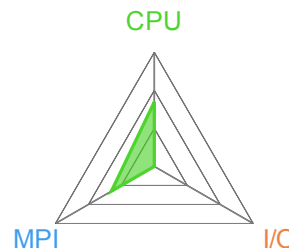


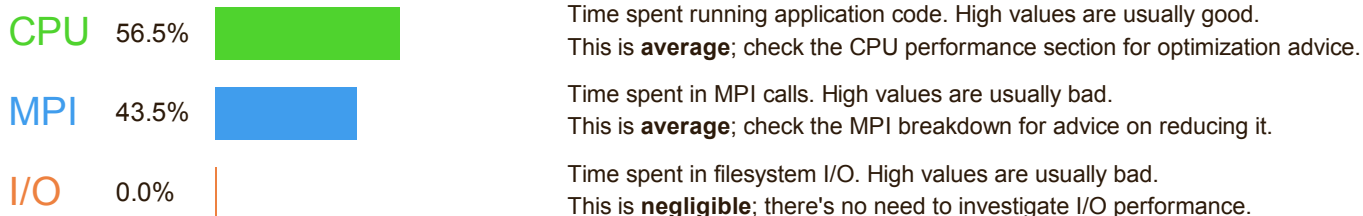


Executable: cp2k.popt  
Resources: 256 processes, 16 nodes  
Machine: cray-one  
Start time: Tue Oct 27 16:02:12 2013  
Total time: 951 seconds (16 minutes)  
Full path: /users/allinea/cp2k/exe/CRAY-XE6-gfortran-hwtopo  
Notes: H2O benchmark



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

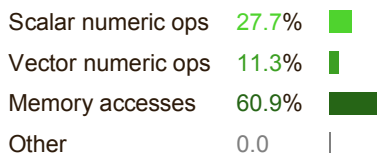
The total wallclock time was spent as follows:



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:

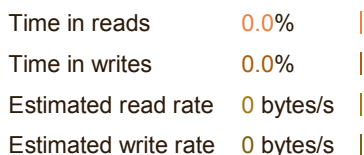


The per-core performance is **memory-bound**. Use a profiler to identify time-consuming loops and check their cache performance.

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

### I/O

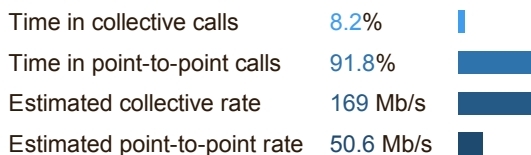
A breakdown of how the **0.0%** total I/O time was spent:



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

### MPI

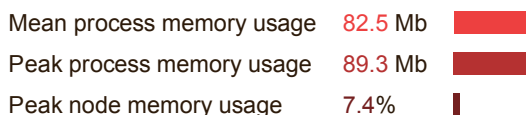
Of the **43.5%** total time spent in MPI calls:



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.