Using CrayPAT and Apprentice2: A Step- by-step guide

Abstract

This tutorial introduces HPE Cray users to the Cray Performance Analysis Tool and its Graphical User Interface, Apprentice2. The examples are based on the code supplied in the tarball, however, the techniques can easily be applied to any application that is compiled and executed on a HPE Cray supercomputer.

Introduction

The Cray Performance Analysis Tool (CrayPAT) is a powerful framework for analysing a parallel application's performance on Cray supercomputers. It can provide very detailed information on the timing and performance of individual application procedures, directly incorporating information from the raw hardware performance counters available on AMD Rome processors.

Sampling vs. Tracing

CrayPAT has two modes of operation, Sampling and Tracing. Sampling takes regular snapshots of the application, recording which routine the application was in. This can provide a good overview of the important routines in an application without interfering with the run time, however it has the potential to miss smaller functions and cannot provide the more detailed information like MPI messaging statistics or information from hardware performance counters.

Tracing involves instrumenting each subroutine with additional instructions that can record this extra information when they enter and exit. This approach ensures full capture of information, but can result in high overheads, especially where individual functions and subroutines are very small (as is typical in Objected Oriented languages like C++), it can also generate very large amounts

of data which become difficult to process and visualise.

CrayPAT's Automatic Program Analysis aims to capture the most important performance information without distorting the results by over instrumentation or generating large volumes of data. APA uses two steps, the first uses sampling to identify important functions in the application, it then uses this data, along with information about the size and number of calls to generate a modified binary with tracing included. This approach aims to cover the vast majority of application runtime with the minimum of overhead and provides a quick and straightforward method of analysing an application's performance on Cray supercomputers.

A step-by-step guide to using APA

This step-by-step guide demonstrates how to profile an application using CrayPAT's Automatic Program Analysis.

First, after logging on to the main system, users should load the perftools module.

module load perftools

The perftools module has to be loaded while all source files are compiled and linked. Next, load the NetCDF and HDF5 module (required by VH1):

module load cray-netcdf

module load cray-hdf5

The VH1 can be built with a simple call to:

cd src; make

To instrument then the binary, run the **pat_build** command with the **-O apa** option. This will generate a new binary with **+pat** appended to the end.

cd ../bin;

pat_build -O apa vh1-mpi-cray

You should now run the new binary on the backend using the **run**. **sh** script in the run directory. In this example you should edit the batch script change the

name of the executable to **vh1-mpi-cray+pat**. You should then submit this executable to run on the Cray backend.

sbatch --reservation=XXXX run.sh

(Replace the XXXX with the reservation name given to you by the course organisers). Once this has run, you will see that the run has generated an extra directory, **vh1-mpi-cray+pat+<number>s** in a directory <jobid_number>. This file contains the raw sampling data from the run and needs to be post processed to produce useful results. This is done using the pat_report tool which converts all the raw data into a summarised and readable form.

pat_report vh1-mpi-cray+pat+2681227-198s

Table 1: Profile by Function

This tool can generate a large amount of data, so you may wish to capture the data in an output file, either using a shell redirect like >, or adding the -o <file> option to the command.

```
Samp% | Samp | Imb. | Imb. | Group
       | Samp | Samp% | Function
      100.0% | 2,359.3 | -- | -- |Total
|-----
| 57.7% | 1,361.6 | -- | -- | USER
| 20.0% | 472.2 | 38.8 | 7.9% | parabola_
| 12.7% | 298.7 | 43.3 | 13.2% | riemann_
| 5.9% | 140.2 | 20.8 | 13.5% |sweepz_
| 5.6% | 133.2 | 33.8 | 21.1% | remap_
| 3.2% | 76.3 | 9.7 | 11.8% |sweepy_
| 3.0% | 71.5 | 14.5 | 17.6% | paraset_
| 1.9% | 45.8 | 14.2 | 24.8% | evolve
| 1.9% | 44.2 | 14.8 | 26.2% | states
| 1.1% | 27.1 | 7.9 | 23.5% | flatten_
| 1.0% | 22.8 | 11.2 | 34.4% |sweepx1
| 37.6% | 887.8 | -- | -- |MPI
||-----
|| 36.5% | 861.8 | 83.2 | 9.2% |mpi_alltoall
| 4.2% | 100.0 | -- | -- |ETC
||-----
|| 2.6% | 60.3 | 13.7 | 19.3% |__cray_sset_SNB
| 1.5% | 34.4 | 8.6 | 20.9% | cray scopy SNB
```

Table 1 - User functions profiled by samples

Table 1 above shows the results from sampling the application. Program functions are separated out into different types, USER functions are those defined by the application, MPI functions contains the time spent in MPI library functions, ETC functions are generally library or miscellaneous functions included. ETC function can include a variety of external functions, from mathematical functions called in by the library (as is this case) to system calls.

The raw number of samples for each code section is show in the second column and the number as an absolute percentage of the total samples in the first. The third column is a measure of the imbalance between individual processors being sampled in this routine and is calculated as the difference between the average number of samples over all processors and the maximum samples an individual processor was in this routine.

The profile also generated two other files that are useful in the profiling directory, one with the extension .ap2 which holds the same data as the .xf but in the post processed form. The other file has a .apa extension and is a text file with a suggested configuration for generating a traced experiment. You are welcome and encouraged to review this file and modify its contents in subsequent iterations, however in this first case we will continue with the defaults.

This .apa file acts as the input to the pat_build command and is supplied as the argument to the -O flag.

pat_build -O build_options.apa

This will produce a third binary with extension +apa. Copy this binary into the bin/directory. This binary should once again be run on the back end, so the input run.sh script should be modified and the name of the executable changed to vh1-mpi-cray+apa. The script is then submitted to the backend.

sbatch -- reservation=XXXX run.sh

(Replace the XXXX with the reservation name given to you by the course organisers). Again, a new profile directory will be generated by the application, which should be processed by the pat_report tool. As this is now a tracing experiment it will provide more information than before

pat_report vh1-mpi-cray+apa+2681298-198s

Table 1: Profile by Function Group and Function

```
Time | Imb. | Imb. | Calls | Group
          | Time | Time% | Function
              100.0% | 67.740903 | -- | -- | 7,373,686.5 | Total
| 76.4% | 51.733412 | -- | -- | 7,372,951.0 | USER
| 24.8% | 16.776085 | 2.516269 | 13.6% | 460,800.0 | remap_
| 11.1% | 7.529205 | 3.421455 | 32.6% | 1.0 | vhone
| 11.0% | 7.447873 | 0.953479 | 11.8% |
                                        50.0 |sweepz
| 10.6% | 7.186668 | 0.967835 | 12.4% | 100.0 | sweepy
  9.3% | 6.289532 | 2.906604 | 33.0% | 4,147,200.0 |parabola_
  4.5% | 3.048572 | 0.517124 | 15.1% | 460,800.0 | riemann_
  1.6% | 1.104668 | 0.641691 | 38.3% | 921,600.0 | paraset_
 1.4% | 0.964630 | 0.366043 | 28.7% | 460,800.0 | evolve_
 1.1% | 0.727949 | 0.346536 | 33.7% | 460,800.0 | flatten_
 1.0% | 0.658229 | 0.320822 | 34.2% | 460,800.0 | states_
| 21.9% | 14.863376 | -- | -- | 363.2 |MPI_SYNC
|| 17.5% | 11.826659 | 9.977789 | 84.4% | 300.0 |mpi_alltoall_(sync)
\parallel \ \ 3.9\% \ | \ \ 2.608508 \ | \ \ 2.592821 \ | \ \ 99.4\% \ | \qquad 51.0 \ | mpi\_allreduce\_(sync)
| 1.7% | 1.144092 | -- | -- | 371.3 |MPI
\parallel 1.6\% \mid 1.086442 \mid 0.023866 \mid 2.2\% \mid 300.0 \mid mpi\_alltoall
|-----
```

Table 2 – User functions profiled using tracing

The updated table above (Table 2) is the version generated from tracing data instead of the previous sampling data table (Table 1). This version makes true timing information is available (averages per processor) and the number of times each function is called. Table 3 shows the information available for individual functions. Timings are more accurate and features like the number of calls are available. Information from the Rome hardware performance counters is also available.

USER / remap

Time% 24.8% Time 16.776085 secs Imb. Time 2.516269 secs Imb. Time% 13.6% 460,800.0 calls 0.025M/sec Calls CPU_CLK_UNHALTED:THREAD_P 87,504,487,183 CPU_CLK_UNHALTED:REF_P 2,979,085,085 DTLB_LOAD_MISSES:MISS_CAUSES_A_WALK 20,952,547 DTLB_STORE_MISSES:MISS_CAUSES_A_WALK 7.282.943 1,714,128,948 L1D:REPLACEMENT L2 ROSTS:ALL DEMAND DATA RD 1,861,959,568 L2_RQSTS:DEMAND_DATA_RD_HIT 1,747,562,343 FP_COMP_OPS_EXE:SSE_SCALAR_DOUBLE 1,642 FP_COMP_OPS_EXE:SSE_FP_SCALAR_SINGLE 772,302,817 FP_COMP_OPS_EXE:X87 845,393,483 FP_COMP_OPS_EXE:SSE_PACKED_SINGLE 127,020,303 SIMD_FP_256:PACKED_SINGLE 5,099,855,700 User time (approx) 18.663 secs 50,407,589,746 cycles 100.0% Time CPU_CLK 2.94GHz HW FP Ops / User time 2,300.039M/sec 42,924,624,751 ops 10.6%peak(DP) Total SP ops 2,254.740M/sec 42,079,229,626 ops Total DP ops 45.299M/sec 845,395,124 ops MFLOPS (aggregate) 55.200.93M/sec D2 cache hit, miss ratio 93.3% hits 6.7% misses D2 to D1 bandwidth 6,089.462MiB/sec 119,165,412,368 bytes Average Time per Call 0.000036 secs

Table 3 – Per function hardware performance counter information

11.7%

Additional documentation is available for CrayPAT and can be accessed either through the man pages for individual commands or through the interactive CrayPAT command (requires perftools to be loaded):

pat_help

CrayPat Overhead: Time

Or though man pages:

man intro_pat man pat_build man pat_report

Apprentice2

Apprentice2 is the Graphic User Interface and visualisation suite for CrayPAT's performance data. It reads the .ap2 files from the profile output directory generated by pat_report's the profile files. It is launched from the command line with:

app2 profile_directory>

Figure 1 shows a screenshot of the call tree information available from CrayPAT. It shows how time is spent along the call tree, inclusive time corresponds to the width of boxes, excluding time to the height. Yellow represents the load imbalance time between processors. Extra information is provided by holding the mouse over areas of the screen, the "?" box will provide hints on how to interpret the information displayed.

Accessing Temporal Information

Tracing an application can potentially generate very large amounts of data, to reduce this volume the CrayPAT will, by default, summarise the data over the entire application run. To see more detailed information about the timing of individual events (like the sequencing of MPI messages between processors or the number of hardware counter events in a time interval) CrayPAT has to be instructed to store all data from throughout the run. This is controlled by the PAT_RT_SUMMARY environment variable, setting it to 0 in run.sh will prevent summarising and allow access to even more data.

export PAT_RT_SUMMARY=0

Warning! Running tracing experiment on a large number of processors for a long period of time will generate VERY large files! Most tracing experiments should be conducted on a small number of processors (<= 256) and over a short wall clock time period (< 5 minute).

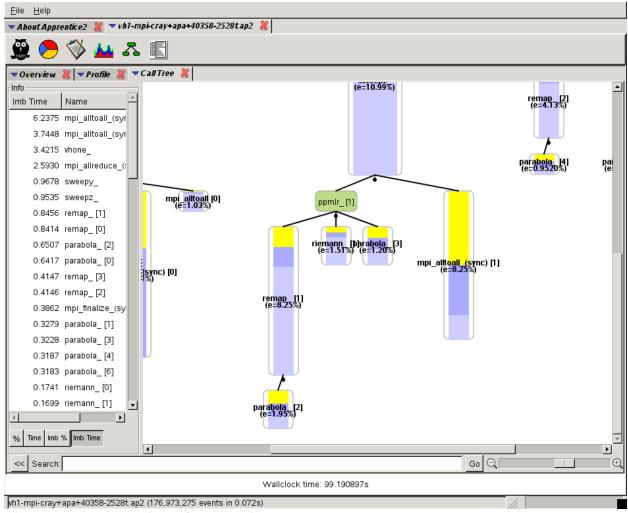


Figure 1 – A screenshot of Apprentice 2.