Monitoring the Cray XC30 Power Management Hardware Counters

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1. Introduction

This document is concerned with how to record and analyse the data provided by the power monitoring hardware counters on ARCHER, a Cray XC30 platform. Basic descriptions of these counters can be obtained by running `papi_native_avail` on the compute nodes of the host system using the `aprun` command.

There are two groups of power monitoring counters, running average power limit (RAPL) and power management (PM), see the following two tables.

Table 1: Running average power limit counters

Name	**Description**	**Units**
UNITS:POWER	Scaling factor for power (3)	n/a
UNITS:ENERGY	Scaling factor for energy (16)	n/a
UNITS:TIME	Scaling factor for time (10)	n/a
THERMAL_SPEC	Thermal specification (130)	W
MINIMUM_POWER	Minimum power (64)	W
MAXIMUM_POWER	Maximum power (200)	W
MAXIMUM_TIME_WINDOW	Maximum time window (0.046)	s
PACKAGE_ENERGY	Energy used by chip package	nJ
DRAM_ENERGY	Energy used by package DRAM	nJ
PP0_ENERGY	Power-plane zero package energy	nJ

The counters have a time resolution of 100 ms [4]. The term *package* relates to the compute node processor: each node has two 12-core processors and therefore two packages. This means there is one set of RAPL counters per socket, whereas for PM counters, there is one set per node (or per two sockets). The PP0 package energy counter value is a summation of the energy used by all the cores (including processor caches) within a package [6]. Note, several of the hardware counters are by definition fixed (e.g., UNITS:POWER) and so only ever have one value, which is given in brackets at the end

Table 2: Power management counters

Name	Description	Units
PM_POWER_CAP:NODE	Compute node power cap	W
PM_POWER:NODE	Compute node point-in-time power	W
PM_ENERGY:NODE	Compute node accumulated energy	J
PM_POWER_CAP:ACC	Accelerator power cap	W
PM_POWER:ACC	Accelerator point-in-time power	W
PM_ENERGY:ACC	Accelerator accumulated energy	J
PM_FRESHNESS	Number of times HSS has updated data structure	n/a
PM_GENERATION	Number of times a power cap change was made	n/a
PM_STARTUP	Timestamp of the last startup	cycles
PM_VERSION	Version of sysfs directory tree	n/a

of the counter description.

Two molecular modelling codes (DL_POLY v4.05 and CP2K v2.6.14482) are used to show how to access power management data for simulation jobs that run over multiple compute nodes. The former application achieves parallelism through MPI exclusively, and can be built for all three programming environments available on ARCHER (Cray, Intel and gnu). We would expect that the choice of compiler should not impact energy use, nevertheless this paper will confirm whether this is indeed the case. The second code, CP2K, will be run in a mixed OpenMP/MPI mode (using the gnu environment): this provides a more useful case as we explore whether or not adding more threads raises or lowers the energy use.

2. CrayPat

We begin with the Cray Performance and Analysis Tool (CrayPat) as the most straightforward way to obtain power management data. This tool requires that the application code is instrumented before it is submitted to the job launcher. Before the code is compiled the perftools software module must be loaded.

```
module load perftools
```

Then, after compilation, the application executable is instrumented by the `pat_build` command.

```
pat_build DLPOLY.Z
```

This produces a new executable with a `+pat` suffix. It is this instrumented program that is launched via the `aprun` command and controlled according to various properties supplied by the job submission script, an excerpt of which follows.

```
module load perftools

export PAT_RT_SUMMARY=1
export PAT_RT_PERFCTR=UNITS:POWER,UNITS:ENERGY,UNITS:TIME, /
THERMAL_SPEC,MINIMUM_POWER,MAXIMUM_POWER,MAXIMUM_TIME_WINDOW, /
PACKAGE_ENERGY,PP0_ENERGY,DRAM_ENERGY, /
PM_POWER_CAP:NODE,PM_POWER:NODE,PM_ENERGY:NODE, /
PM_FRESHNESS,PM_GENERATION,PM_STARTUP,PM_VERSION

export OMP_NUM_THREADS=1

aprun -n 96 ./DLPOLY.Z+pat >& stdouterr
```

Note, the ACC power management counters are missing from the list assigned to the `PAT_RT_PERFECTR` environment variable. Although those three counters are returned by `papi_native_avail`, CrayPat reports an error, insisting that those performance counter event names do not exist. Having the summary flag set to one will generate one set of values for the counters listed in the submission script. If the code runs successfully, one of the output files will have a `.xf` extension, which can then be analysed via the `pat_report` command.

```
pat_report ./DLPOLY.Z+pat+43271-13s.xf
```

Something like the following output is then generated.

```
...
Table 3:  Program HW Performance Counter Data
...
THERMAL_SPEC 130 W
MINIMUM_POWER 64 W
MAXIMUM_POWER 200 W
MAXIMUM_TIME_WINDOW 0.046 s
PACKAGE_ENERGY 530.413 J
PP0_ENERGY 387.626 J
DRAM_ENERGY 58.021 J
PM_POWER:NODE 286 W
PM_ENERGY:NODE 767.219 J
PM_FRESHNESS 28.417
PM_STARTUP 1414408518017769 cycles
...
```

In the previous example, the DL_POLY code was run over four nodes, and so, by default the energies are averages, whereas the powers (also by default) are maximum values: e.g., PACKAGE_ENERGY is the average energy used by the eight processors, and PM_POWER:NODE is the maximum point-in-time power recorded (for one node) during the execution run. The `pat_report` tool has the flexibility to accept different aggregations [4].

Unfortunately, it doesn't seem possible to record multiple counter readings during execution on a per node basis. A CrayPat sampling job is specified by using the `-S` option with the `pat_build` command and by adding two extra options to the job script, see below.

```
export PAT_RT_EXPERIMENT=samp_pc_time
export PAT_RT_INTERVAL=1000
```

The interval is in microseconds. This setup does not generate a set of sampling data that could be used to investigate how energy use varies throughout the run; the only data generated specific to the selected counters appears to be in aggregate form only.

3. PM MPI Library

Hart et al. [3] have provided a library that allows one to monitor the power management (hereafter PM) counters directly. This library, pm_lib, accesses the actual counter files, located at `/sys/cray/pm_counters`. There are five counters available, instantaneous power and cumulative energy for normal nodes and for accelerated nodes — these measurements cover CPU, memory and any other hardware contained on the processor daughter card; any consumption due to the Aries network controllers and beyond is excluded however. The fifth counter is the freshness counter, which should always be read before reading the other counters. After a set of readings have been taken, the freshness counter is read again and if the value is unchanged, we know we have a consistent set of measurements: i.e., the power and energy were taken at the same time. The counters have a temporal resolution of 100 ms. The library can be linked with Fortran and C/C++ programs: however, for codes running on several multi-core nodes it is necessary to extend the library in two significant ways. First, only one MPI process per node must use pm_lib to access the PM counters on that node; and second, only one MPI process (e.g., rank 0) should collate the data, writing it to a single file.

The result of these extensions is a new library called pm_mpi_lib, which has an interface featuring just three functions, defined in Appendix A. When instrumenting a code for the first time, the area of interest is the main loop that controls how the simulation progresses. For DL_POLY, this is the loop at the start of the `./VV/w_md_v.f90` source file, which can be instrumented as follows. A call to the pm_mpi_lib function, `pm_mpi_open`, should be placed immediately before the loop. This function establishes the MPI rank of the calling process and then obtains the unique number of the node on which the process is running via `MPI_Get_processor_name`. The node number is then used to split the `MPI_COMM_WORLD` communicator: i.e., the node number is used as the *colour* of the sub-communicator, which is effectively a communicator for all processes on the same node. Thus, an appropriate `MPI_Allreduce` can be used to determine which process has the lowest numerical rank value on any given node, thereby choosing the process that will monitor the PM counters. All such monitoring processes (one per node) then go on to create another sub-communicator, one that unites them all, which allows rank 0 to determine the number of monitors. In addition to these tasks, the monitoring processes open their respective PM counter files; rank 0 also gets the current MPI time.

The second pm_mpi_lib function call, `pm_mpi_monitor`, can be placed at various points within the application loop. As the name suggests, this function allows all monitoring processes to read the PM counters; for all other processes, no read is performed and the holding variables are set to zero. A subsequent `MPI_Allreduce` can then be used to sum the counter values over all nodes; thus the total cumulative energy can be obtained. For the point-in-time power counters however, the sum is divided by the number of monitoring processes in order to calculate an average. Rank 0 then writes this data to the output file, see Appendix A for a description of the output format.

Finally, the third and last call, `pm_mpi_close`, is placed immediately outside the main application loop: this call ensures that each monitoring process closes its PM counter files and that rank 0 also closes the output file.

4. Results

The three functions of the pm_mpi_lib library have been used to instrument the DL_POLY and CP2K codes mentioned earlier, such that the PM counters for cumulative energy and point-in-time power are read for each node (four for DL_POLY and eight for CP2K). The data is then collated and output as a total energy and as an average power for each time step of the simulation.

4.1. Compiler Dependence

Figure 1 shows histograms of energy use per simulation step, defined as one iteration of the loop at the start of the DL_POLY source file, `./VV/w_md_v.f90`. There are three sets of histograms, one for each compiler environment: grey represents the Cray compiler, blue is Intel and red is gnu. For each run, the number of nodes assigned (4) and the input data set were the same: the latter was taken from the standard DL_POLY test case 40 (ionic liquid dimethylimidazolium chloride), see Section 8.1 of the user manual [5]. Furthermore, the molecular simulation defined by the test case was extended by increasing the value of the steps parameter in the `CONTROL` file from 750 to 20 000.

The histograms do not correspond with a single normal distribution: in general, there is one main peak and two minor ones appearing at lower energies, see Figure 1 (left column). In addition, there are high-energy simulation steps that occur every one thousand iterations (right column): this is how often the `DL_POLY` restart files are written to disk. The same DL_POLY job was run six times for each compiler environment and an average performance was calculated in order to tease out any compiler dependence. Repeatedly running exactly the same executable with the same input data will produce some variation in energy usage: however, we expect this variation to be mitigated by the fact that all jobs were run on the ARCHER test development server, where resource contention is minimal.

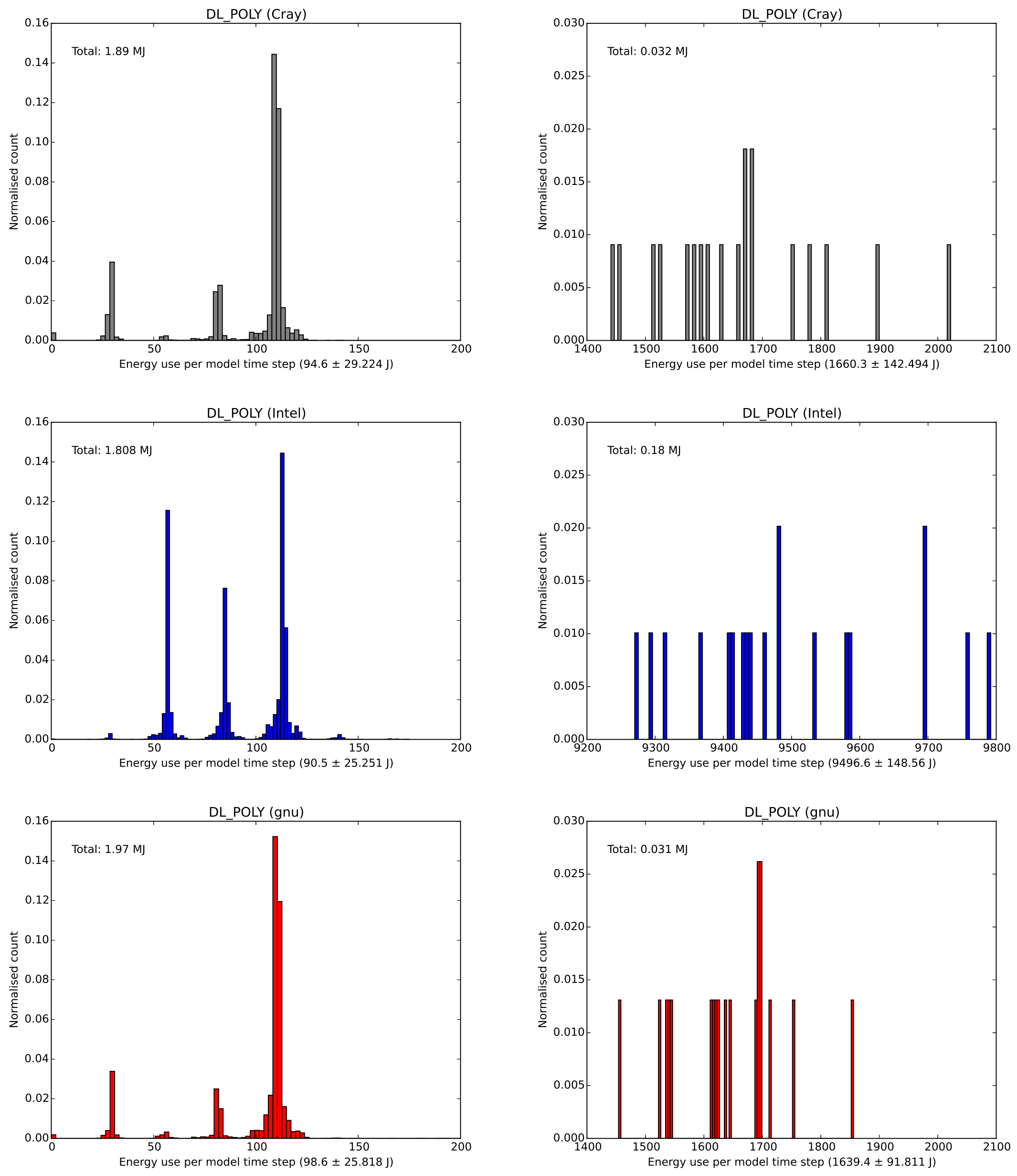


Figure 1: Histograms of energy used per DL_POLY simulation step over 0 – 200 J (left column) and > 200 J (right column). Plots are based on results obtained from the third run of six for each compiler environment, e.g., Cray (top row), Intel (middle row) and gnu (bottom row).

The Cray-compiled code had the lowest energy usage (1.92 ± 0.02 `MJ` over 1748 ± 2.6 `s`), followed by the Intel-compiled code (1.97 ± 0.01 `MJ` over 1770 ± 2.7 `s`), and lastly, the gnu-compiled code (2 ± 0.02 `MJ` over 1823 ± 2 `s`). The Cray energy usage is approximately 3% lower ($1.92/1.97 \approx 0.97$) than the Intel result and 4% lower than the mean result for the gnu runs. Unsurprisingly, energy usage follows execution time. However, the Intel runs show a marked difference as regards the high-energy iterations: for the Cray and gnu runs, these high-energy iterations are a factor of sixteen higher than the energy used for 99.9% of the simulation steps, whereas for the Intel runs, this factor increases to around ninety-five. Note, the Intel-compiled code would be the most energy efficient, if the total for the high-energy iterations (0.18 `MJ`) was reduced such that it matched the high-energy totals achieved by the Cray and gnu runs: in fact, this hypothetical reduction would make the Intel runs the most efficient ($\sim$ 5% lower than the Cray energy usage).

In order to understand more fully the impact of execution times on energy consumption, we show the distributions of execution times per simulation step (Figure 2) for the same runs as those featured in Figure 1. Again, the distributions are divided into two groups, short iterations (left column) and long iterations (right column) occurring every 1000 simulation steps (i.e., the restart dumps). The high energy steps consume more energy because those iterations take longer to execute; also, the Intel high-energy iterations run for the longest (by almost an order of magnitude).

Figure 3 presents example point-in-time power histograms. Unlike the cumulative energy results, these histograms correspond with a single normal distribution, giving a meaningful average and deviation, see the x-axis labels. Hence, the normal distributions inferred by the power histograms for all eighteen runs are also given in the bottom right plot. The Cray and gnu compiled codes have similar distributions as regards power measurements: therefore, the difference in energy usage for these two codes can be attributed to execution time. Overall, the Intel runs show the highest mean power and we also know that the high-energy iterations for the Intel runs are the most time consuming. Nevertheless, the Intel energy usage is mitigated by the fact that the majority low-energy iterations execute the fastest on average: in the left column of Figure 2, the Intel distribution is

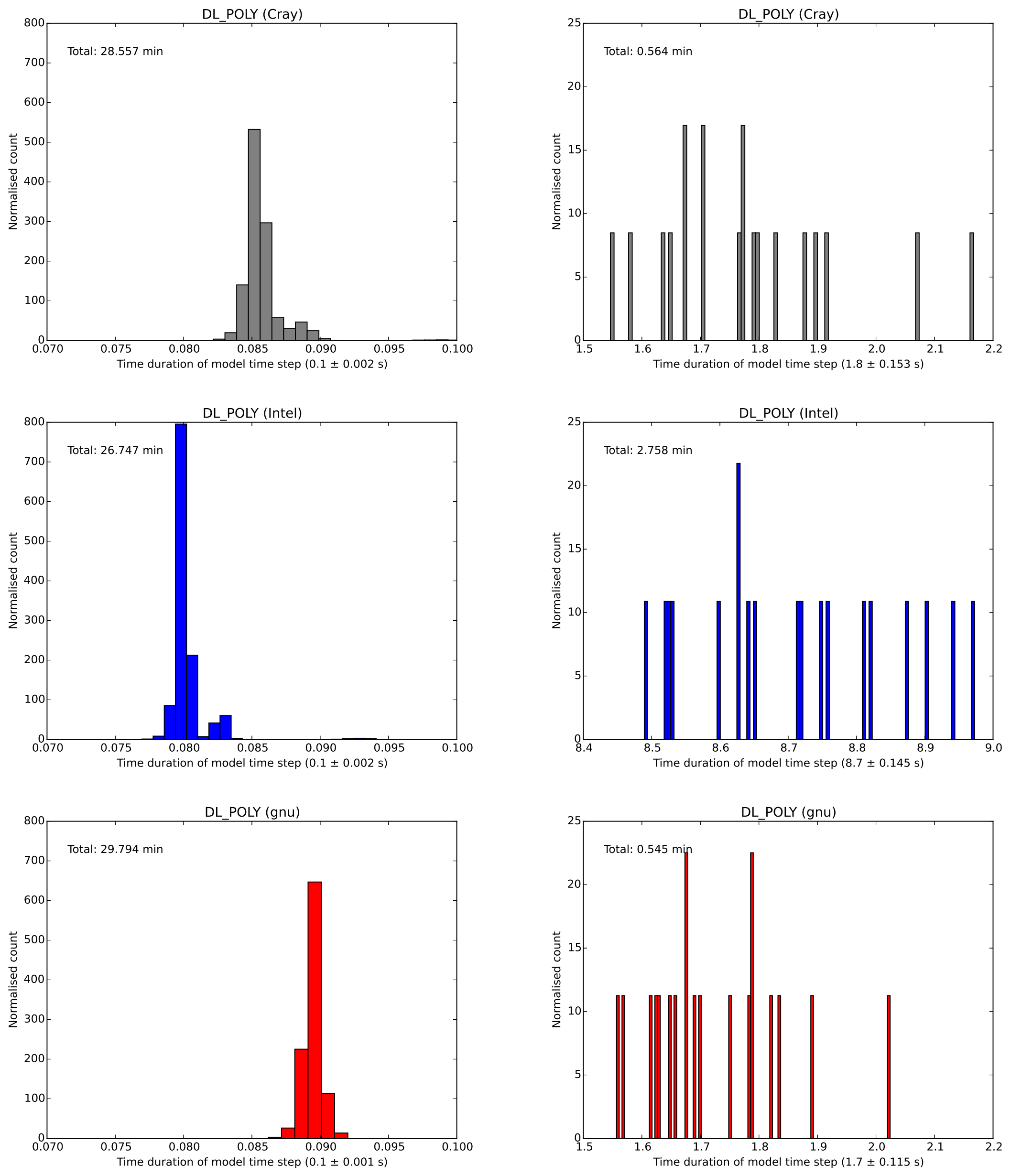


Figure 2: Histograms of time duration per DL_POLY simulation step over < 0.1 s (left column) and > 0.1 s (right column). Plots are based on results obtained from the third run of six for each compiler environment, e.g., Cray (top row), Intel (middle row) and gnu (bottom row).

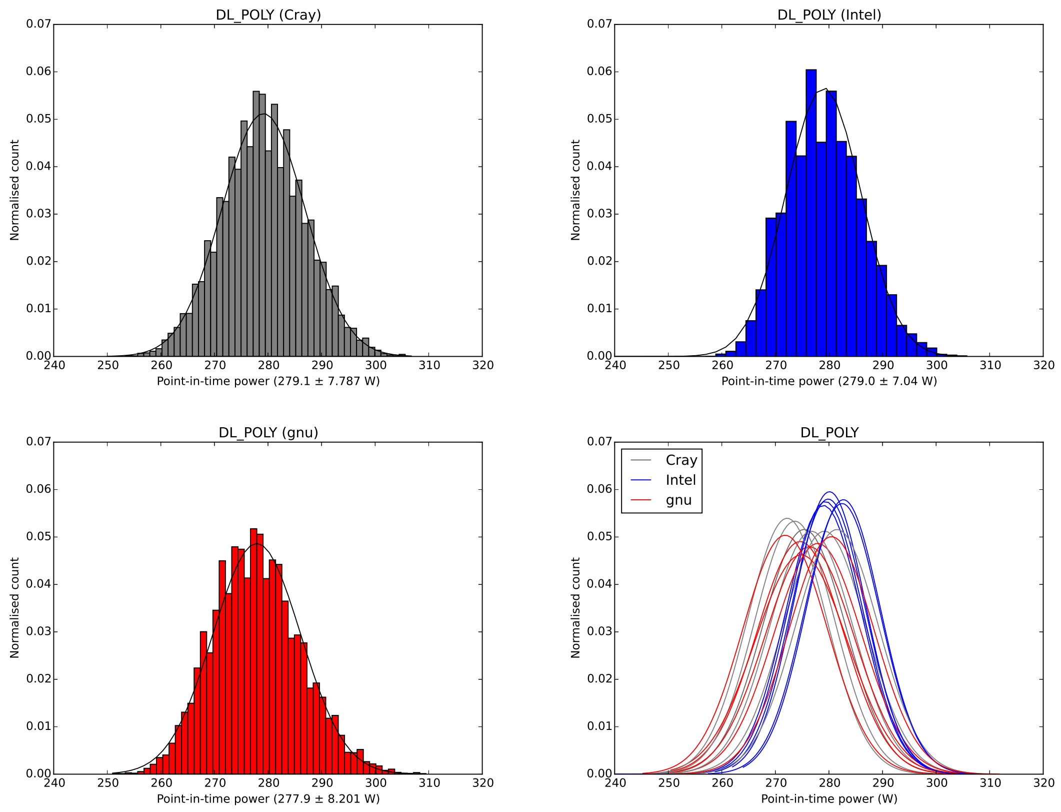


Figure 3: The point-in-time power histograms based on results obtained from the second run of six for each compiler environment. The plot at bottom right compares the normal distributions inferred from the power histograms of all eighteen runs.

furthest to the left. This mitigating factor is perhaps the reason why the Intel runs do not show the highest energy consumption.

4.2. OpenMP Threads

This section examines the impact of OpenMP thread count on energy usage when running the gnu-compiled CP2K code with the input data set entitled `H2O-1024.inp`, which can be found in the `./tests/QS/benchmark/` folder that resides within the CP2K installation directory. A particular loop within the CP2K source file, `./src/motion/md_run.F`, was instrumented with the three pm_mpi_lib functions mentioned earlier. The loop in question is labelled `Real MD Loop` and exists within the `qs_mol_dyn_low` subroutine. In addition, the value of the `MOTION.MD.STEPS` input parameter (i.e., the number of loop iterations) was changed from 10 to 100. The results were generated by running the CP2K code over eight nodes for a variety of threading options. Table 3 reveals an energy-usage

Table 3: Cumulative energies and run times for different CP2K threading options

`aprun` options	**Cumulative Energy [MJ]**	**Run Time [hr]**
`-n 192 -N 24 -S 12 -d 1`	52.263	5.4
`-n 96 -N 12 -S 6 -d 2`	49.727	5.94
`-n 64 -N 8 -S 4 -d 3`	45.052	5.27
`-n 48 -N 6 -S 3 -d 4`	48.819	6.26
`-n 32 -N 4 -S 2 -d 6`	54.284	7.47
`-n 24 -N 3 -d 8`	71.54	11.57
`-n 16 -N 2 -S 1 -d 12`	91.342	16.72

sweet spot for 3 threads per MPI process; increasing the thread count further causes the performance to deteriorate. The `aprun` option, `-ss`, was also set for six of the seven cases: this option was not used for the eight thread case, since it is not possible to evenly divide three MPI processes over two NUMA regions.

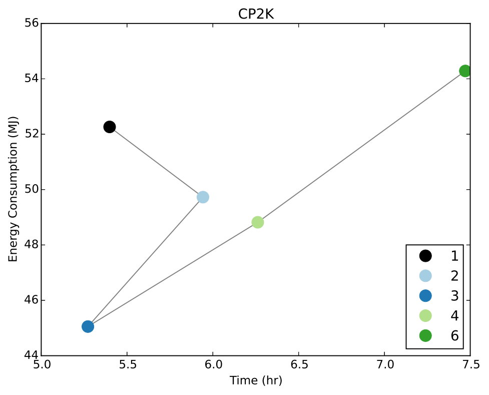


Figure 4: CP2K energy consumption against runtime for different OpenMP threading options (1-4 and 6 threads).

Figure 4 allows the reader to see the change in energy consumption and runtimes when increasing the thread count from one to six. Further increases in the thread count merely lengthen the runtime, thereby consuming more energy, see the last two rows of Table 3. Interesting behaviour occurs for low thread counts, e.g., when changing from one to two threads, the energy use comes down even though the runtime has increased. At three threads, both the runtime and energy consumption are reduced — this is the sweet spot.

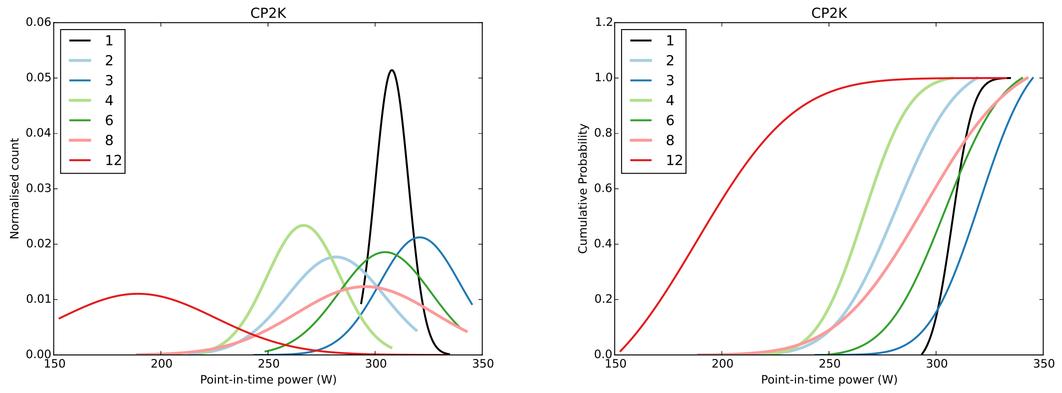


Figure 5: The normal distributions (left) and the cumulative distribution functions (right) inferred from the point-in-time power histograms across all OpenMP threading counts used for the CP2K code. A colour-blind safe version of this figure can be found in Appendix B.

The deviation in power readings becomes much more pronounced when the number of threads per MPI process is greater than one, see Figure 5 (left). Single-threaded execution gives a sharply defined peak at around 310 W. The power distributions increase in width for thread counts of 2-6, and then become even wider for the highest thread counts of 8 and 10. From left to right, the distribution peaks (and CDF curves) correspond to 12, 4, 2, 8, 6, 1 and 3 threads: this means that specifying 12 threads per MPI process draws the lowest mean power, whereas 3 threads results in the highest power usage.

5. Conclusions and Further Work

The DL_POLY results show the expected correlation between energy use and runtime. The choice of compiler does produce noticeable differences in energy usage: the Cray-compiled code uses the least energy, followed by Intel then gnu. However, the results also show that the evenly-spaced restart write iterations (19 out of 20 000) run for significantly longer, and furthermore, this disparity is more extreme for the Intel runs. Closer examination of the data, reveals that the Intel runs would use the least energy, if the compiler options could be set such that the Intel high-energy iterations had runtimes comparable with the Cray and gnu results.

Energy use will depend on the number of threads per MPI process: using multiple threads can reduce runtimes and energy usage but not beyond a certain thread count. Three threads is the optimum thread count for CP2K running over eight nodes with the `H2O-1024.inp` data set. Further work could investigate the importance of node assignment within the ARCHER dragonfly topology [1] as regards energy consumption. For example, running with three threads per MPI process, one could compare energy usages for the following scenarios.

1. All eight nodes from the same chassis.
2. Four nodes from one chassis and four nodes from a different chassis.
3. Same as scenario two but involving a chassis from a different group.

The first scenario involves communication within the rank 1 network only, the second will also feature communication over the rank 2 network, whereas the final scenario will involve communication over the optical rank 3 network. It is assumed that runtimes will increase should more communication hops between nodes be required: hence, these different scenarios should result in different node energies being recorded. The usefulness of this work would be in understanding the energy cost of communicating via the rank 2 and/or rank 3 networks. This work would of course need to be done on ARCHER itself as opposed to the test and development server (tds), which comprises only one group containing two cabinets. Note, the CP2K tests involving thread counts of 4 and 12 were performed on nodes that resided in different cabinets; the other CP2K tests involved nodes within the same chassis, thereby utilising the rank 1 network only. Regarding the DL_POLY results, 16 out of 18 runs were executed on nodes within the same chassis: the remaining two runs (one Cray and one gnu) featured a single node in the second tds cabinet.

A PM MPI Library

The source code is held in a Git repository [2] together with a makefile, and two small test harnesses that demonstrate how to call the library functions from Fortran and C codes. There is also a test folder containing `readme.txt` files that explain exactly how to integrate the pm_mpi_lib source with the DL_POLY and CP2K source codes. The following text describes the interface provided by the three functions of the pm_mpi_lib library.

1. `void pm_mpi_open(char* pmc_out_fn)`: the parameter, `pmc_out_fn`, points to a null-terminated string that specifies the name of the file that will hold the PM counter data: a `NULL` parameter will set the output file name to `./PMC`. The open function also calls `pm_mpi_monitor(0)` in order to determine a baseline for the cumulative energy. In addition, rank 0 establishes a temporal baseline by calling `MPI_Wtime` and also writes a one-line header to the output file, which gives the library version followed by the names of the data items that will appear in the subsequent lines.

2. `void pm_mpi_monitor(int nstep)`: the parameter, `nstep`, allows the client to label each set of counter values that are output by rank 0. The output file comprises lines of space-separated fields. A description of each field follows (the C-language data type is given in square brackets).

   Time [double]: the time as measured by `MPI_Wtime` (called by rank zero) that has elapsed since the last call to `pm_mpi_open`.

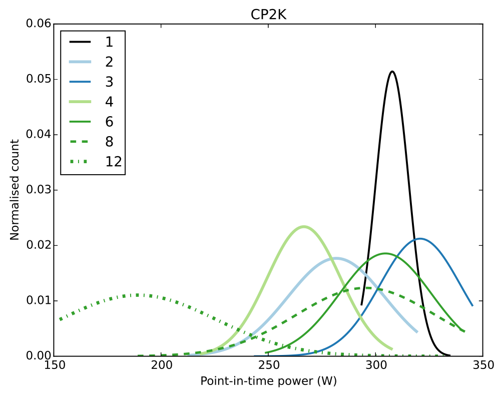
   Step [int]: a simple numerical label: e.g., the iteration count, assuming `pm_mpi_monitor` is being called from within a loop.

   Point-in-time power [double]: the average power reading across all assigned compute nodes.

   Energy [unsigned long long int]: the energy used by all assigned compute nodes since the last call to `pm_mpi_open`.

3. `void pm_mpi_close(void)`: calls `pm_mpi_monitor(nstep+1)`. All counter files are closed, then rank 0 closes the output file.

B Colour-blind Safe Version of Figure 5



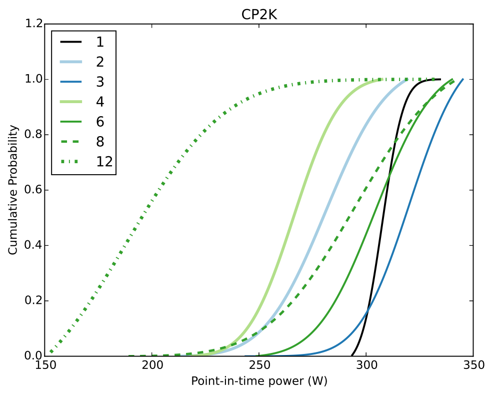


Figure 6: The normal distributions (left) and the cumulative distribution functions (right) inferred from the point-in-time power histograms across all OpenMP threading counts used for the CP2K code.

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