

Executable: cp2k.popt

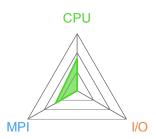
Resources: 256 processes, 16 nodes

Machine: cray-one

Start time: Tue Oct 27 16:02:12 2013 Total time: 951 seconds (16 minutes)

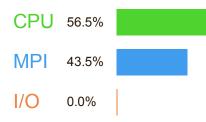
Full path: /users/allinea/cp2k/exe/CRAY-XE6-gfortran-hwtopo

Notes: H20 benchmark



Summary: cp2k.popt is CPU-bound in this configuration

The total wallclock time was spent as follows:



Time spent running application code. High values are usually good.

This is average; check the CPU performance section for optimization advice.

Time spent in MPI calls. High values are usually bad.

This is average; check the MPI breakdown for advice on reducing it.

Time spent in filesystem I/O. High values are usually bad.

This is **negligible**; there's no need to investigate I/O performance.

This application run was CPU-bound. A breakdown of this time and advice for investigating further is in the CPU section below.

CPU

A breakdown of how the 56.5% total CPU time was spent:

Scalar numeric ops 27.7% Vector numeric ops 11.3% Memory accesses 60.9% Other 0.0

The per-core performance is memory-bound. Use a profiler to identify time-consuming loops and check their cache performance.

Little time is spent in vectorized instructions. Check the compiler's vectorization advice to see why key loops could not be vectorized.

MPI

Of the 43.5% total time spent in MPI calls:

Time in collective calls

Time in point-to-point calls

Estimated collective rate

169 Mb/s

Estimated point-to-point rate

50.6 Mb/s

The point-to-point transfer rate is low. This can be caused by inefficient message sizes, such as many small messages, or by imbalanced workloads causing processes to wait. Use an MPI profiler to identify the problematic calls and ranks.

I/O

A breakdown of how the 0.0% total I/O time was spent:

Time in reads 0.0%
Time in writes 0.0%
Estimated read rate 0 bytes/s
Estimated write rate 0 bytes/s

No time is spent in I/O operations. There's nothing to optimize here!

Memory

Per-process memory usage may also affect scaling:

Mean process memory usage 82.5 Mb

Peak process memory usage 89.3 Mb

Peak node memory usage 7.4%

The peak node memory usage is low. You may be able to reduce the total number of CPU hours used by running with fewer MPI processes and more data on each process.