CP2K PARALLELISATION AND OPTIMISATION

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Overview

- Overview of Parallel Programming models
  - Shared Memory
  - Distributed Memory

- CP2K Algorithms and Data Structures

- Parallel Performance

- CP2K Timing Report

Parallel Programming Models

- Why do we need parallelism at all?
- Parallel programming is (even) harder than sequential programming
- Single processors are reaching limitations
  - Clock rate stalled at ~2.5 GHz (due to heat)
  - Full benefits of vectorisation (SIMD) can be hard to realise
  - Chip vendors focused on low-power (for mobile devices)

Parallel Programming Models

- But we need *more* speed!
  - Solve problems faster (strong scaling)
  - Solve bigger problems in same time (weak scaling)
  - Tackle new science that emerges at long runtimes / large system size
  - Enables more accurate force models (HFX, MP2, RPA …)

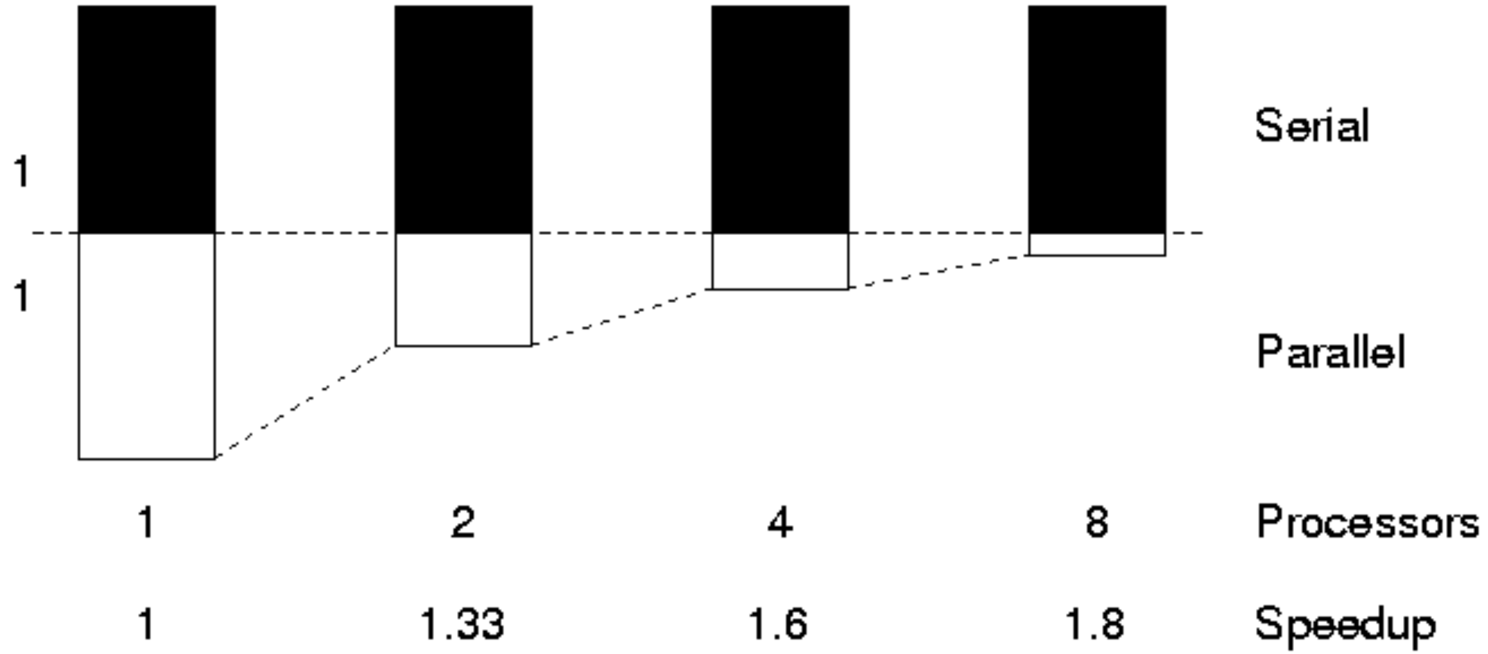
- Need strategies to split up our computation between different processors

- Ideally our program should run P times faster on P processors - but not in practice!
  - Some parts may be inherently serial (Amdahl's Law)
  - Parallelisation *will* introduce overheads e.g. communication, load imbalance, synchronisation…

Parallel Programming Models

"The performance improvement to be gained by parallelisation is limited by the proportion of the code which is serial"

Gene Amdahl, 1967

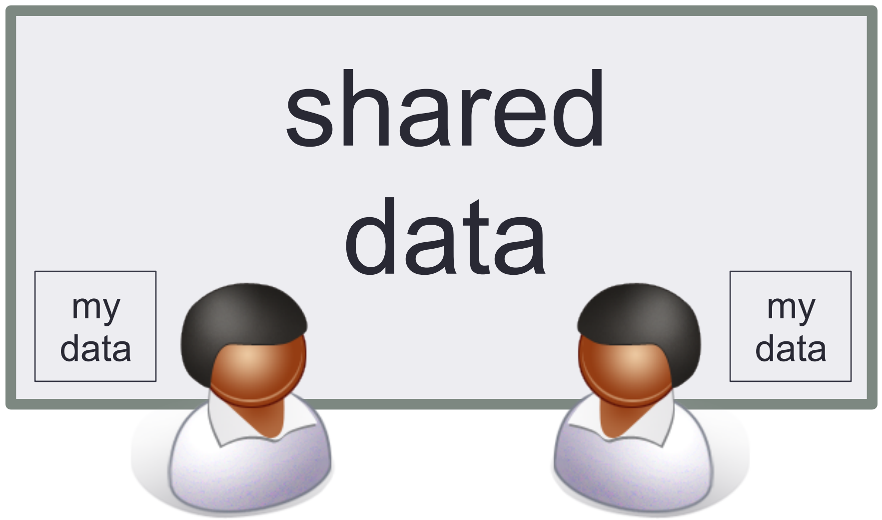


Parallel Programming Models

- Almost all modern CPUs are multi-core
  - 2,4,6… CPU cores, sharing access to a common memory
- This is Shared Memory Parallelism
  - Several processors executing the same program
  - Sharing the same address space i.e. the same variables
  - Each processor runs a single ‘thread’
  - Threads communicate by reading/writing to shared data
- Example programming models include:
  - OpenMP, POSIX threads (pthreads)

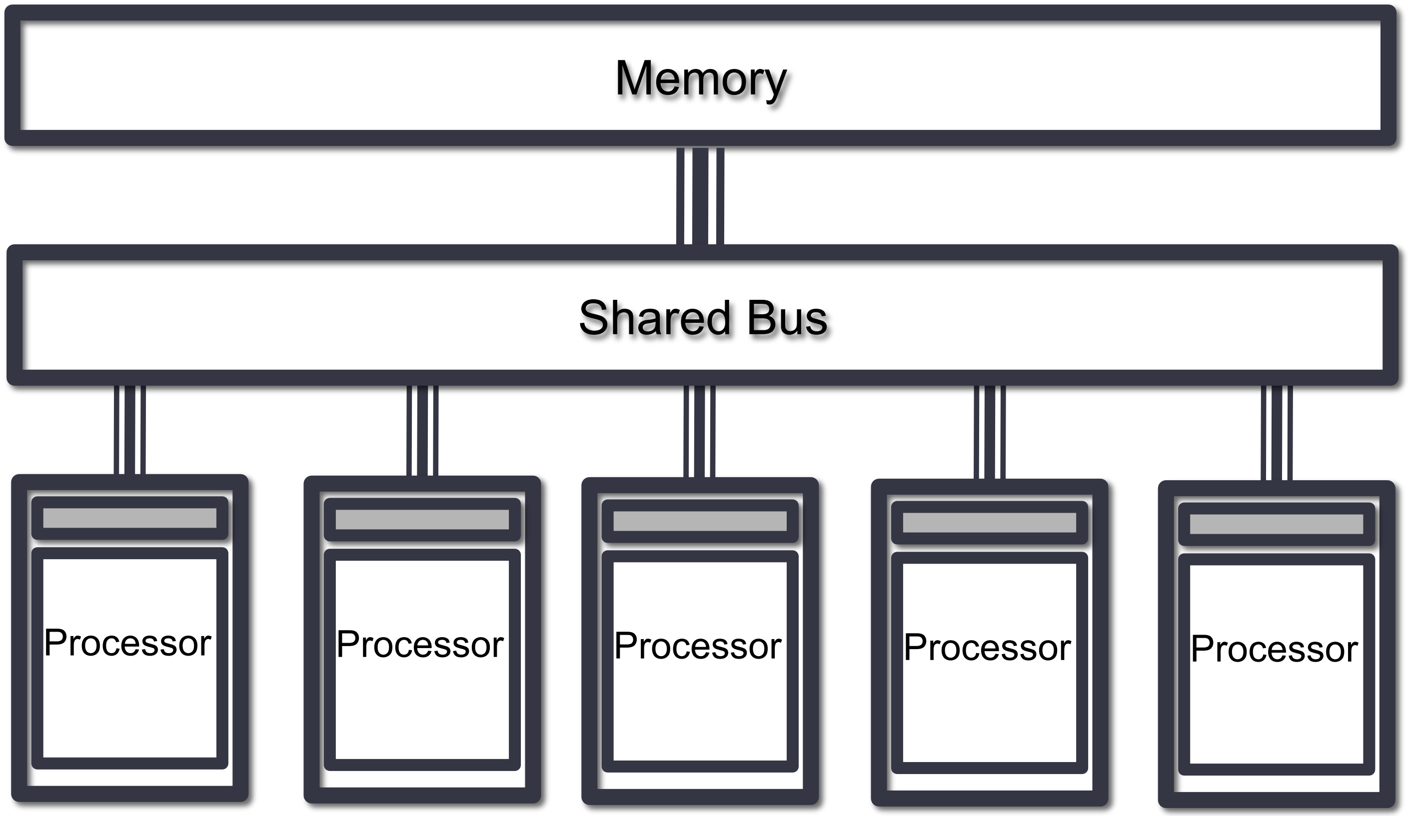
Analogy

- One very large whiteboard in a two-person office
  - the shared memory
- Two people working on the same problem
  - the threads running on different cores attached to the memory
- How do they collaborate?
  - working together
  - but not interfering
- Also need *private* data



Hardware

- Needs support of a shared-memory architecture



Parallel Programming Models

- Most supercomputers are built from 1000s of nodes
  - Each node consists of some CPUs and memory
  - Connected together via a network

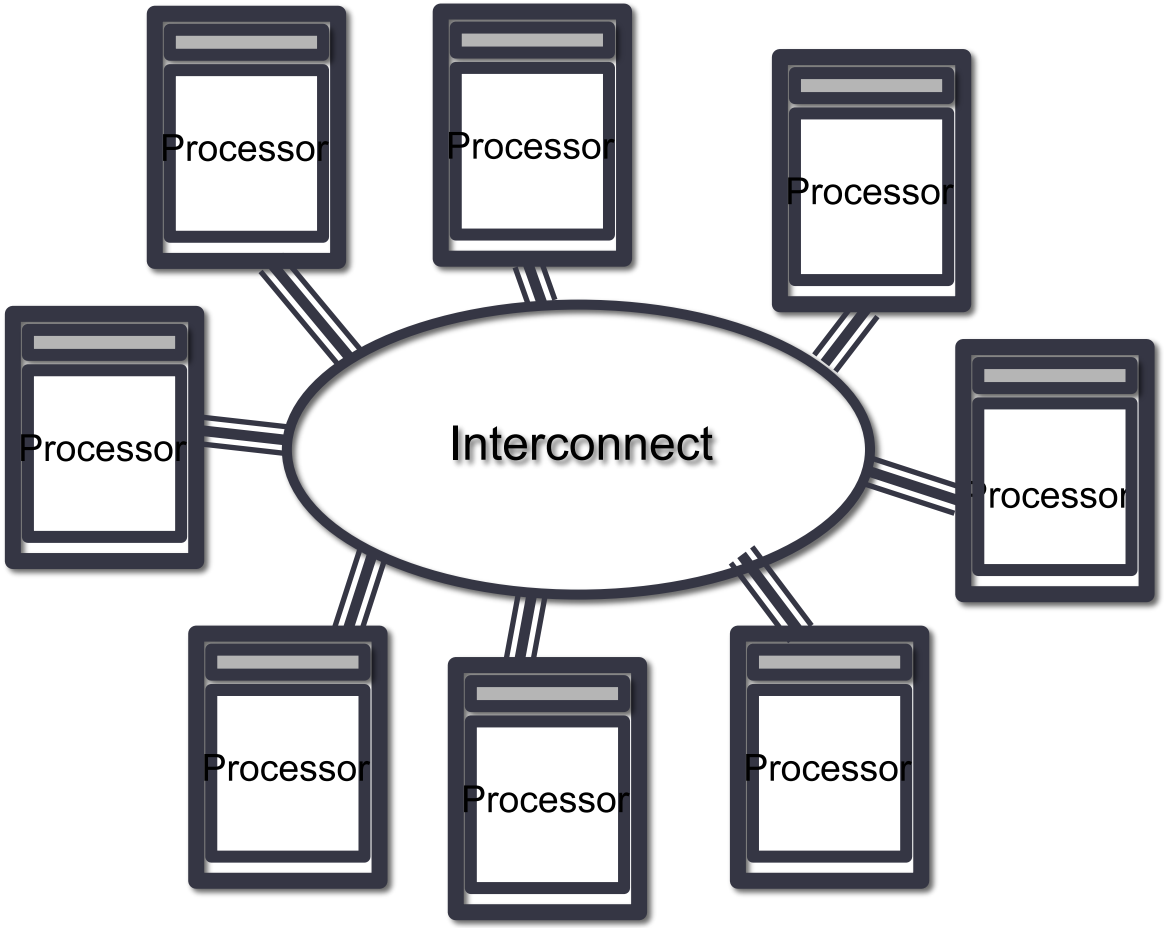
- This is Distributed Memory Parallelism
  - Several processors executing (usually) the same program
  - Each processor has it’s own address space
  - Each processor runs a single ‘process’
  - Threads communicate by passing messages
- Example programming models include:
  - MPI, SHMEM

Analogy

- Two whiteboards in different single-person offices
  - the distributed memory
- Two people working on the same problem
  - the processes on different nodes attached to the interconnect

- How do they collaborate?
  - to work on single problem
- Explicit communication
  - e.g. by telephone
  - no shared data

Hardware



- Natural map to distributed-memory
  - one process per processor-core
  - messages go over the interconnect, between nodes/OS's

Parallel Programming Models

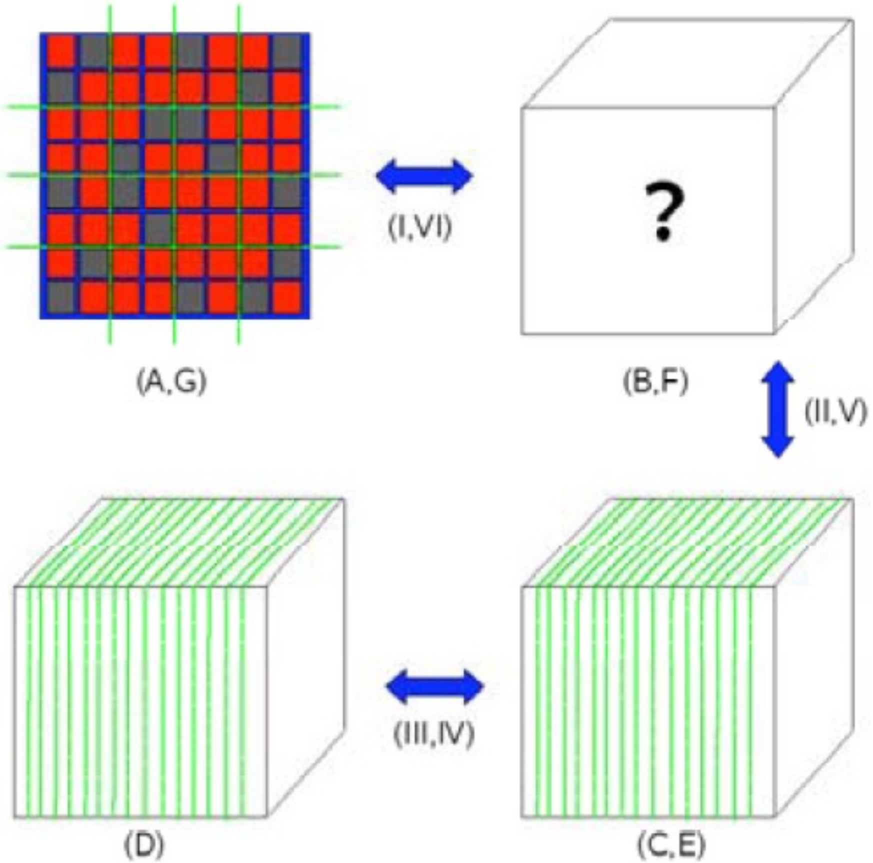
- Support both OpenMP *or* MPI (`ssmp` and `popt`)
  - Use OpenMP for desktop PCs with multi-cores *or*
  - MPI for clusters and supercomputers
  - Maybe also support for Accelerators (GPUs)

- May also combine MPI *and* OpenMP (`psmp`)
  - Called hybrid or mixed-mode parallelism
  - Use shared memory within a node (with several processors)
  - Use message passing between nodes
  - Usually only useful for scaling to 10,000s of cores!

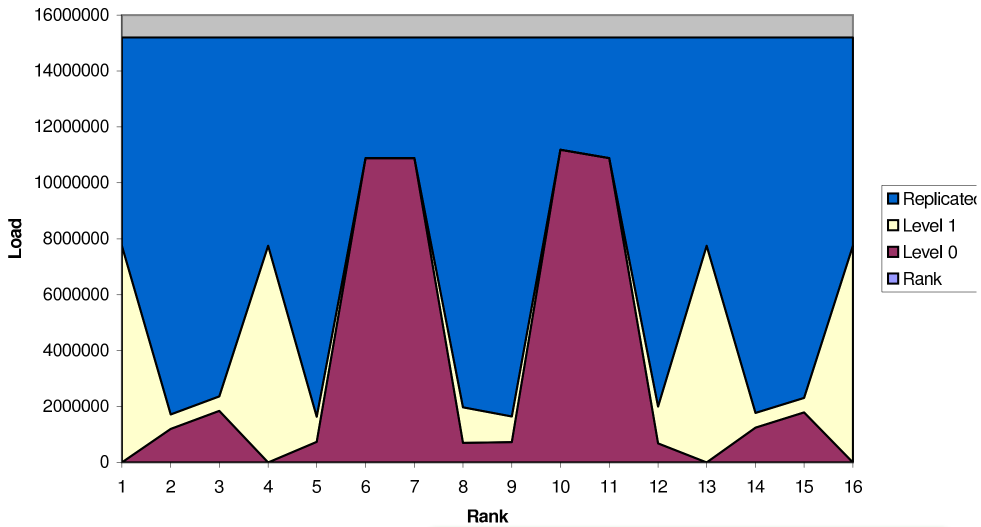
CP2K Algorithms and Data Structures

- (A,G) – distributed matrices
- (B,F) – realspace multigrids
- (C,E) – realspace data on planewave multigrids
- (D) – planewave grids

- (I,VI) – integration/ collocation of gaussian products
- (II,V) – realspace-to-planewave transfer
- (III,IV) – FFTs (planewave transfer)

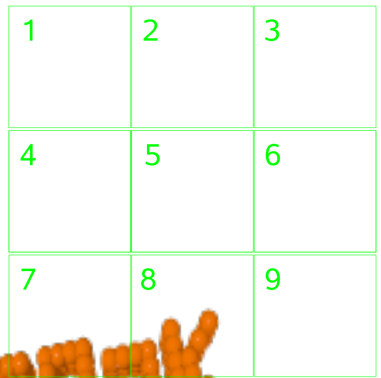


CP2K Algorithms and Data Structures

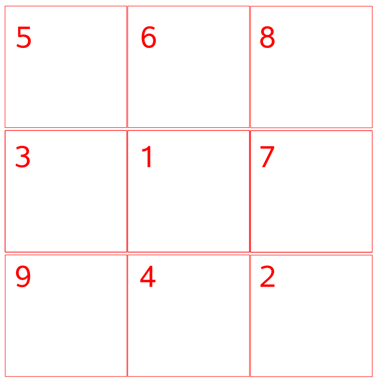


- Distributed realspace grids
  - Overcome memory bottleneck
  - Reduce communication costs
  - Parallel load balancing
    - On a single grid level
    - Re-ordering multiple grid levels
    - Finely balance with replicated tasks

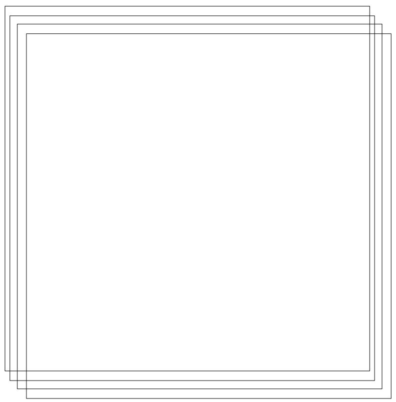
Level 1, fine grid, distributed



Level 2, medium grid, dist



Level 3, coarse grid, replicated



- `libgrid` for optimised collocate/integrate routines
- ~5-10% speedup typical

CP2K Algorithms and Data Structures

- Fast Fourier Transforms
  - 1D or 2D decomposition
  - FFTW3 and CuFFT library interface
  - Cache and re-use data
    - FFTW plans, cartesian communicators

- `GLOBAL%FFTW_PLAN_TYPE MEASURE | PATIENT`
- Up to 5% Speedup possible

- DBCSR
  - Distributed MM based on Cannon's Algorithm
  - Local multiplication recursive, cache oblivious

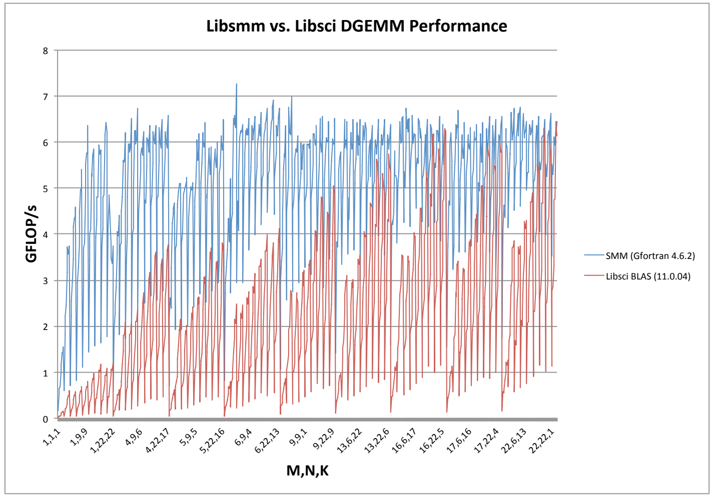
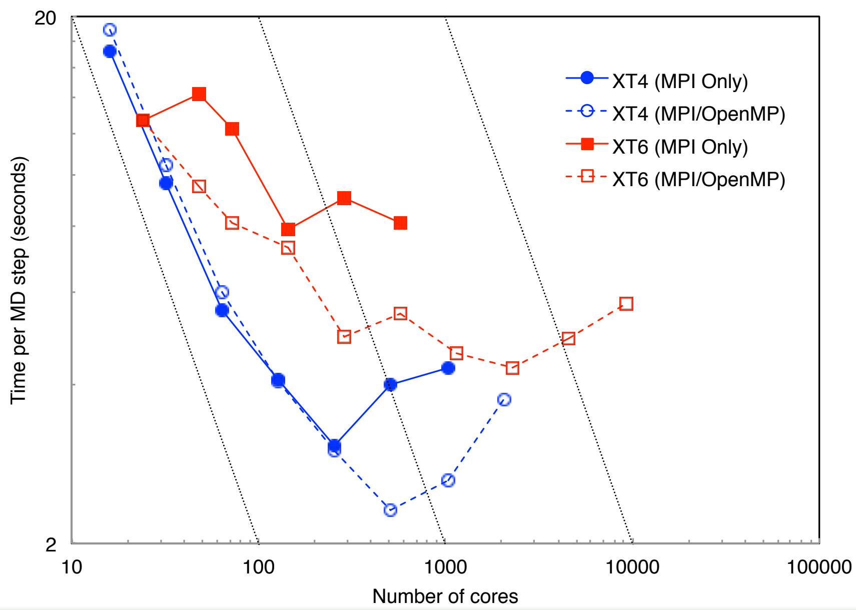


Figure 5: Comparing performance of SMM and Libsci BLAS for block sizes up to 22,22,22

- `libsmm` for small block multiplications

CP2K Algorithms and Data Structures

- OpenMP
  - Now in all key areas of CP2K
  - FFT, DBCSR, Collocate/ Integrate, Buffer Packing
  - Incremental addition over time
    - Usually 2 or 4 threads per process
- Dense Linear Algebra
  - Matrix operations during SCF
  - GEMM - ScaLAPACK
  - SYEVD – ScaLAPACK / ELPA

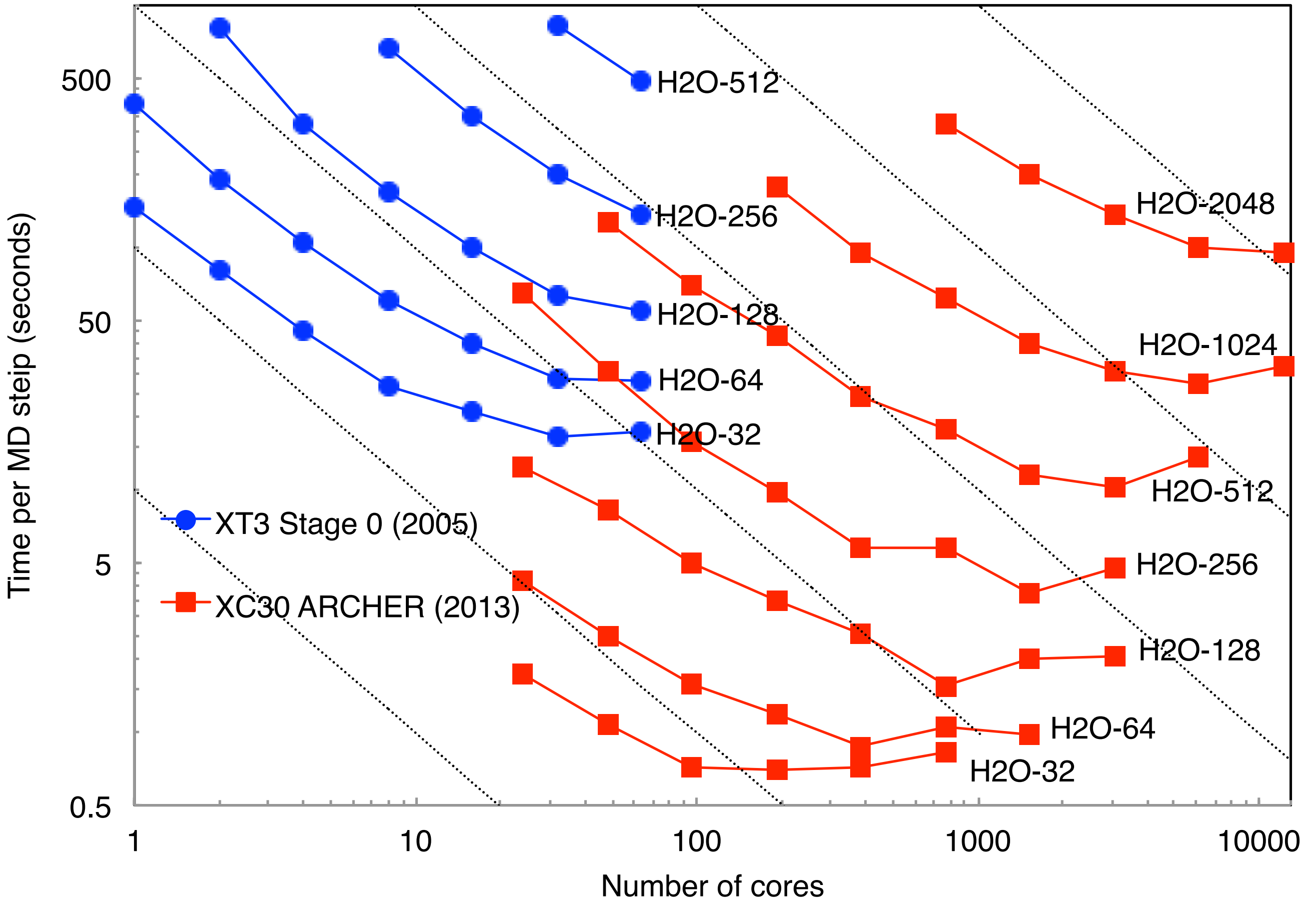


- `-D__ELPA2` and link library to enable
- `GLOBAL%PREFERRED_DIAG_LIBRARY ELPA`
- Up to ~5x Speedup for large, metallic systems

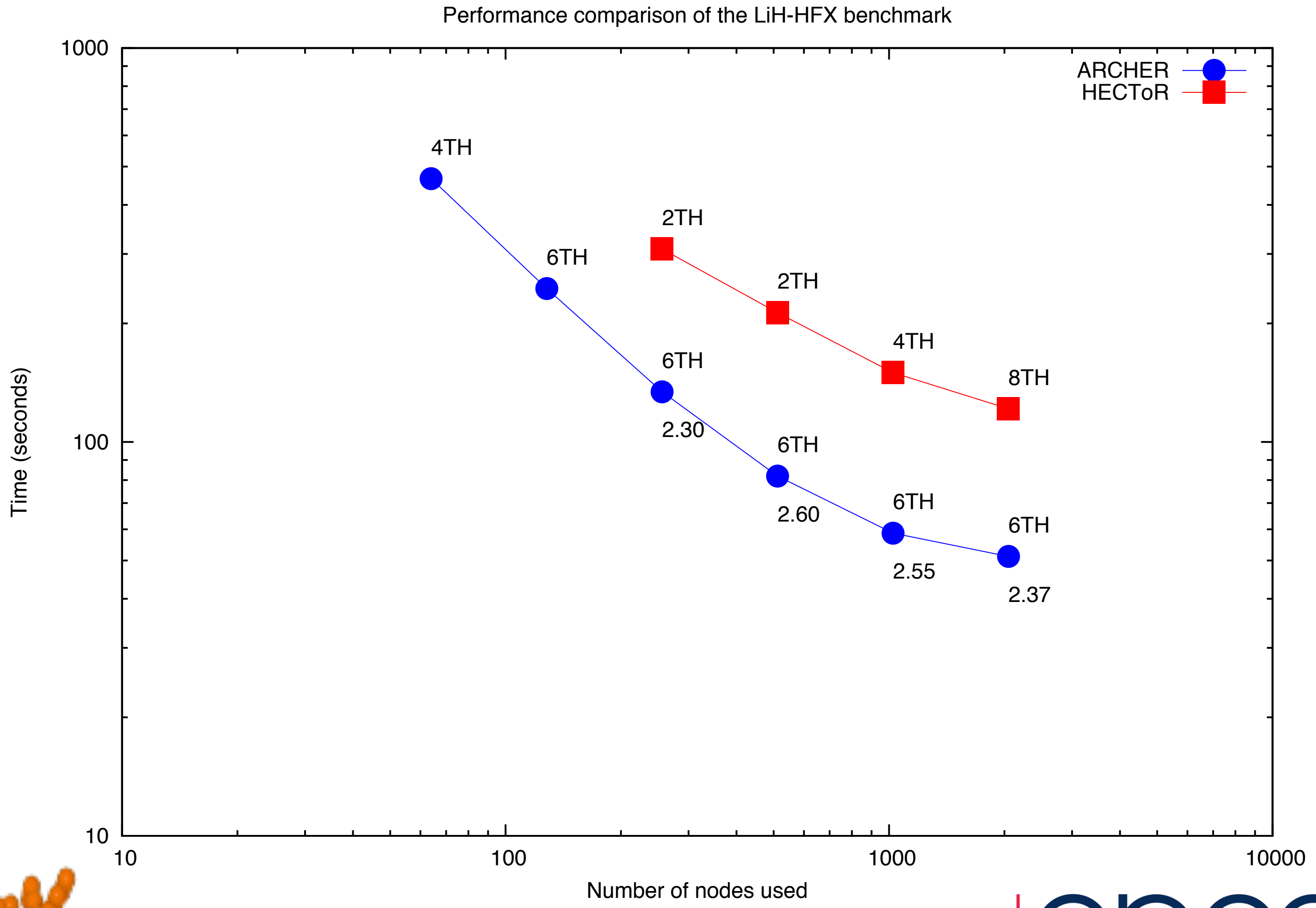
Parallel Performance

- Different ways of comparing time-to-solution and compute resource…
- Speedup: $S = T_{ref} / T_{par}$
- Efficiency: $E_p = S_p / p$,   ‘good’ scaling is $E > 0.7$
- If $E < 1$, then using more processors uses more compute time (AUs)
- Compromise between overall speed of calculation and efficient use of budget
  - Depends if you have one large or many smaller calculations

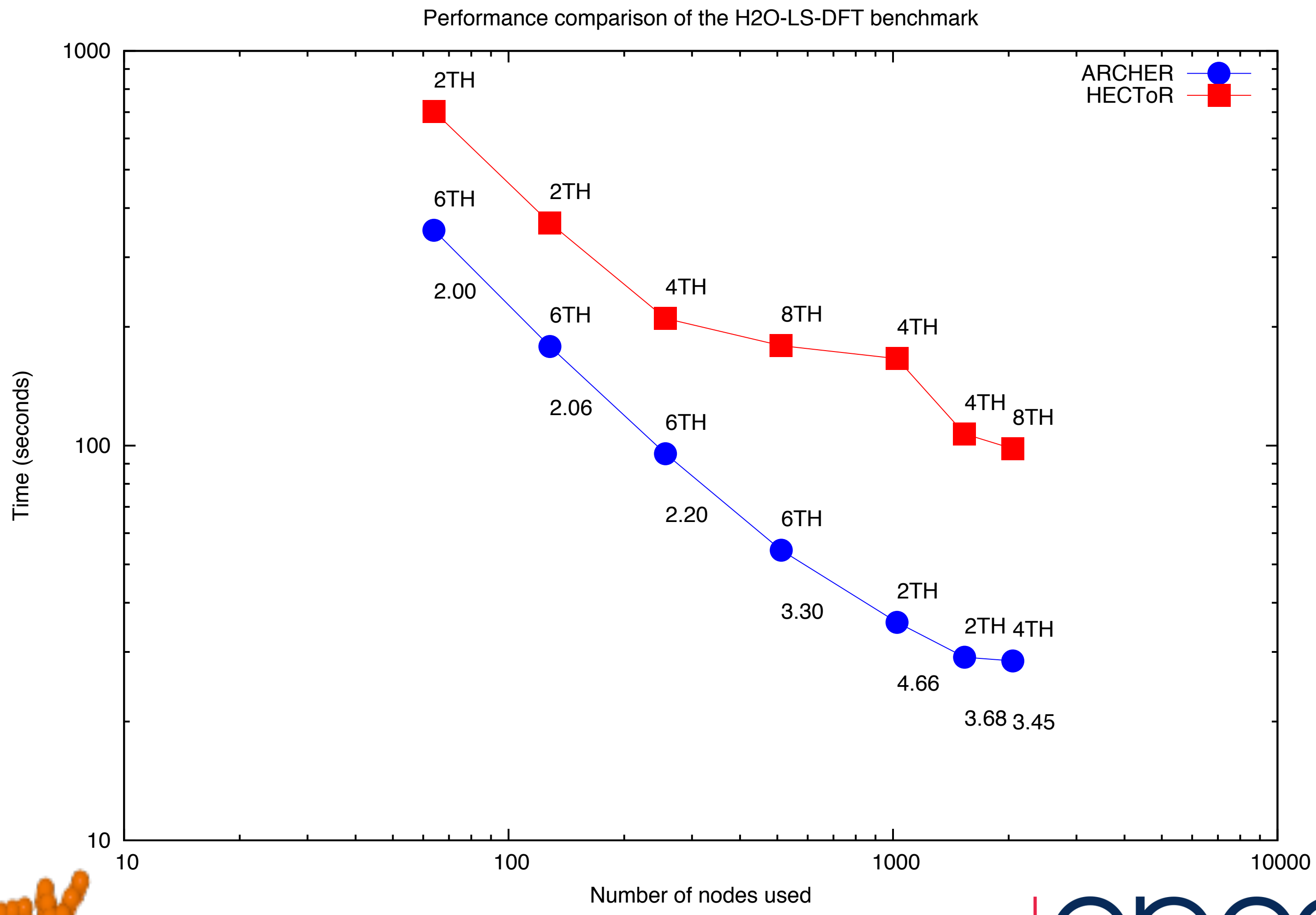
Parallel Performance : H2O-xx



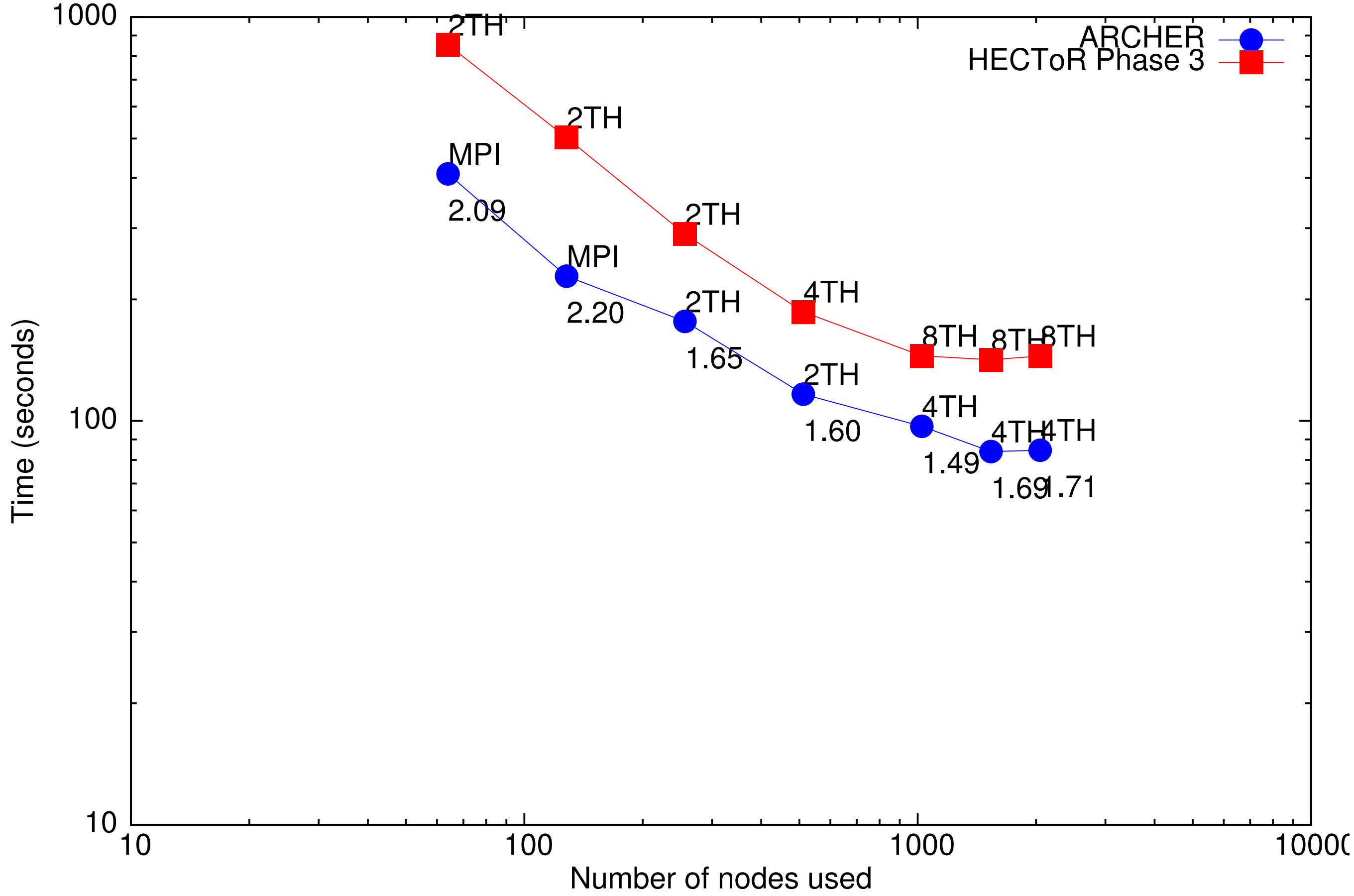
Parallel Performance: LiH-HFX

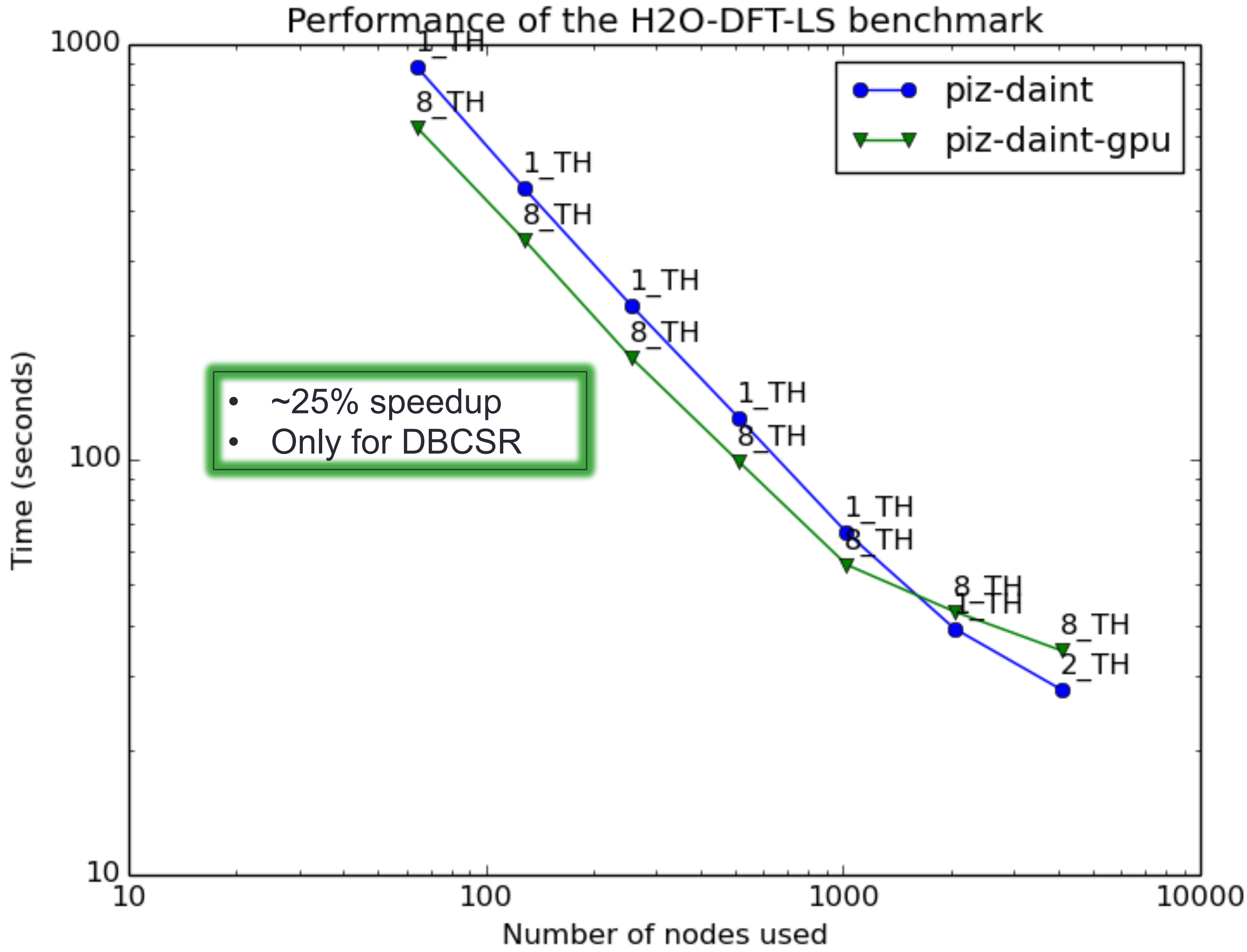


Parallel Performance: H2O-LS-DFT



Parallel Performance: H2O-64-RI-MP2





Performance of the H2O-DFT-LS benchmark
Time (seconds)
Number of nodes used
1000
100
10
10
100
1000
10000
piz-daint
piz-daint-gpu
1_TH
8_TH
1_TH
8_TH
1_TH
8_TH
1_TH
8_TH
1_TH
8_TH
8_TH
1_TH
8_TH
2_TH
• ~25% speedup
• Only for DBCSR

CP2K Timing Report

- CP2K measures are reports time spent in routines and communication
  - timing reports are printed at the end of the run

```
-------------------------------------------------------------------------------
-                                                                             -
-                         MESSAGE PASSING PERFORMANCE                         -
-                                                                             -
-------------------------------------------------------------------------------

ROUTINE             CALLS  TOT TIME [s]  AVE VOLUME [Bytes]  PERFORMANCE [MB/s]
MP_Group                4         0.000
MP_Bcast              186         0.018             958318.             9942.82
MP_Allreduce         1418         0.619               2239.                5.13
MP_Gather              44         0.321              21504.                2.95
MP_Sync              1372         0.472
MP_Alltoall          1961         5.334          323681322.           119008.54
MP_ISendRecv       337480         0.177               1552.             2953.86
MP_Wait            352330         5.593
MP_comm_split          48         0.054
MP_ISend            39600         0.179              14199.             3147.38
MP_IRecv            39600         0.100              14199.             5638.21
-------------------------------------------------------------------------------
```

CP2K Timing Report

```
-------------------------------------------------------------------------------
-                                                                             -
-                                T I M I N G                                  -
-                                                                             -
-------------------------------------------------------------------------------
SUBROUTINE                               CALLS  ASD         SELF TIME        TOTAL TIME
                                       MAXIMUM       AVERAGE  MAXIMUM  AVERAGE  MAXIMUM
CP2K                                         1  1.0    0.018    0.018   57.900   57.900
qs_mol_dyn_low                               1  2.0    0.007    0.008   57.725   57.737
qs_forces                                   11  3.9    0.262    0.278   57.492   57.493
qs_energies_scf                             11  4.9    0.005    0.006   55.828   55.836
scf_env_do_scf                              11  5.9    0.000    0.001   51.007   51.019
scf_env_do_scf_inner_loop                   99  6.5    0.003    0.007   43.388   43.389
velocity_verlet                             10  3.0    0.001    0.001   32.954   32.955
qs_scf_loop_do_ot                           99  7.5    0.000    0.000   29.807   29.918
ot_scf_mini                                 99  8.5    0.003    0.004   28.538   28.627
cp_dbcsr_multiply_d                       2338 11.6    0.005    0.006   25.588   25.936
dbcsr_mm_cannon_multiply                  2338 13.6    2.794    3.975   25.458   25.809
cannon_multiply_low                       2338 14.6    3.845    4.349   14.697   15.980
ot_mini                                     99  9.5    0.003    0.004   15.701   15.942
-------------------------------------------------------------------------------
```

CP2K Timing Report

- Not just for developers!
  - Check that communication is < 50% of total runtime
  - Check where most time is being spent:
    - Sparse matrix multiplication - `cp_dbcsr_multiply_d`
    - Dense matrix algebra – `cp_fm_syevd` (`&DIAGONALISATION`), `cp_fm_cholesky_*` (`&OT`), `cp_fm_gemm`
    - FFT – `fft3d_*`
    - Collocate / integrate – `calculate_rho_elec`, `integrate_v_rspace`
- Control level of granularity

```
&GLOBAL
  &TIMINGS
    THRESHOLD 0.00001
  &END TIMINGS
&END GLOBAL
```

Default is 0.02 (2%)

Summary

- First look for algorithmic gains
  - Cell size, SCF settings, preconditioner, choice of basis set, QM/MM , ADMM…
- Check scaling of *your* system
  - Run a few MD steps / reduced `MAX_SCF`
- Almost all performance-critical code is in libraries
  - Compiler optimisation –O3 is good enough
  - Intel vs gfortran vs Cray – difference is close to zero
- Before spending 1,000s of CPU hours, build libsmm, libgrid, ELPA, FFTW3…
  - Or ask your local HPC support team ☺

CP2K Parallelisation and Optimisation

Questions?