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http://tinyurl.com/CP2KSchool2018
#CP2KSummerSchool

CP2K Parallelisation and Optimisation

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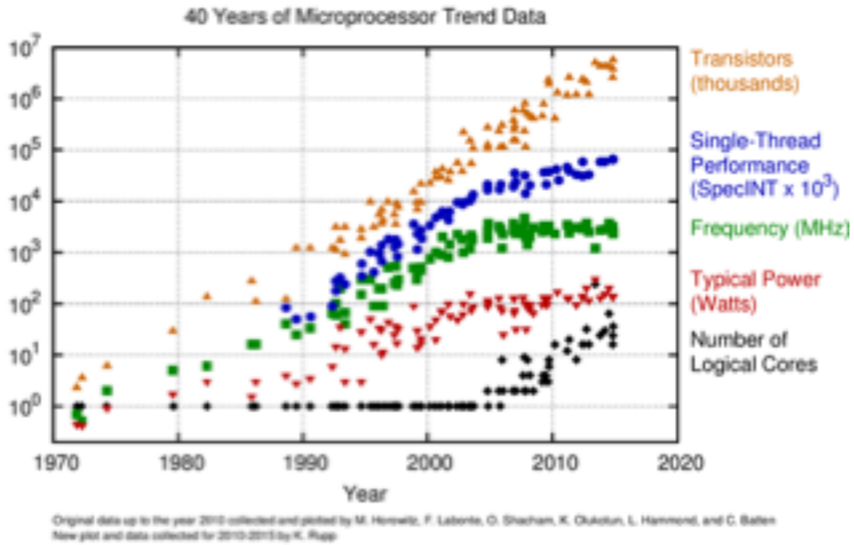
Overview

- 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 …)

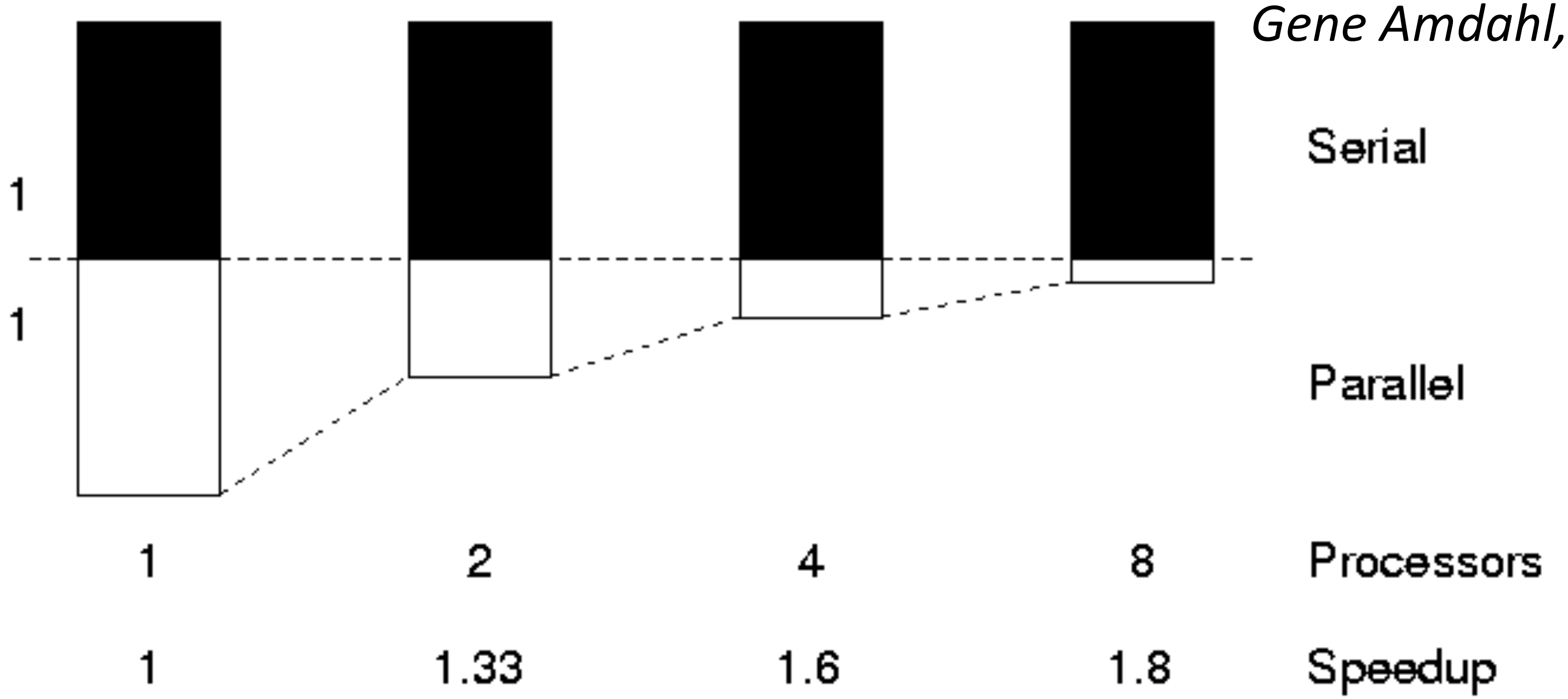
- Need strategies to split up our computation between different processors

- 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



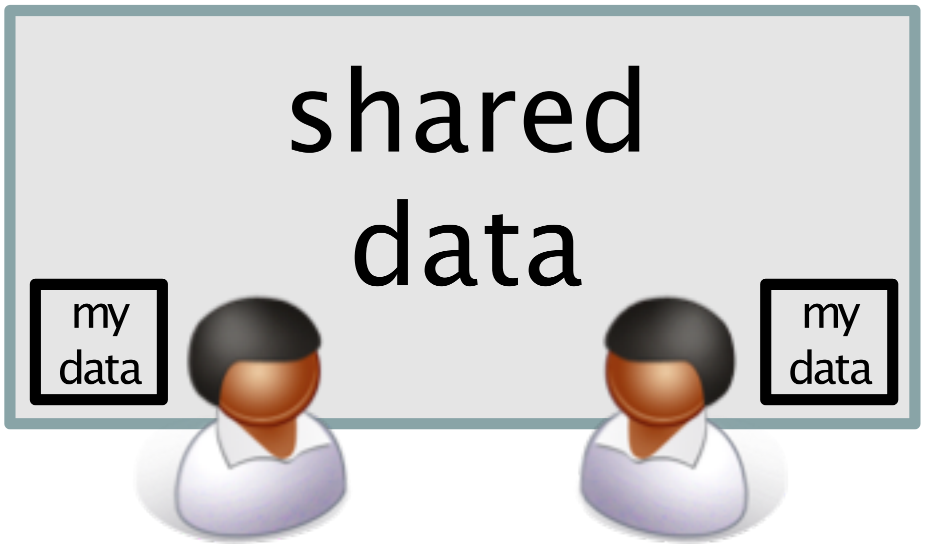
Parallel Programming Models

- 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



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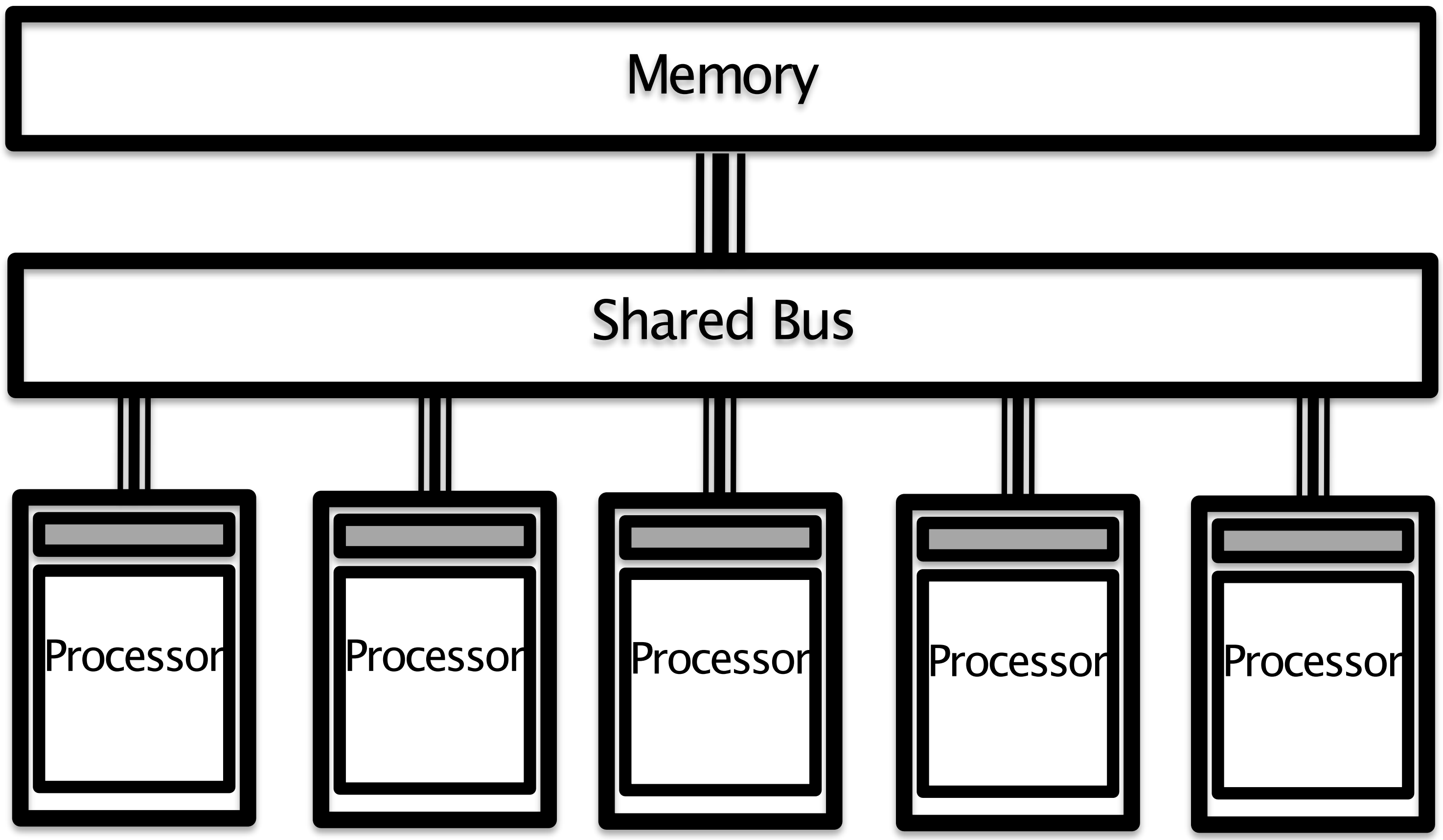
Hardware

Needs support from a shared-memory architecture

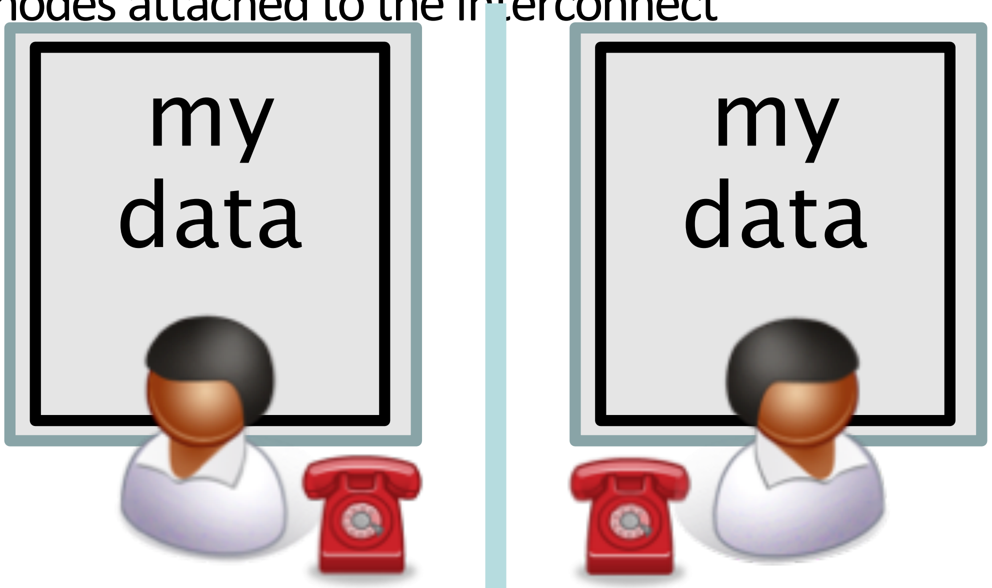


Parallel Programming Models

- 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

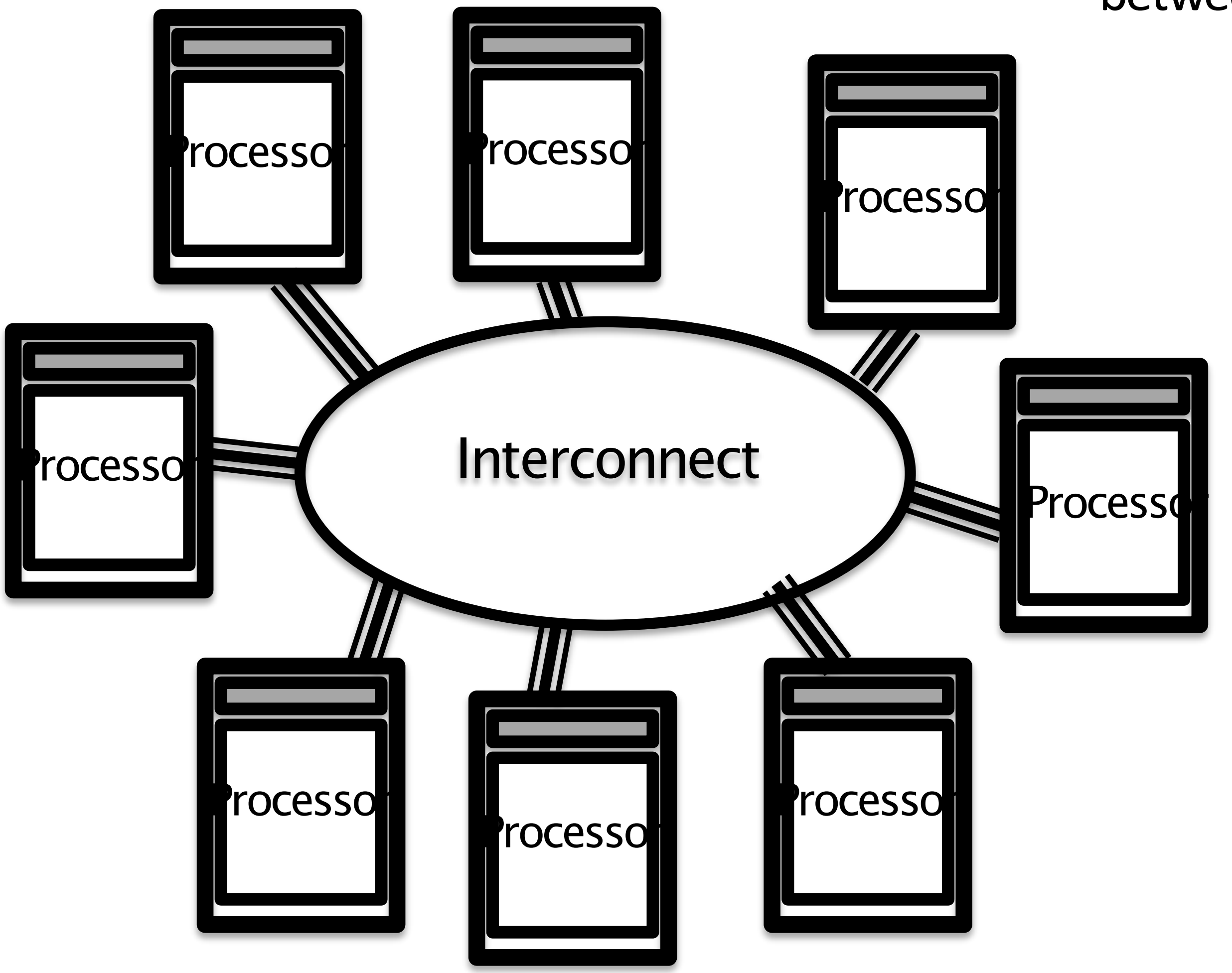
Analogy

- 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

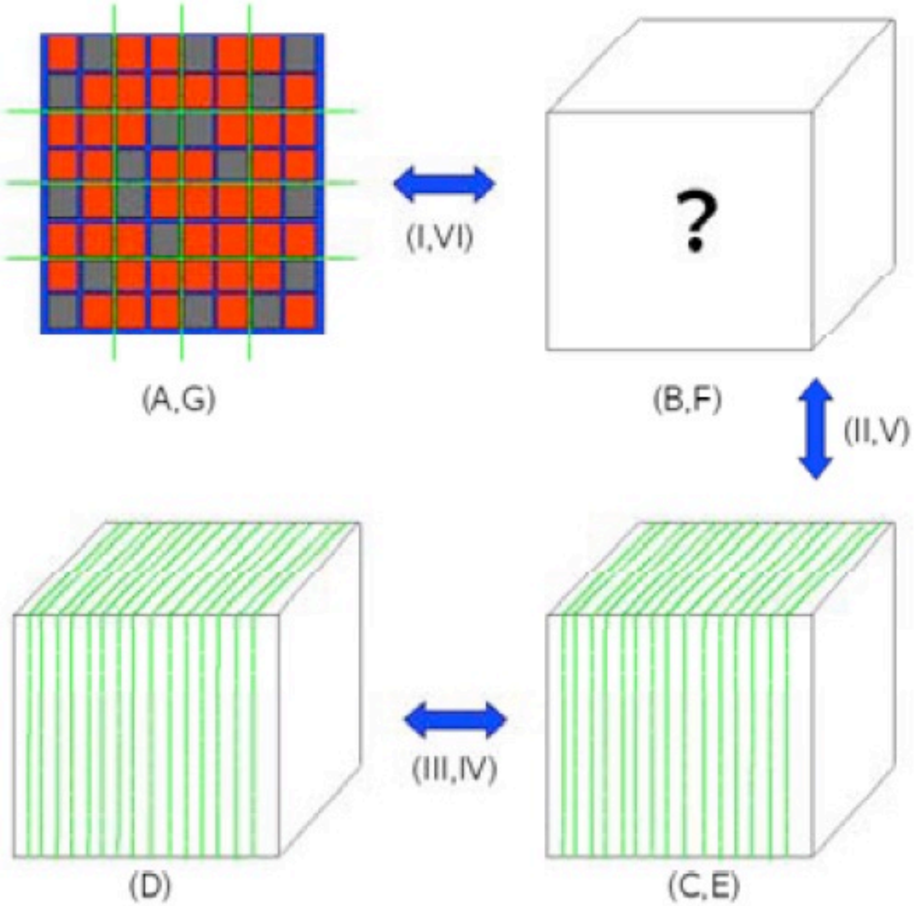
- CP2K can use OpenMP *or* MPI (`ssmp` *or* `popt`)
  - Use OpenMP for desktop PCs with multi-cores *or*
  - MPI for clusters and supercomputers
  - Maybe also support for Accelerators (GPUs)

- 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

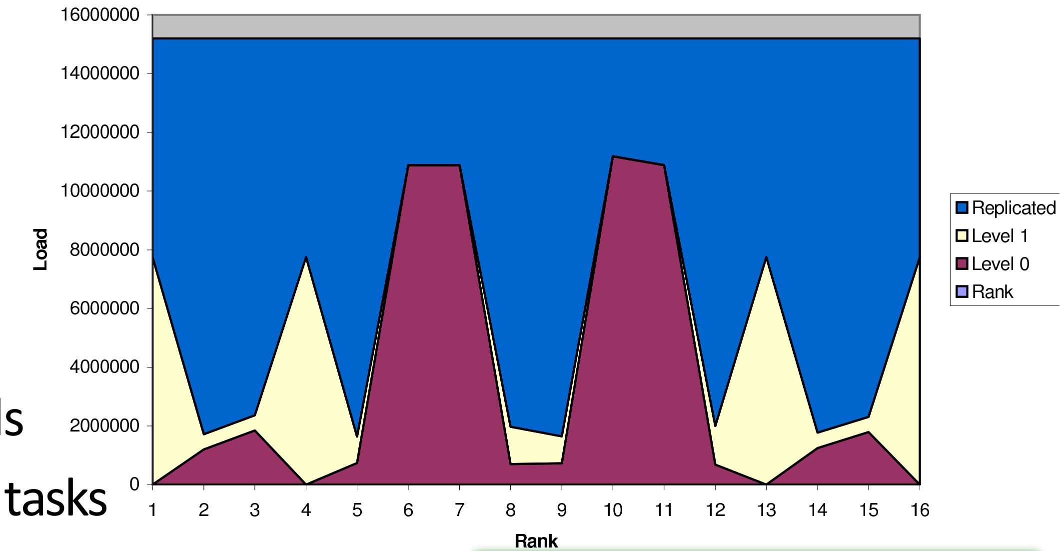
- (A,G) – distributed matrices
- (B,F) – realspace multigrids
- (C,E) – realspace data on planewave multigrids
- (D) – planewave grids

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

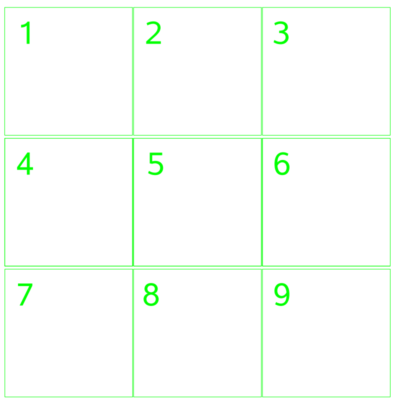


CP2K Algorithms and Data Structures

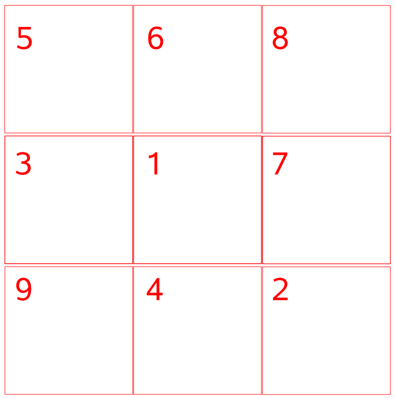
- Distributed realspace grids
  - Overcome memory bottleneck
  - Reduce communication costs
  - Parallel load balancing
    - On a single grid level
    - Re-ordering multiple grid levels
    - Finely balance with replicated tasks



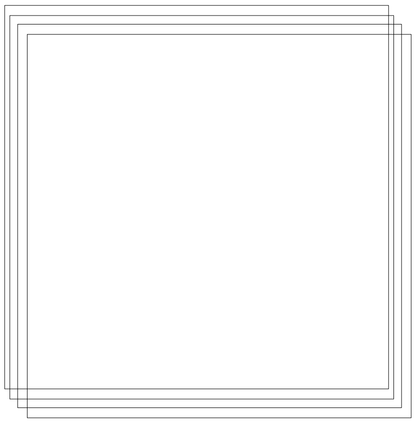
Level 1, fine grid, distributed



Level 2, medium grid, dist



Level 3, coarse grid, replicated



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

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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

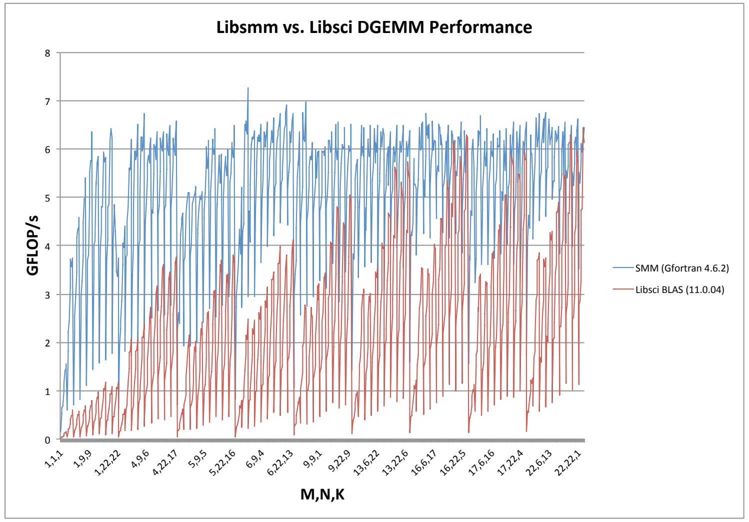

Figure 5: Comparing performance of SMM and Libsci BLAS for block sizes up to 22,22,22

- Run on a square number of processes

- `lib[x]smm` for small block multiplications

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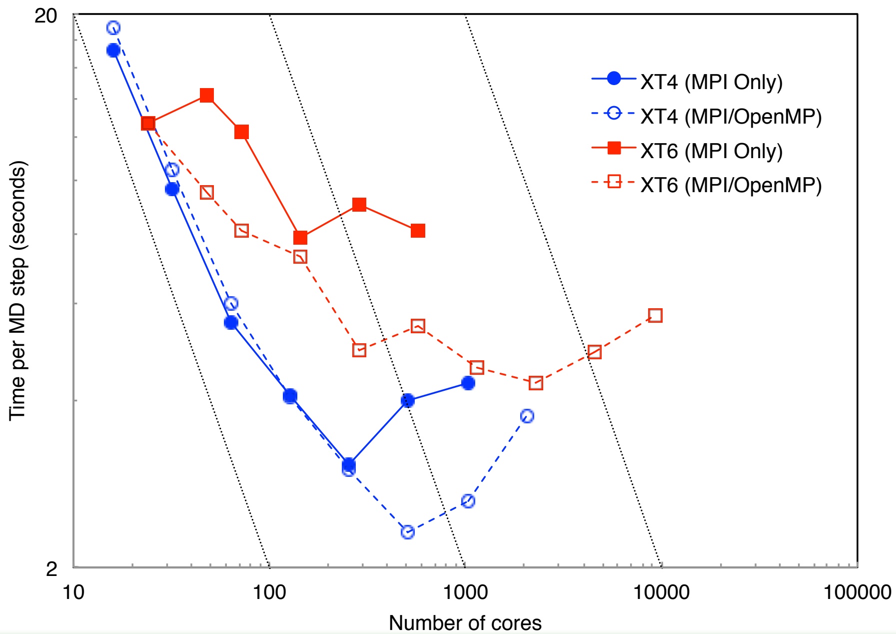
CP2K Algorithms and Data Structures

- OpenMP
  - Now in all key areas of CP2K
  - FFT, DBCSR, Collocate/Integrate,
  - Incremental addition over time
- 1,2 or 4 threads per process



- Dense Linear Algebra
  - Matrix operations during SCF
  - GEMM - ScaLAPACK
  - SYEVD – ScaLAPACK / ELPA

- `-D__ELPA=YYYYMM` 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

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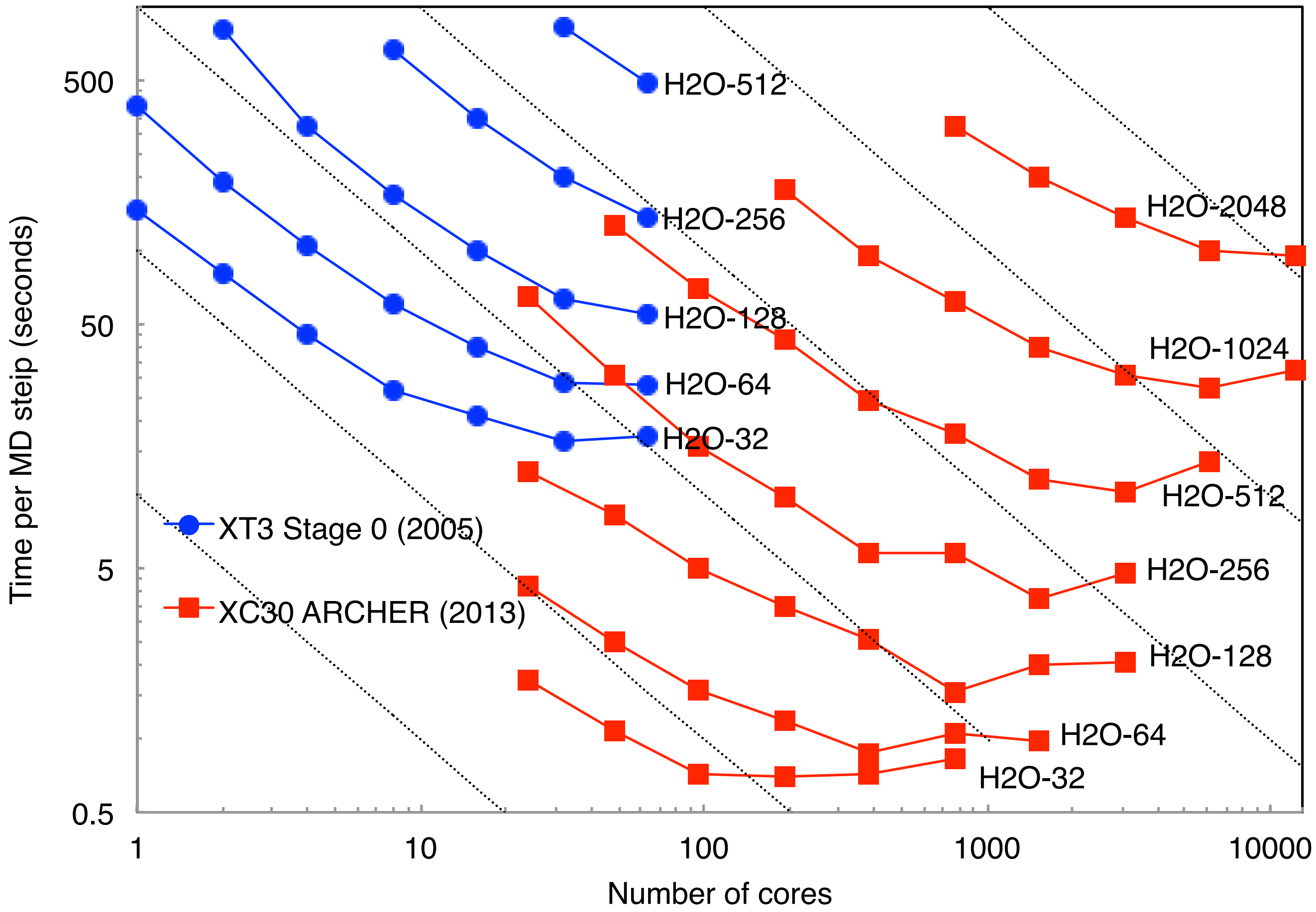
Parallel Performance : H2O-xx



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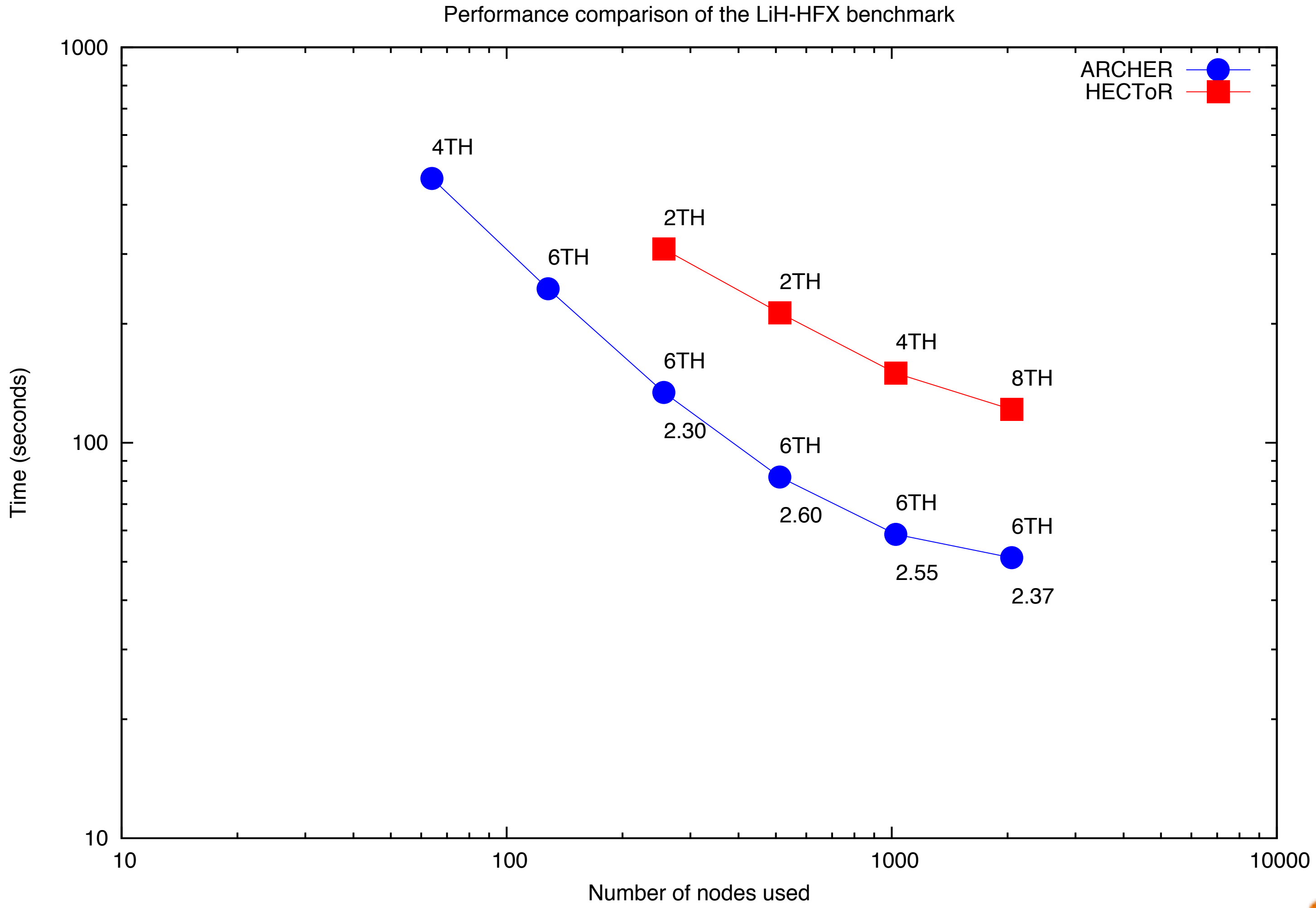
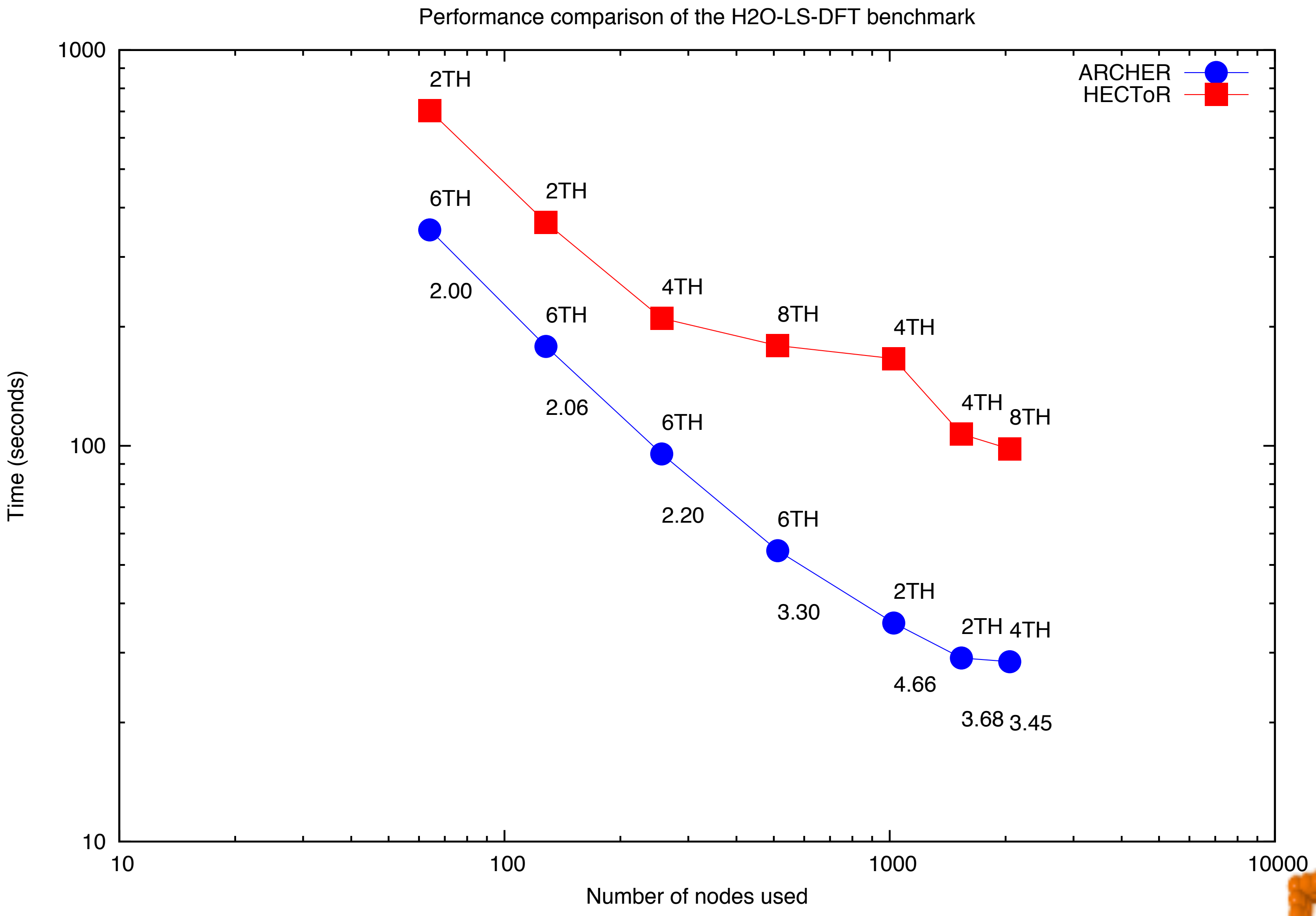
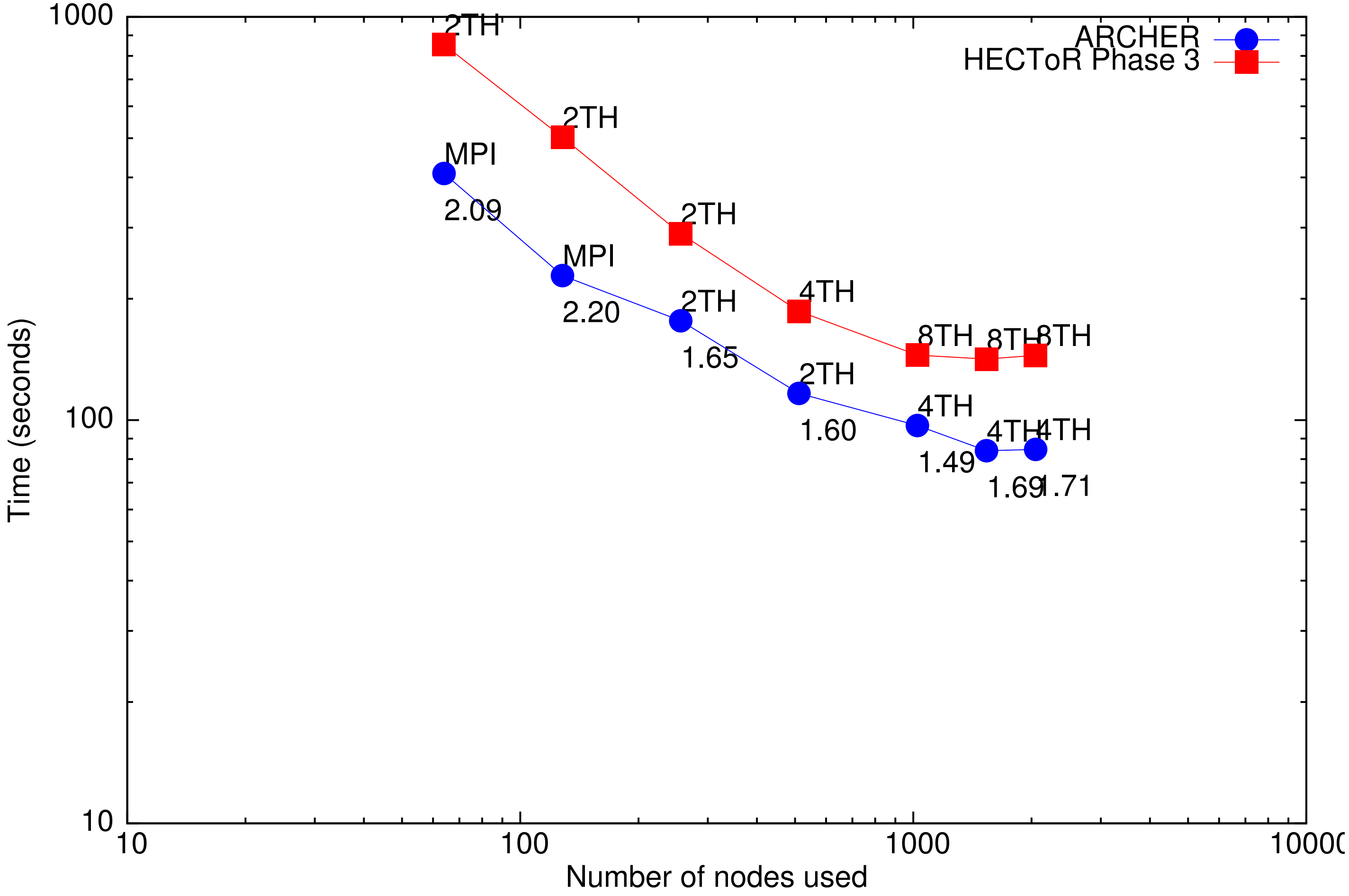
Parallel Performance: LiH-HFX



Parallel Performance: H2O-LS-DFT

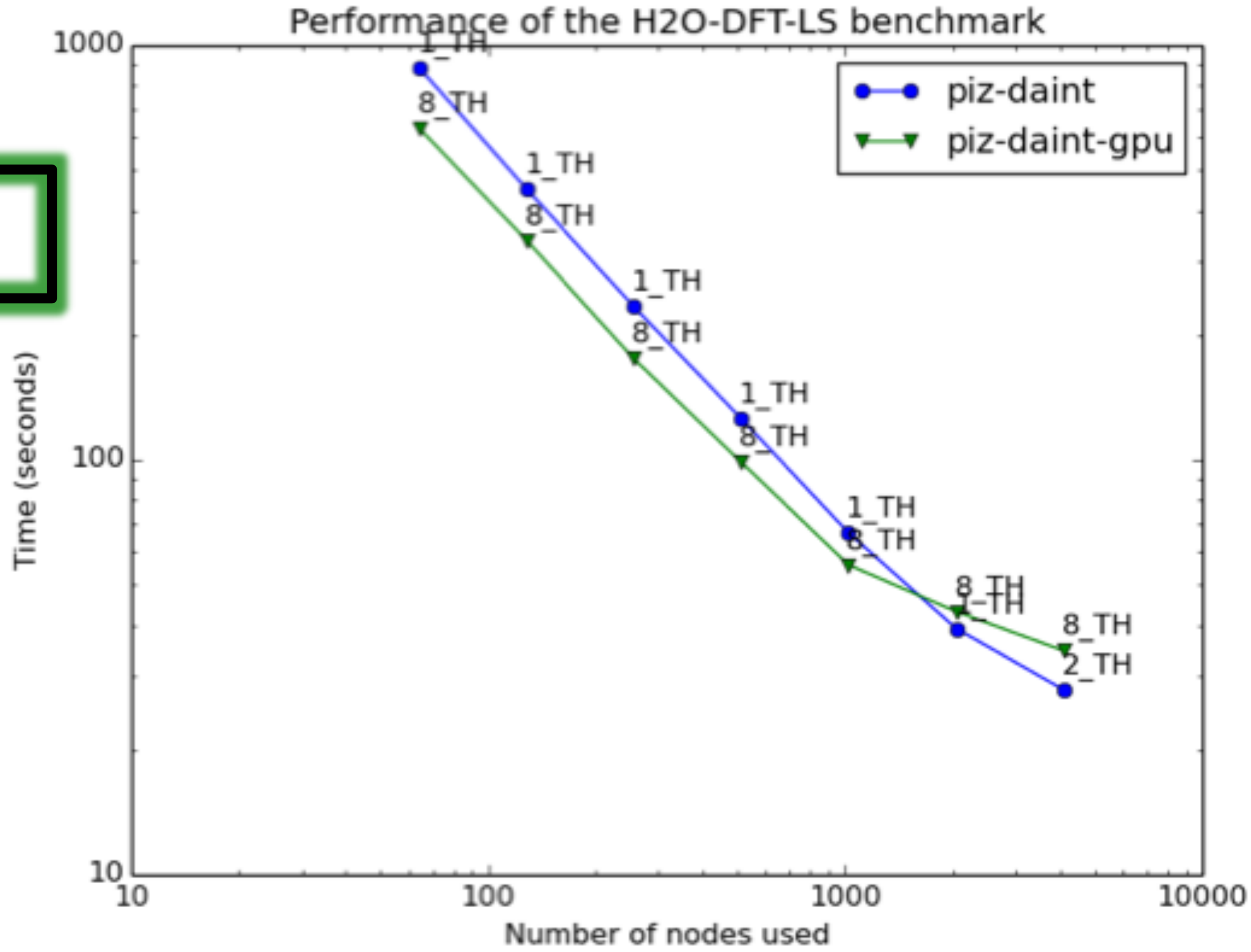


Parallel Performance: $H2O$-64-RI-MP2



Parallel Performance: GPUs

- ~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

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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%)

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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 / GEO_OPT steps
  - Turn off outer SCF, keep inner SCF fixed
- 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 lib[x]smm, libgrid, ELPA, FFTW3…
  - Or ask your local HPC support team ☺

Questions?