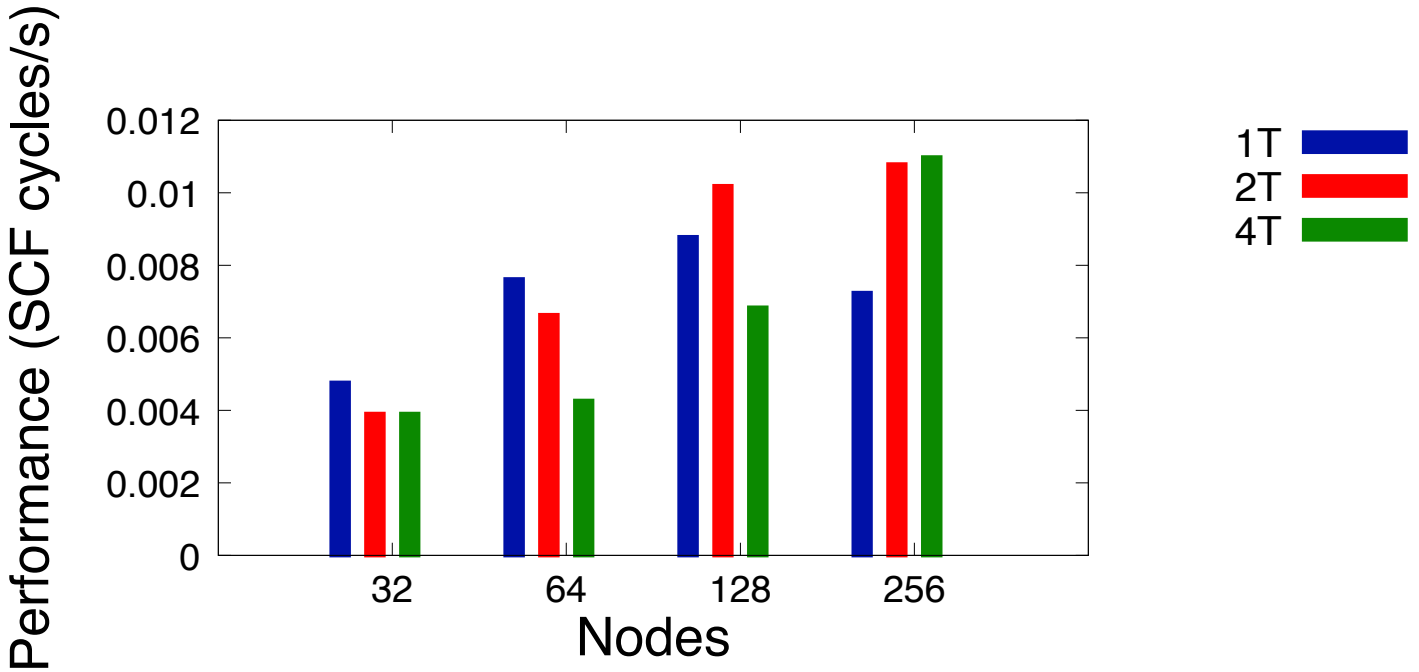
- Hybrid Hartree-Fock exchange calculation which is memory and compute intensive
- 4 or 8 threads per process gives the best performance
- The increase in performance with multiple threads is less significant as this calculation is dominated more by the computation of the integrals rather than comms.

CP2K – LiH-HFX benchmark



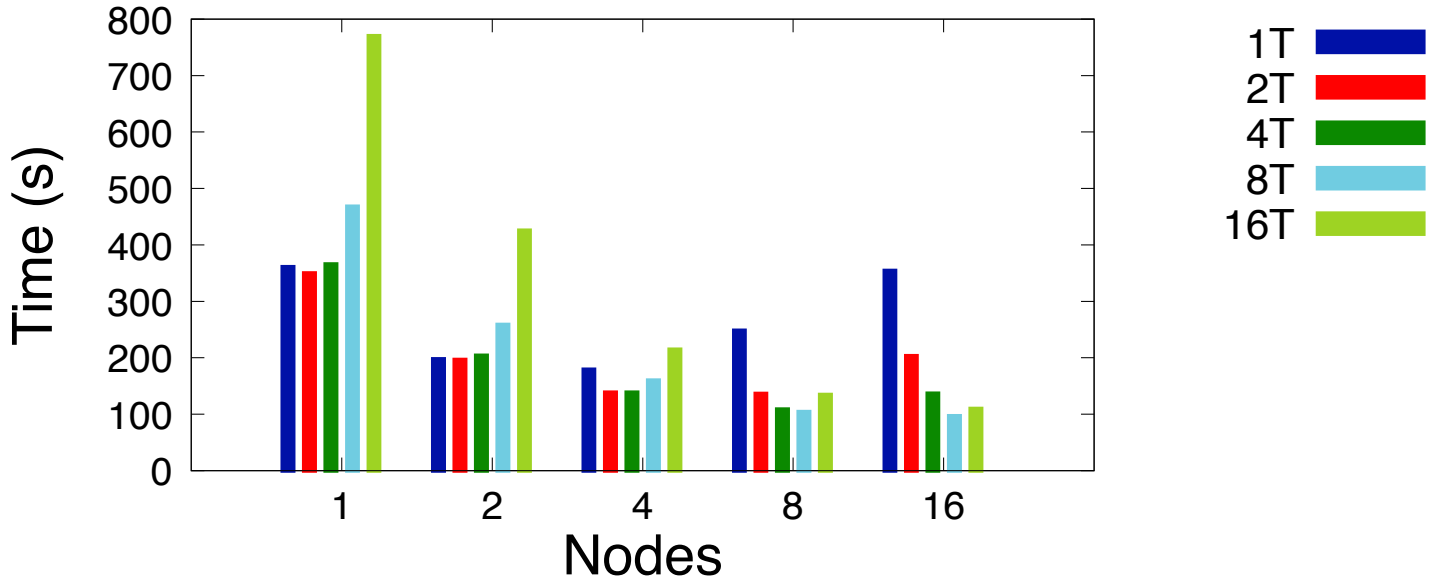
Parallel efficiency	128 nodes	256 nodes
1 thread per process	52%	19%
8 threads per process	68%	49%

CASTEP – DNA benchmark



- Large, memory intensive calculation
- On 32 and 64 nodes using a single thread per process gives the better performance than using multiple threads
- However on 128 and 256 nodes using 2 and 4 threads respectively yields the best performance
- Again MPI collectives dominate in CASTEP

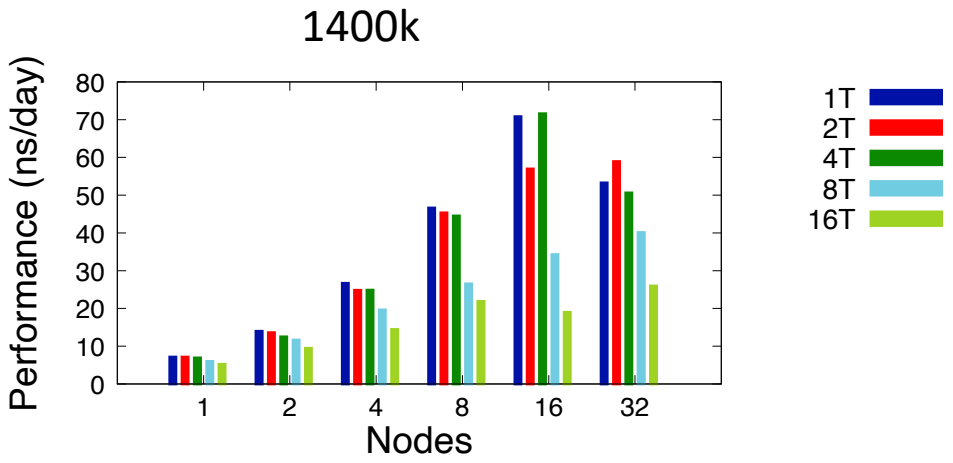
CASTEP – Al3x3 benchmark

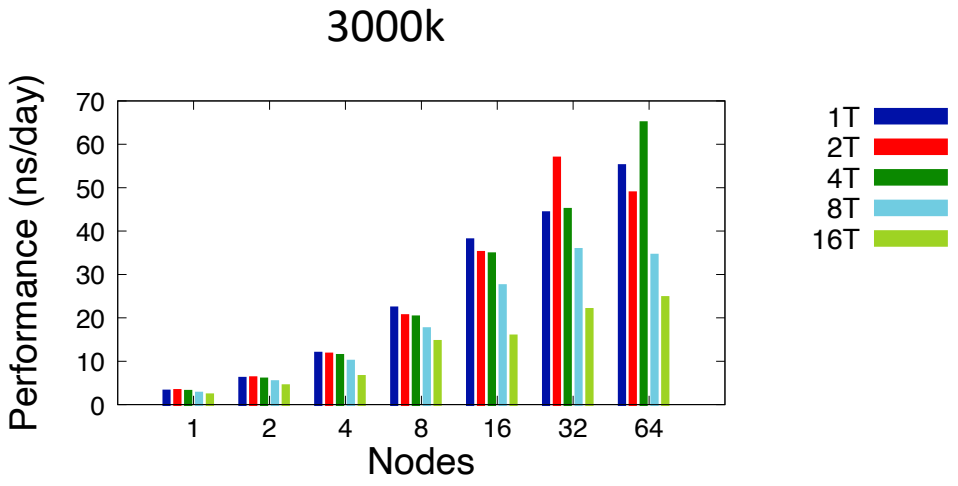


- Smaller system - single point energy calculation
- Using 2 or 4 threads per process gives a performance similar to the single threaded version
- On 4 or more nodes using MPI+OpenMP improves the performance

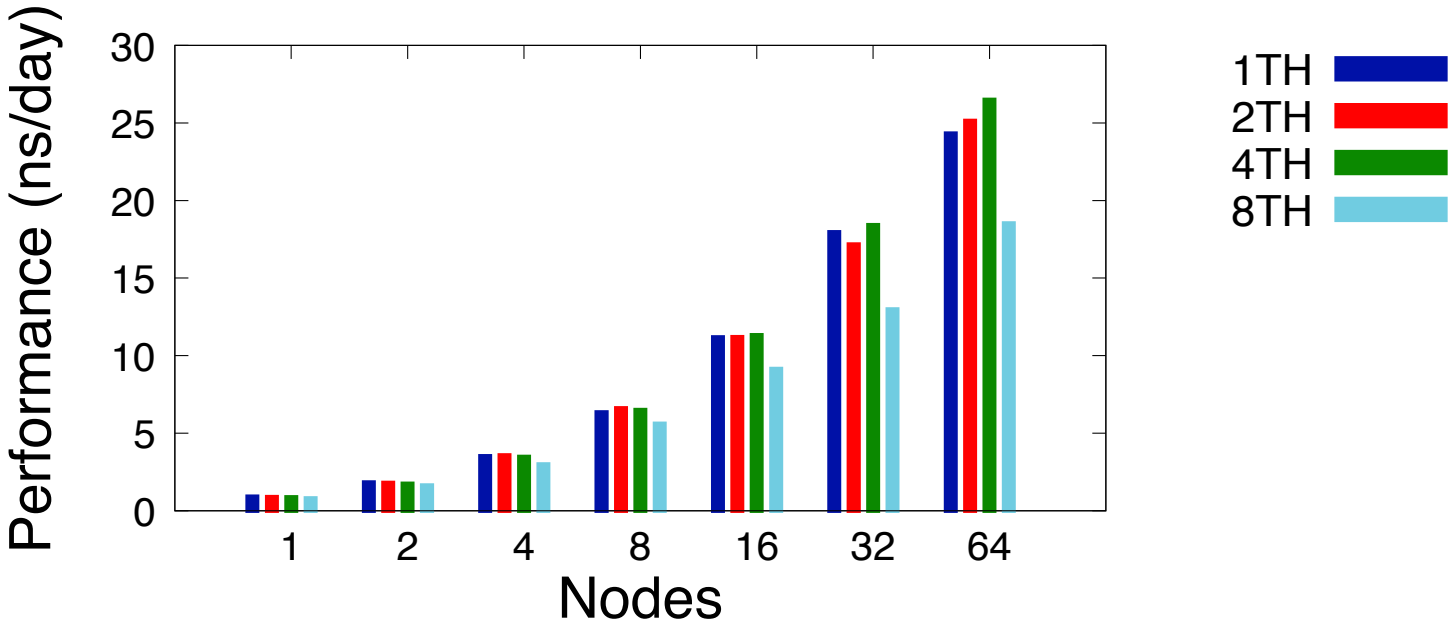
GROMACS – 1400k and 3000k benchmarks

- MD simulations of 1400k and 3000k atoms
- Timing of PME communications become significant at scale
- Using MPI+OpenMP can help reduce the communications cost at the scaling limit
- Performance not great for more than 4 threads
  - Sharing memory beyond the L3 cache



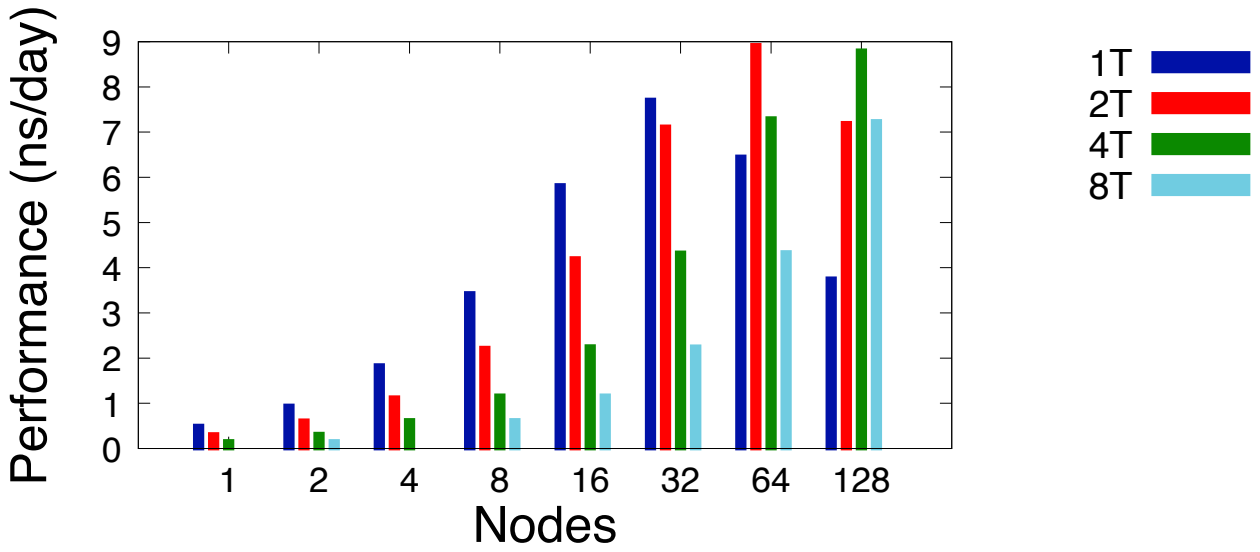


GROMACS – benchPEP benchmark



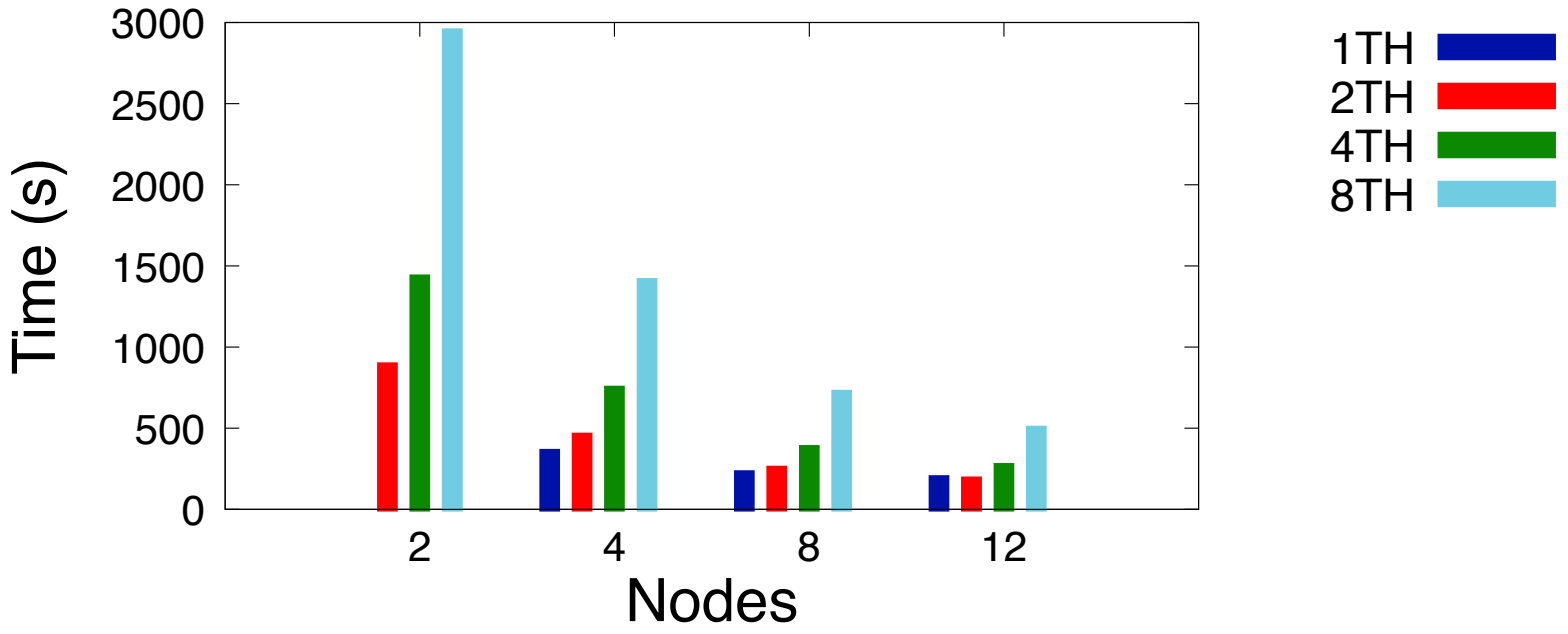
- 12 million atom MD calculation
- For 1 – 16 nodes there is not much performance difference for 1-4 threads
- On 32 and 64 nodes 4 threads per process yields best performance
  - Again with more than 4 threads the performance suffers due to cache effects

LAMMPS – 3000k atom benchmark



- Using a single thread gives the best performance up to 32 nodes.
- Only on 64 and 128 nodes does using MPI+OpenMP improve the performance
- Main overhead on many nodes is writing to file (for checkpointing in LAMMPS) which is poor on many processes – a known issue under investigation
- The performance of this improves with MPI+OpenMP as there are less processes writing to disk

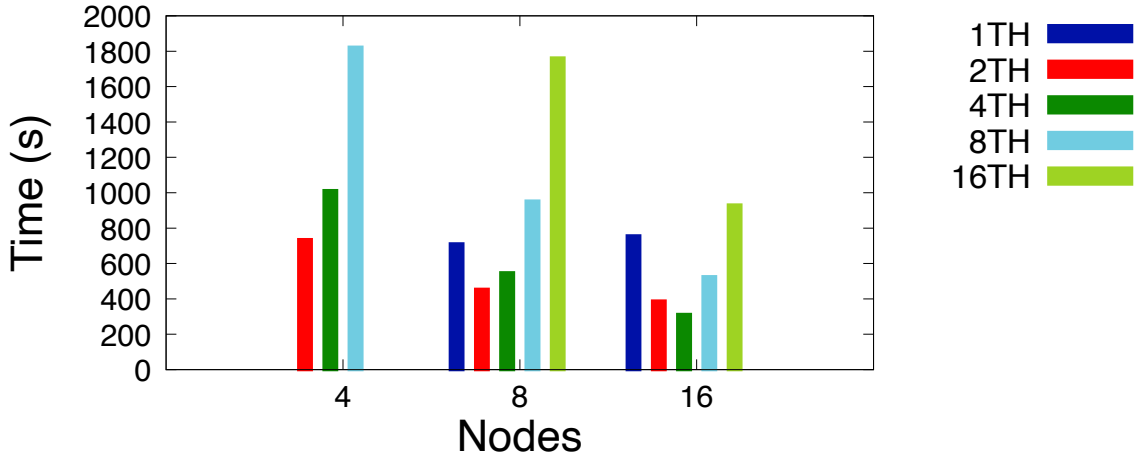
Quantum ESPRESSO – GRIR benchmark



- On 1 node this calculation fails with an out of memory error
- On 2 nodes this fails with OOM on a single thread – not enough memory per process
- Using MPI+OpenMP does not benefit the performance of this calculation – even at the limit of scaling

Quantum ESPRESSO – CNT benchmark

- This test case has very high memory requirements
- Using MPI+OpenMP can prevent OOM errors
- MPI+OpenMP also increases the memory per process, which improves the performance for this system on 8 and 16 nodes
- Underpopulation alone also improves the performance



Threads × PPN	Run time (s)
1 × 128	708
1 × 64	467
2 × 64	454

Test case run time on 8 nodes

Summary

- Quantum chemistry codes CP2K and CASTEP are able to benefit from using MPI+OpenMP in general
  - The run time of these codes are dominated by MPI collective calls
  - MPI+OpenMP reduces the communication overhead
- MPI+OpenMP is useful for Quantum ESPRESSO as it allows more memory per process
  - Calculations can be memory intensive and may require underpopulation to run
- The classical MD codes GROMACS and LAMMPS generally do not benefit much from MPI+OpenMP
  - It can improve the performance, but only at the scaling limit

BENEFITING FROM MPI+OpenMP

How can users benefit?

- Check if your application is MPI+OpenMP enabled
- Performance
  - Applications and test cases where MPI collective communications dominate the run time may benefit from MPI+OpenMP
  - The overhead of MPI communications is reduced as there are less messages between processes
  - At the scaling limit performance can be improved
- Out of memory errors
  - If you have a memory intensive calculation which runs out of memory
  - Requires underpopulation of processes on the node (task-per-node=64)
  - MPI+OpenMP allows more memory per process similar to underpopulation
  - But, using threads as well may give a performance benefit

Using MPI+OpenMP for your application

- Test different values of threads per process for your particular test case to see the effect on the performance
  - 1, 2, 4, 8, 16 threads per process on ARCHER2
  - Usually, 2 or 4 threads
  - Make sure the placement is correct and the processes and threads fully populate the node
- Value for best performance likely to vary depending on:
  - Application
  - Particular problem
  - Number of nodes/cores used
- If underpopulating for memory reasons, then try using multiple threads
  - E.g. 2 threads for half population (64 tasks)

Conclusions

- On ARCHER2 applications can benefit from using MPI+OpenMP
  - Performance benefits – applications which are communications heavy benefit from MPI+OpenMP, particularly on more nodes
  - Aggregation of messages
  - Using 2 or 4 threads per process
- MPI+OpenMP can also help with memory requirements
  - Particularly important in memory limited applications
- MPI+OpenMP might be less useful for classical MD codes
- Overall using MPI+OpenMP on ARCHER2 can be of significant benefit to users – but this is dependent on many factors