Efficient use of MPI+OpenMP on a Cray EX supercomputer

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Introduction

- ARCHER2 is a Cray EX machine based at the University of Edinburgh, UK
  - UK national supercomputing service
  - 5,860 nodes (750,080 cores)
- Consider use of MPI+OpenMP to take 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?
- What information can we get to users for using MPI+OpenMP?

Outline

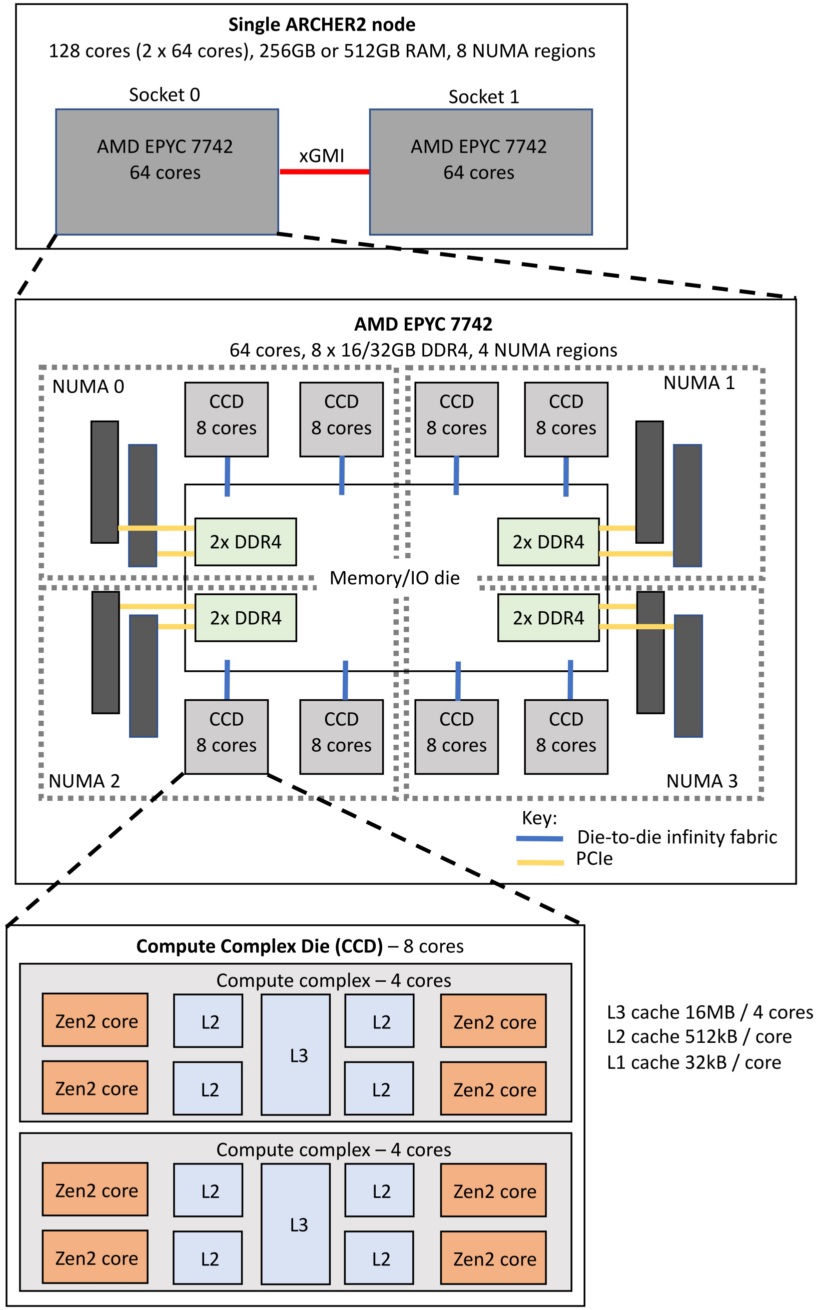
- ARCHER2 overview
- Applications
    - Usage on ARCHER2
    - Applications investigated
    - Application test cases
- Results
- User system benefiting from MPI+OpenMP

ARCHER2

- UK national service used for scientific research
- Supported by the ARCHER2 CSE team
- Runs a range of core applications for different research areas
- 5,860 nodes (750,080 cores)
- 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
- Sensible thread choices of 1, 2, 4, 8, 16



Single ARCHER2 node
128 cores (2 x 64 cores), 256GB or 512GB RAM, 8 NUMA regions

Socket 0: AMD EPYC 7742, 64 cores

xGMI

Socket 1: AMD EPYC 7742, 64 cores

AMD EPYC 7742
64 cores, 8 x 16/32GB DDR4, 4 NUMA regions

Key:
Die-to-die infinity fabric
PCIe

Compute Complex Die (CCD) – 8 cores

Compute complex – 4 cores

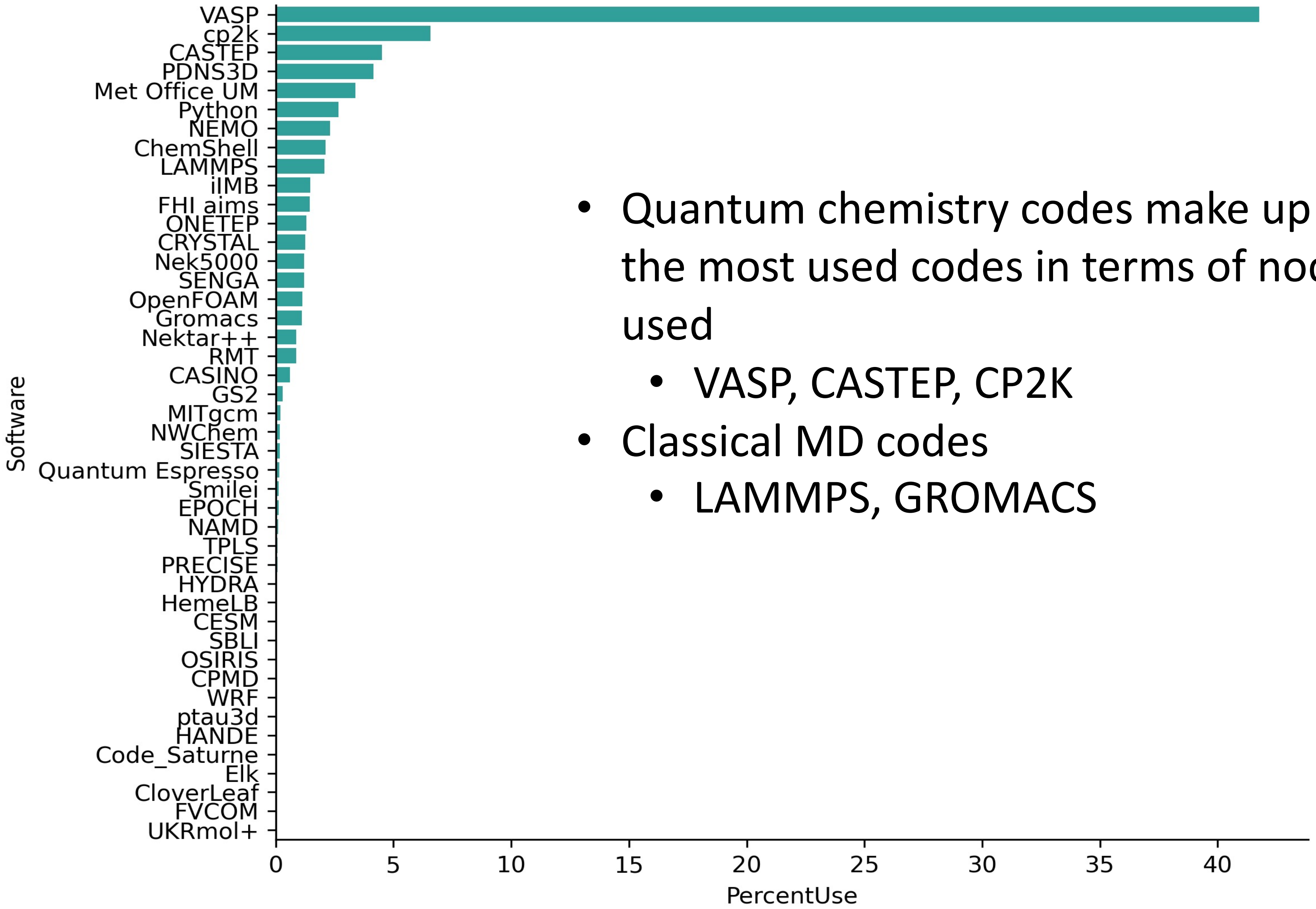
Compute complex – 4 cores

L3 cache 16MB / 4 cores
L2 cache 512kB / core
L1 cache 32kB / core

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 also affect the MPI communication performance
- Using less processes with multiple threads per process (MPI+OpenMP) can maybe help here

ARCHER2 applications usage



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

CP2K

LAMMPS

CASTEP

QUANTUMESPRESSO

GROMACS
FAST. FLEXIBLE. FREE.

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 ESPRESSSO - 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

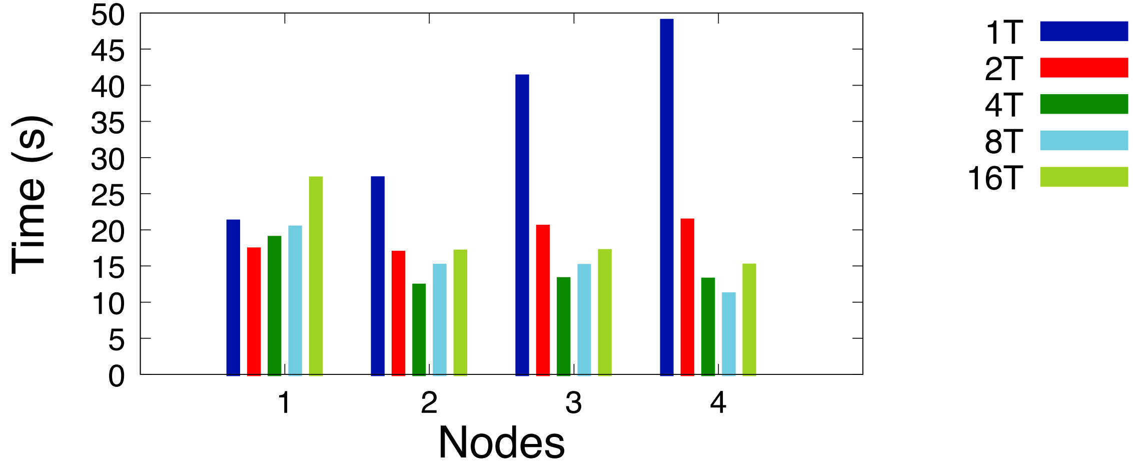
- CASTEP
  - DNA (large memory intensive system)
  - Al3x3 (smaller system)
- CP2K
  - H2O-64 (small water system, LDA)
  - H2O-512 (larger water)
  - LiH-HFX (Hartree Fock exchange, memory intensive)
- GROMACS
  - 1400k and 3000k atom MD simulations
- LAMMPS
  - 3000k atom MD simulation
- Quantum ESPRESSSO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

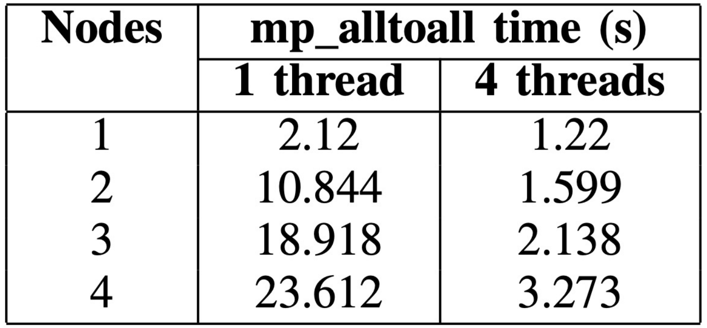
RESULTS

Application benchmark results

CP2K - H2O-64 benchmark

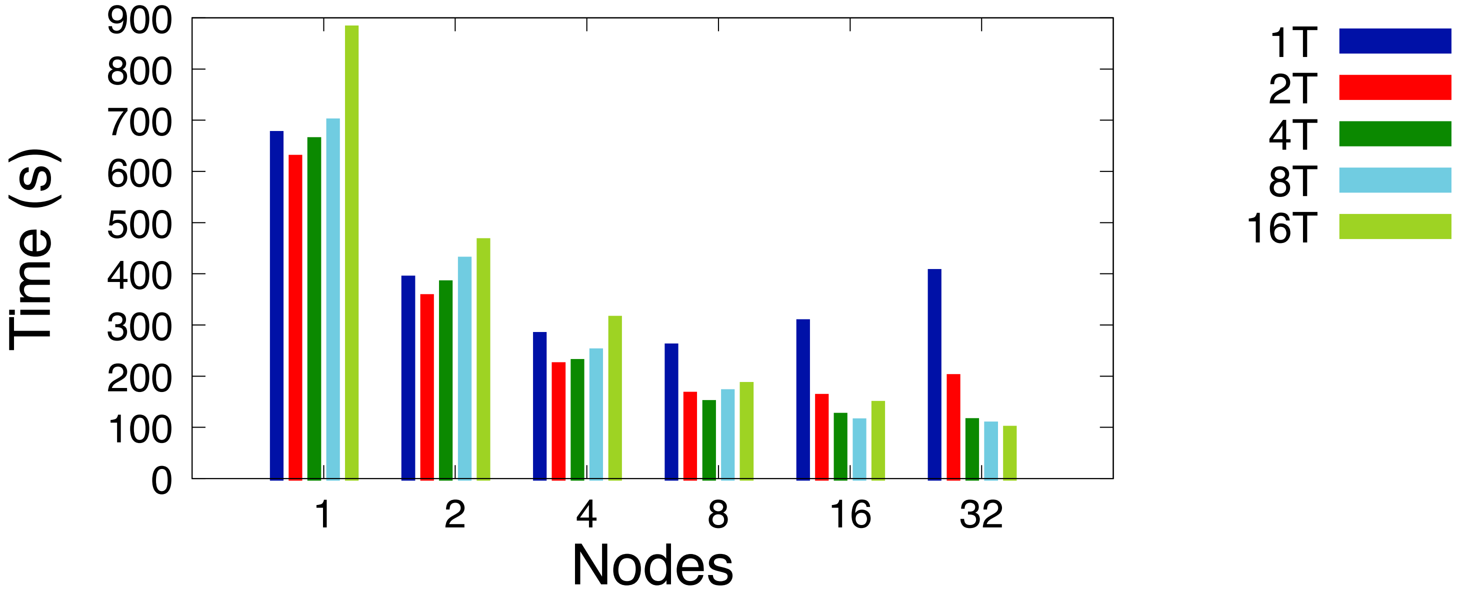
- Small system that does not scale beyond a couple of nodes
- Clear benefit from using multiple threads per process
- Run time dominated by MPI_Alltoall, which contributes more on multiple nodes
- Using MPI+OpenMP reduces the run time of these communications – message aggregation





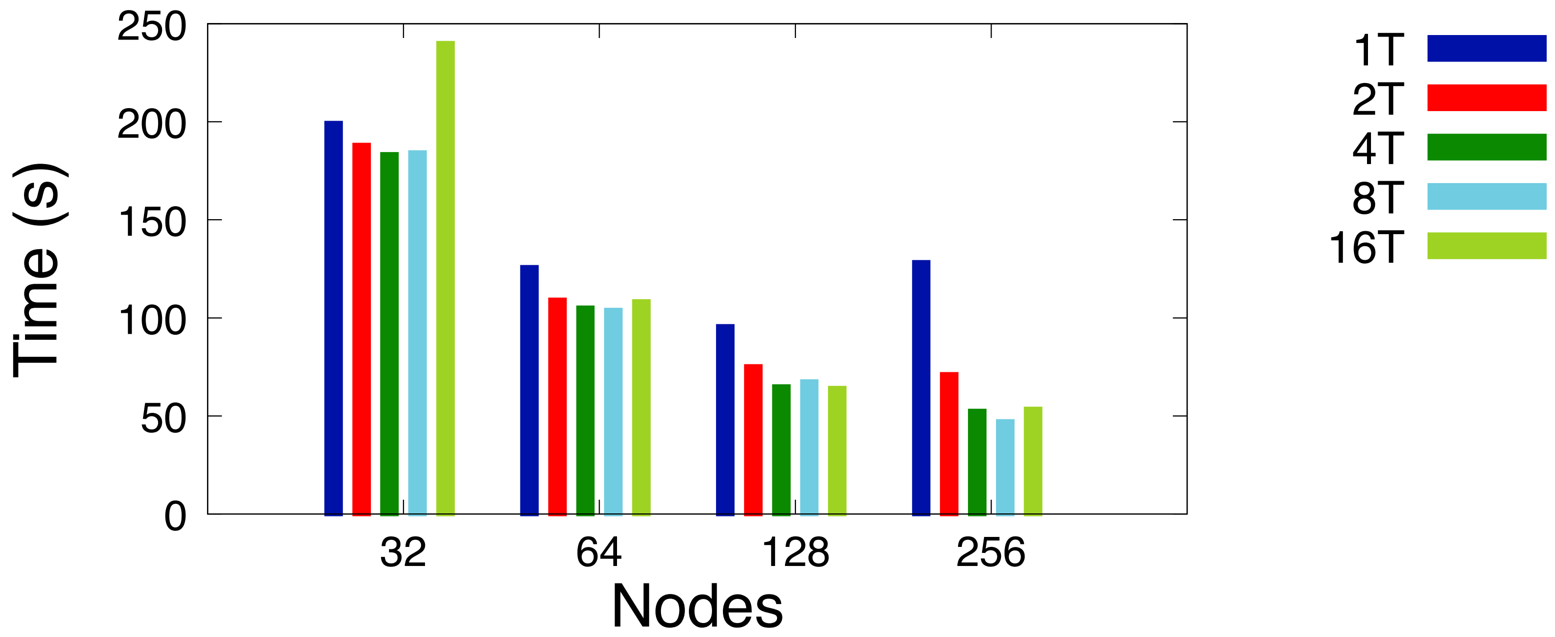
Nodes	mp_alltoall time (s)	
	1 thread	4 threads
1	2.12	1.22
2	10.844	1.599
3	18.918	2.138
4	23.612	3.273

CP2K - H2O-512 benchmark



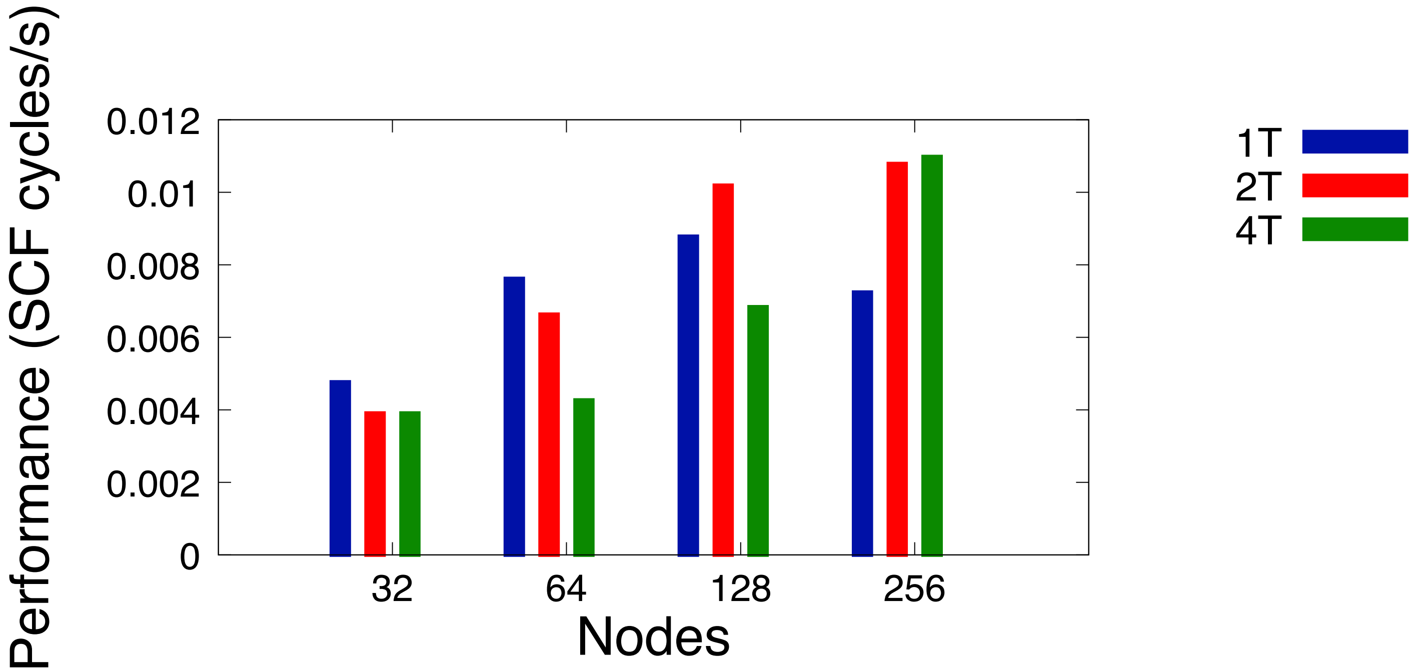
- Larger version of H2O-64 benchmark
- Using multiple threads per process allows for further scaling beyond the single threaded version
- Using 2 or 4 threads per process gives best performance due to reduction in communications overhead

CP2K – LiH-HFX benchmark



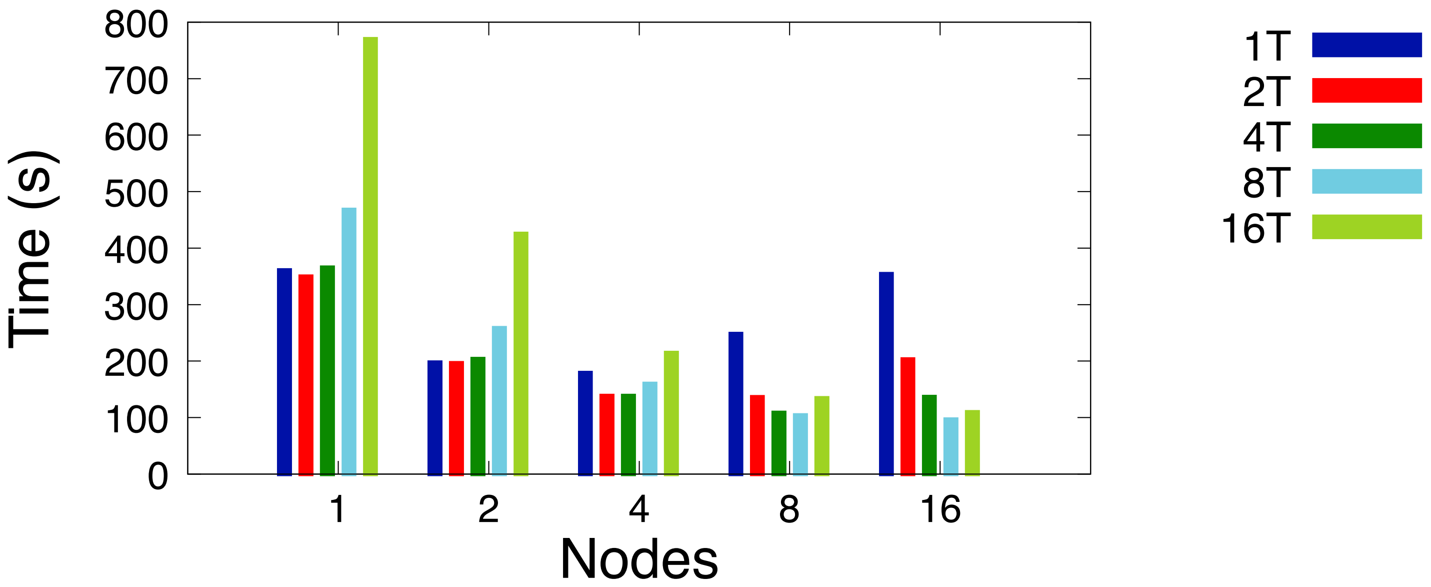
- Hybrid Hartree-Fock exchange calculation which is memory and compute intensive
- 4 or 8 threads per process gives the best performance
- The increase in performance with multiple threads is less significant as this calculation is dominated more by the computation of the integrals rather than comms.

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

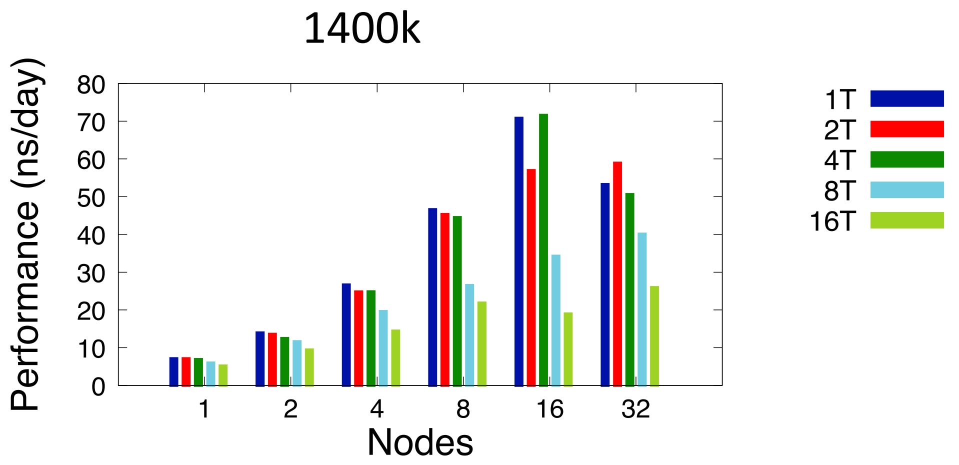
CASTEP – Al3x3 benchmark

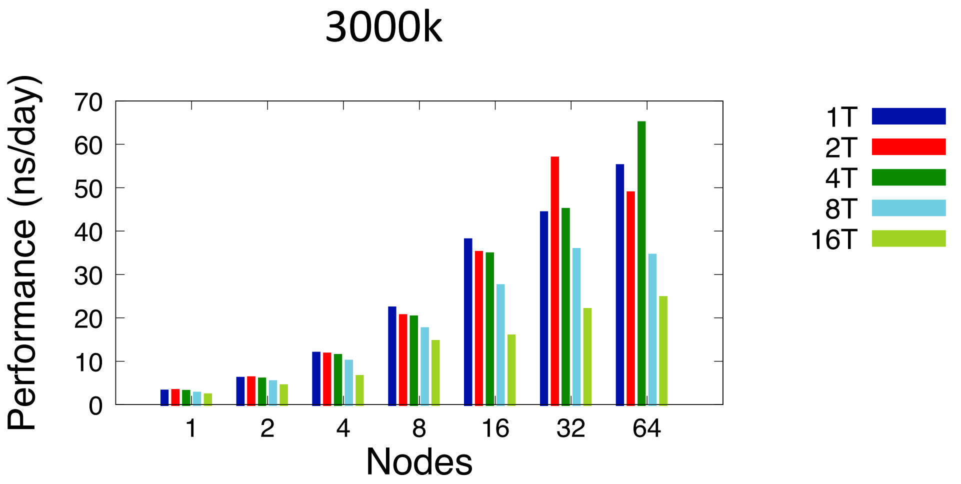


- Smaller system - single point energy calculation
- Using 2 or 4 threads per process gives a performance similar to the single threaded version
- At scale using MPI+OpenMP improves the performance

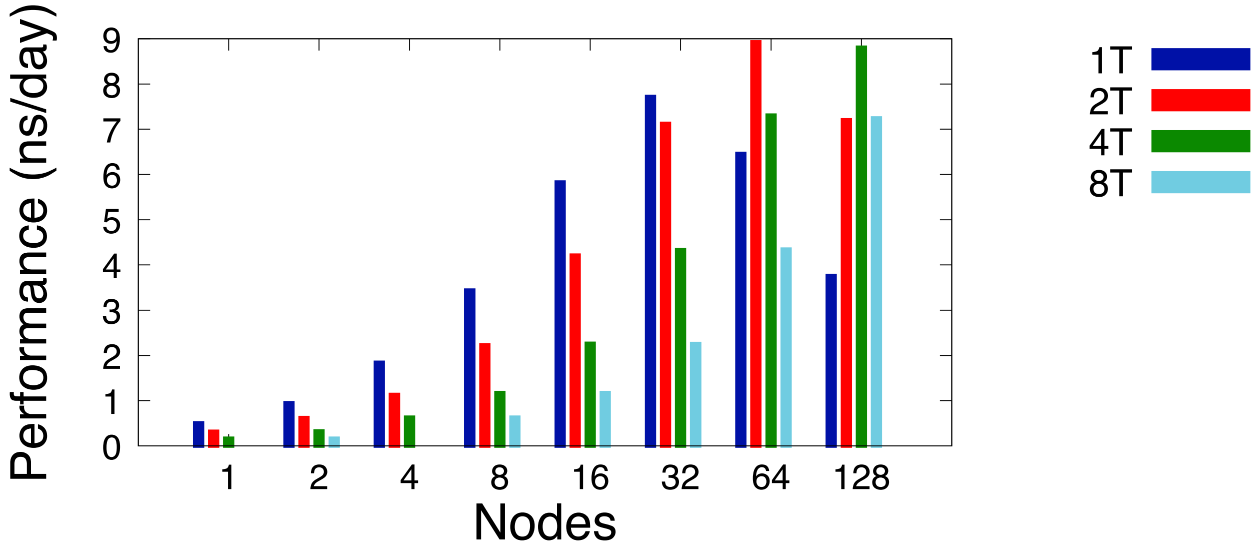
GROMACS – 1400k and 3000k benchmarks

- 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



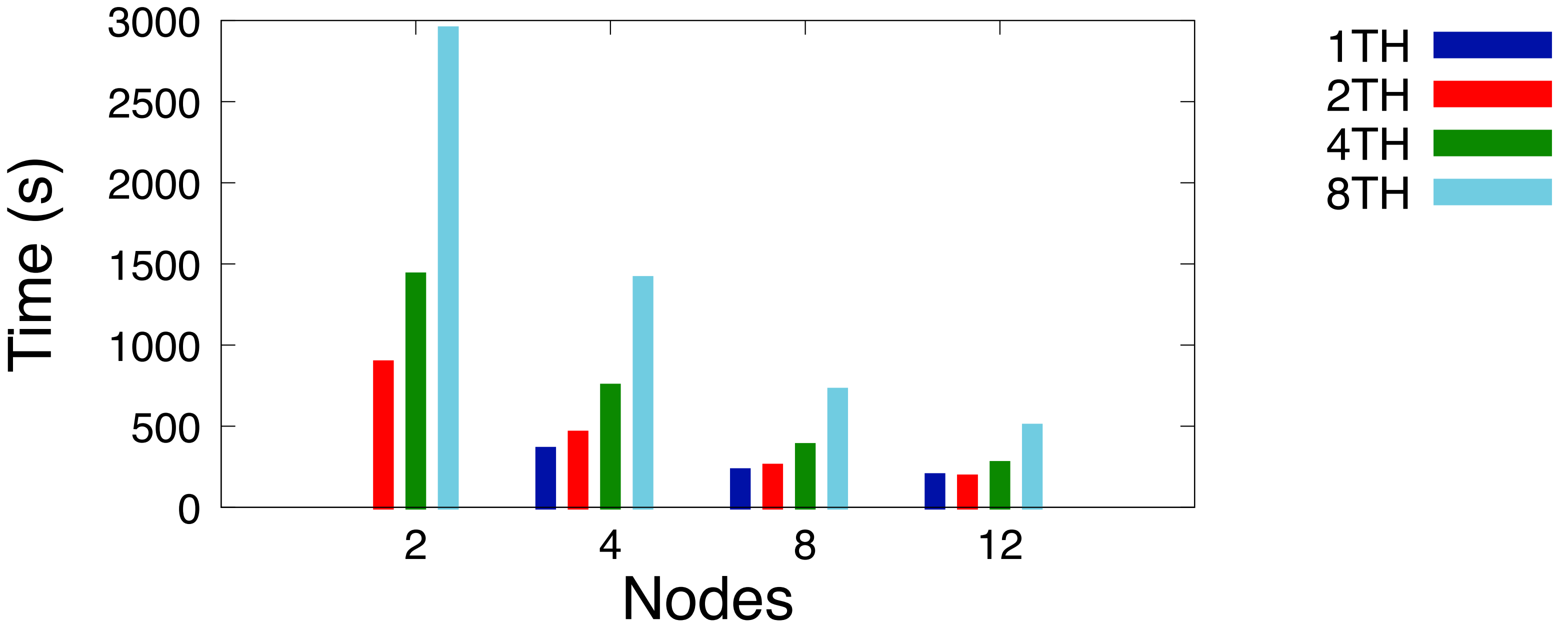


LAMMPS – 3000k atom benchmark



- 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

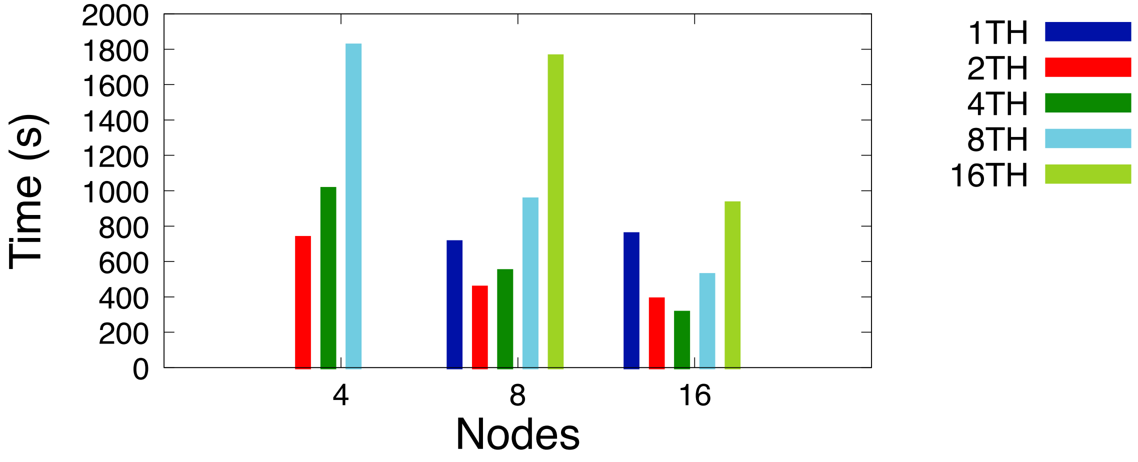
Quantum ESPRESSO – GRIR benchmark

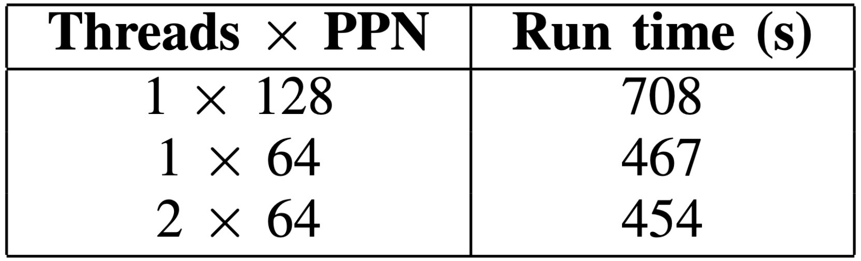


- On 1 node this calculation fails with an out of memory error
- On 2 nodes this fails with OOM on a single thread – not enough memory per process
- Using MPI+OpenMP does not benefit the performance of this calculation – even at the limit of scaling

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

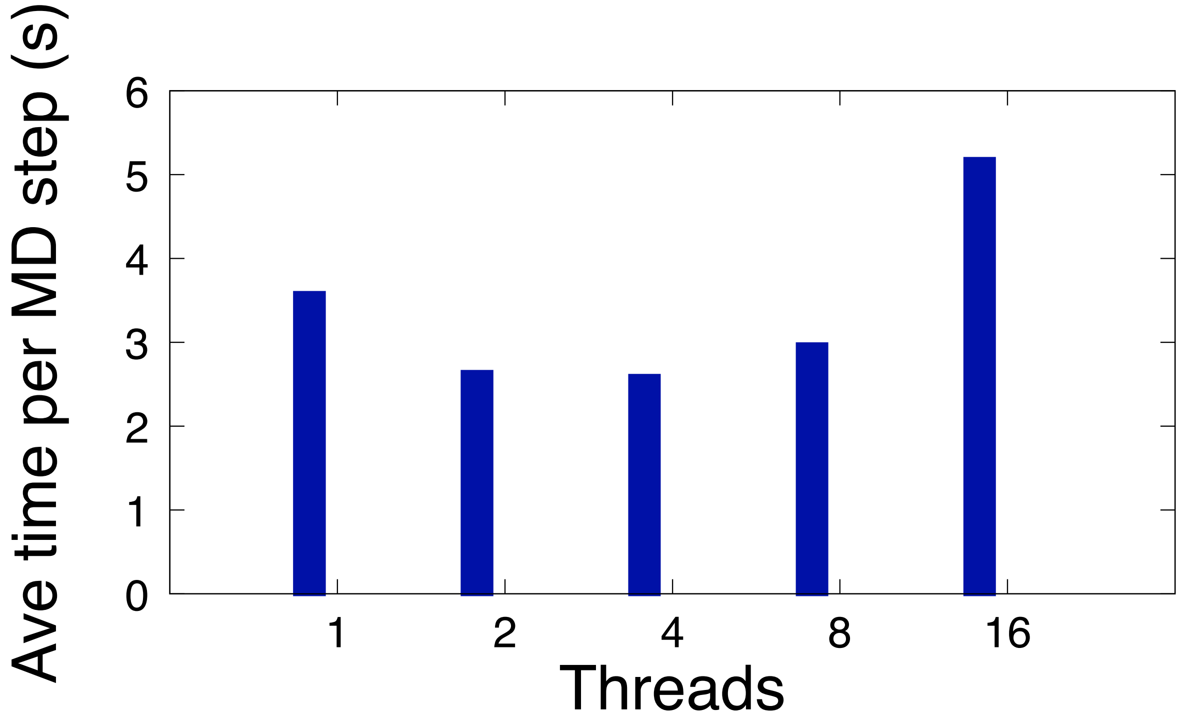
USER EXAMPLE

CP2K calculation

User example system

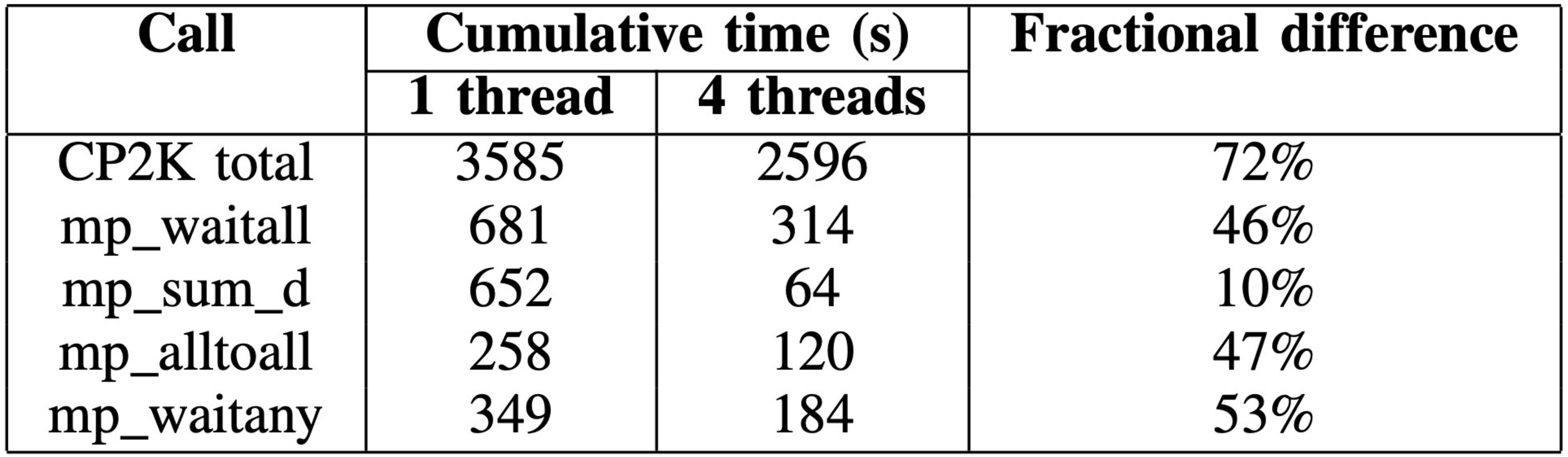
- For CP2K using MPI+OpenMP has been shown to improve the performance of the test cases – but how does this relate to real user simulations?
- This is a real user’s system; a long running molecular dynamics simulation of around 100 water molecules
- Using 4 threads per process was found to greatly increase the performance

User example – average time per MD step on 4 nodes



- Average time per step collected for a 1,000 step MD run
- The time per step on 4 threads is 70% of that of the pure MPI case
- Makes a big difference to run time and resources consumed

User example – MPI communications



Call	Cumulative time (s)		Fractional difference
	1 thread	4 threads	
CP2K total	3585	2596	72%
mp_waitall	681	314	46%
mp_sum_d	652	64	10%
mp_alltoall	258	120	47%
mp_waitany	349	184	53%

- Large reductions in the cumulative time taken for MPI calls
- Adds up to a significant reduction in the total run time

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 is less useful for classical MD codes
- Overall using MPI+OpenMP on ARCHER2 can be of significant benefit to users – but this is dependent on the application