

Executable: cp2k.popt

Resources: 256 processes, 16 nodes

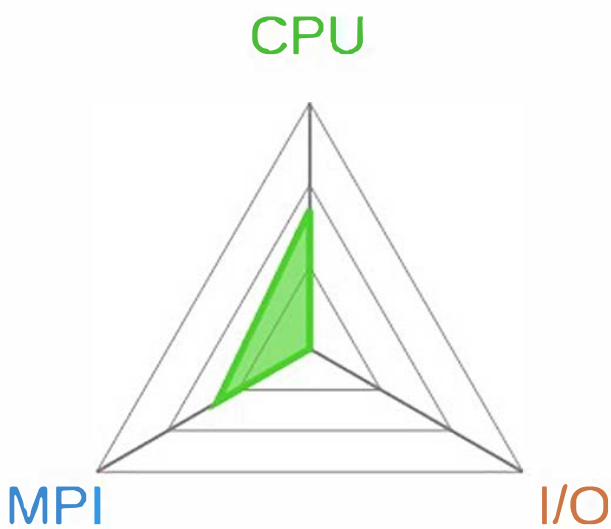
Machine: cray-one

Start time: Tue Oct 27 16:02:12 2013

Total time: 951 seconds (16 minutes)

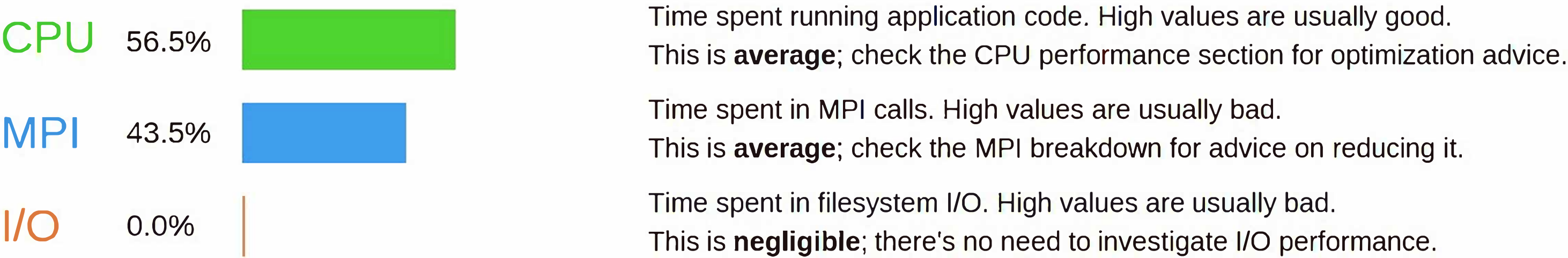
Full path: /users/allinea/cp2k/exe/CRAY-XE6-gfortran-hwtopo

Notes: H2O benchmark



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

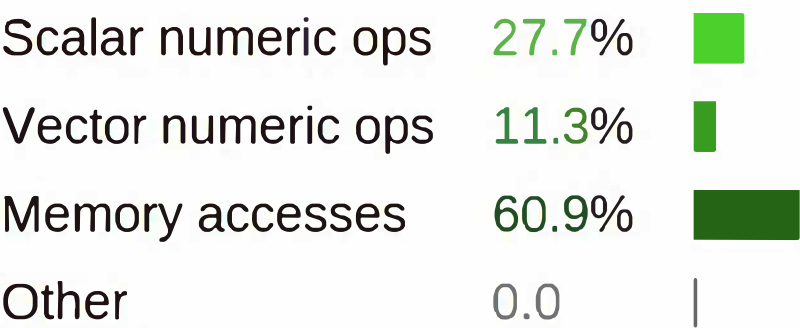
The total wallclock time was spent as follows:



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

CPU

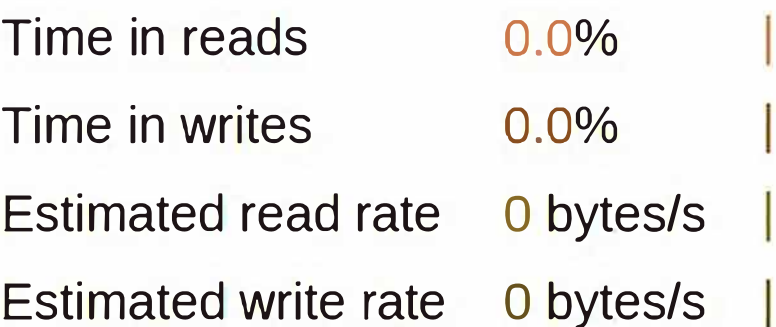
A breakdown of how the 56.5% total CPU time was spent:



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.

I/O

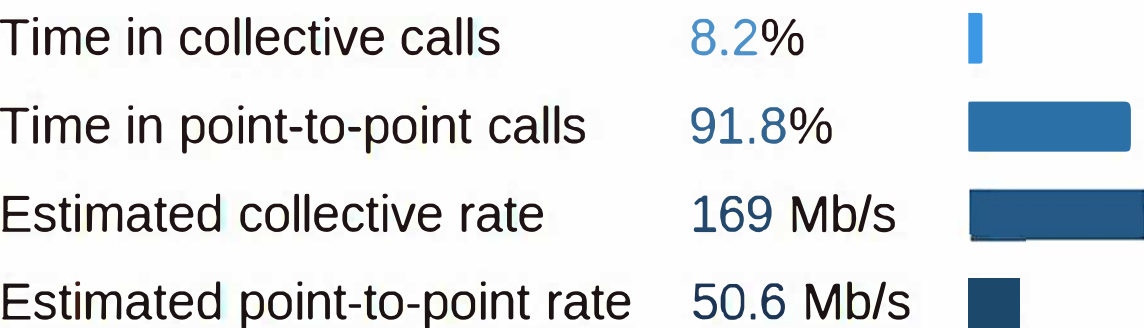
A breakdown of how the 0.0% total I/O time was spent:



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

MPI

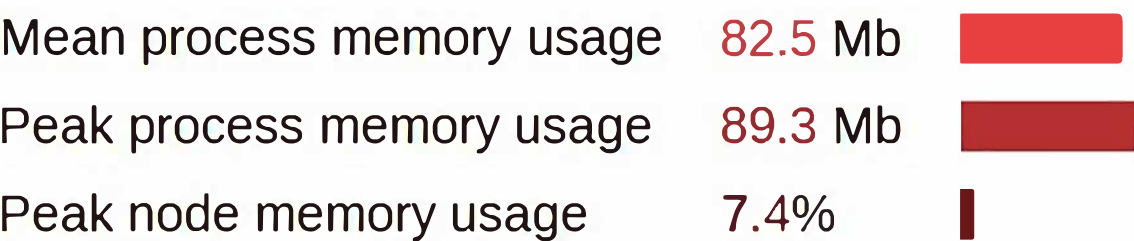
Of the 43.5% total time spent in MPI calls:



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.

Memory

Per-process memory usage may also affect scaling:



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.