Horizon 2020
European Union Funding
for Research & Innovation

CP2K – QM/MM Practical

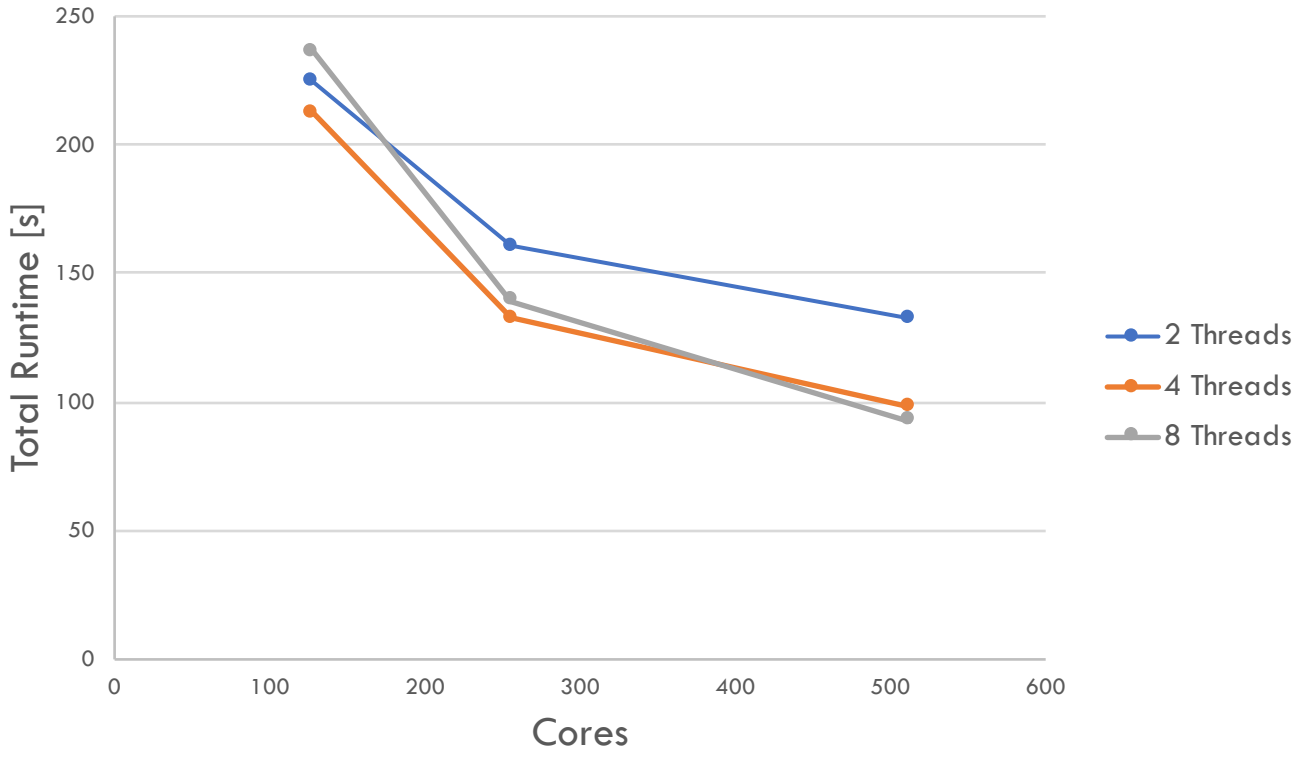
Results – Single node

- Using 1 thread results in out of memory error
  - There is not enough memory per process (128 here)
  - 2 threads allow double the memory per process, remember threads share memory so they do not need their own copy of data
- 4 threads has better performance.
- 32 threads very slow. The threads span 2 memory regions on the node which means data is slow to access

Threads	Time CP2K (s) **T_total**	Time mp_alltoall_z22v (s)	Time mp_sum_dm3 (s)	Time mp_waitany (s)	Total time mp_routines (s) **T_mp**
1	n/a	n/a	n/a	n/a	n/a
2	224.49	18.377	14.758	4.767	37.902
4	212.471	15.599	8.821		24.42
8	236.41	20.451	5.373	7.207	33.031
16	279.018	24.936		24.819	49.755
32	379.674	35.208		26.258	61.466

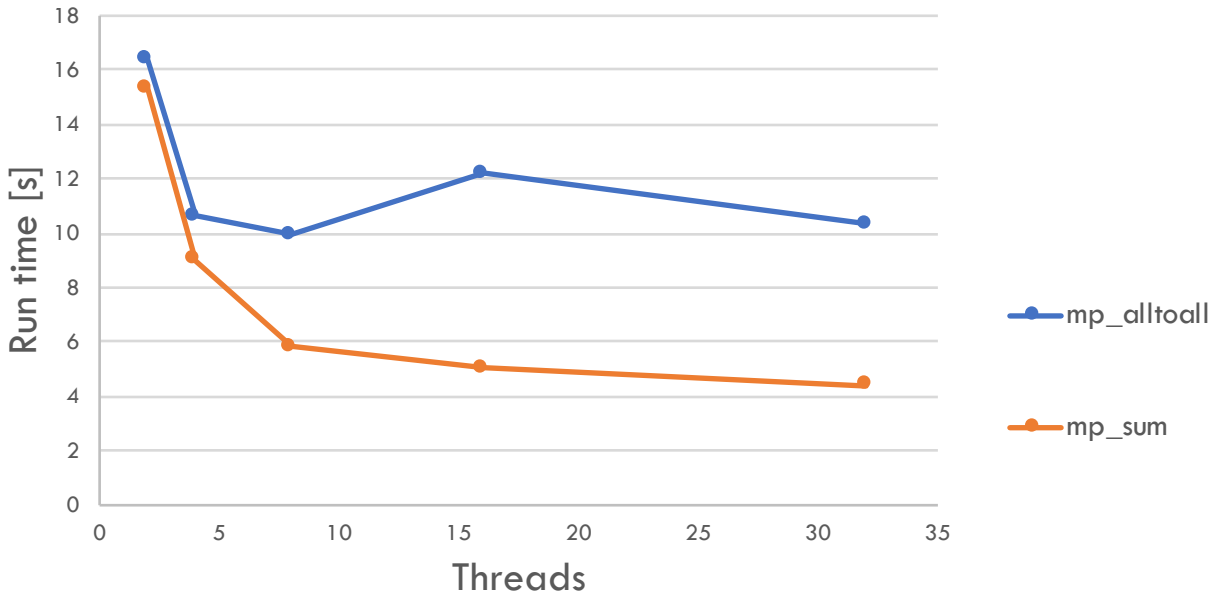
Results – Threading on multiple nodes

- Using 4 threads has the best performance on 1 and 2 nodes
  - 8 threads better on 4 nodes
  - More threads means less processes
  - Potential for less communication overhead
  - Also may exploit threading in areas of code that are not suitable for MPI
- Always a good idea to run tests to see what value is best



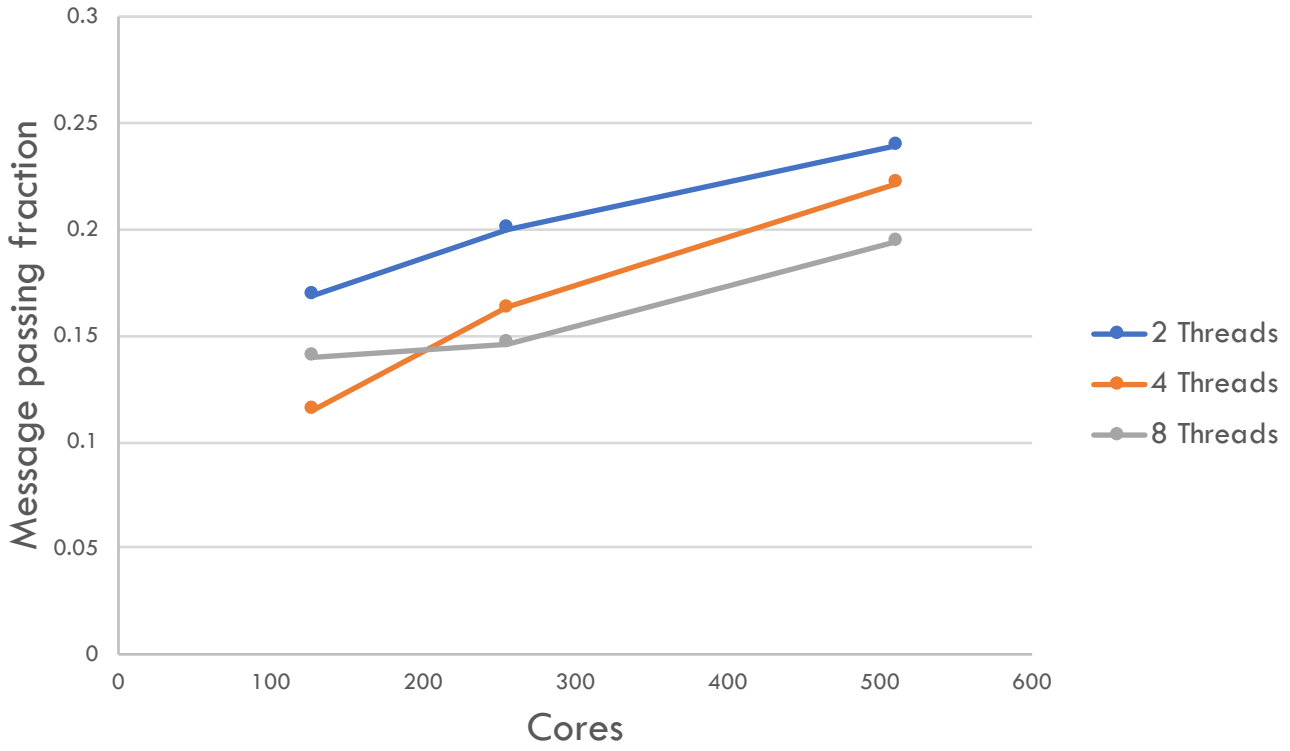
Results – Communications

- Run time of mp_sum decreases with the number of threads
  - Possibly due to less messages being sent
- Run time of mp_alltoall less clear
  - Some improvement with using threads
  - 2-4 threads look to optimal
- Hard to predict how routines and the code as a whole will be affected by changing the number of threads
  - Really have to test this



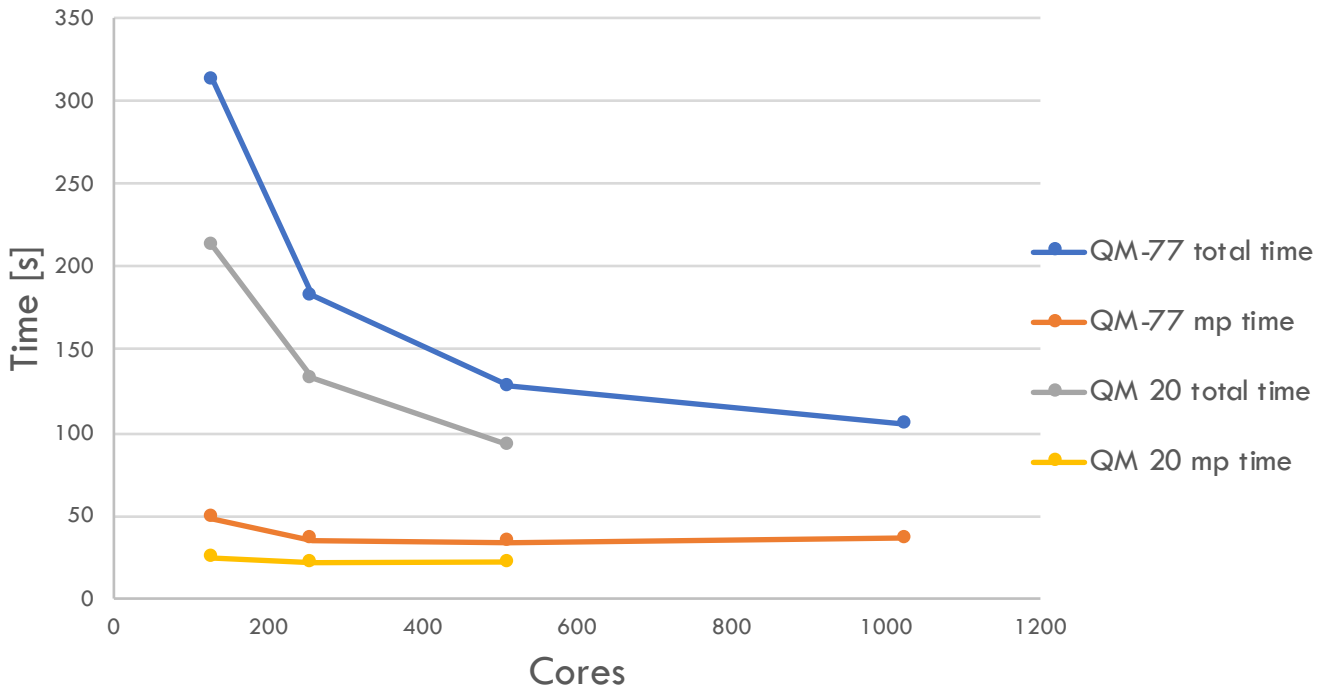
Results – Communications

- Fraction of time spent in MP routines increases with nodes
  - Other areas of the program are improving performance at a greater rate, i.e.. they have greater potential for parallel speed up.
- Changing the number of threads has the potential to reduce this fraction



Results – QM system size

- The large QM system scales better, though perhaps not as well as you would think.
- The system with the large QM region spends a greater fraction of its time doing communications.



BioExcel Partners

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Utrecht University

UNIVERSITY OF JYVÄSKYLA

Horizon 2020
European Union Funding
for Research & Innovation

BioExcel is funded by the European Union Horizon 2020 program under grant agreements 675728 and 823830.