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Performance Analysis on ARCHER using CrayPAT

ARCHER Virtual Tutorial, 11th March 2015

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Outline

- Overview of CrayPAT
- Perftools-lite
- Sampling Experiments
- Tracing Experiments
 - Automated Profile Analysis
 - Hardware counters
- CrayPAT GUI
- Using the CrayPAT API



Further Help

- ARCHER Best Practice Guide:
 - <http://www.archer.ac.uk/documentation/best-practice-guide/performance.php>
- CrayDoc:
 - <http://docs.cray.com>
 - Search "Using Cray Performance Measurement and Analysis Tools"
- Online help:
 - Man pages for the tools
 - `pat_help` utility
- ARCHER training archive:
 - <http://www.archer.ac.uk/training/courses/craytools/>



Why profile?

- For developers:
 - Understand what the most time-consuming parts of a program are
 - Understand communication patterns & problems
 - E.g. load imbalance, synchronisation costs
 - Tool to help direct development effort to for maximum benefits
- For users?
 - Understand why your program performs in a certain way
 - Help with choice of appropriate parameters, MPI processes...



Overview of CrayPAT

- Cray's Performance Analysis Toolkit (PAT)
 - Measuring and understanding performance of parallel codes on Cray systems
- Parallel Programming languages / APIs:
 - MPI, OpenMP, CUDA, CAF, Chapel, Global Arrays, DMAPP, SHMEM...
- Libraries:
 - BLAS/LAPACK/ScaLAPACK, FFTW, PETSc...
- I/O:
 - ADIOS, HDF5, NetCDF, POSIX I/O, (MPI I/O)...



Overview of CrayPAT

- Compared with other tools
 - e.g. Alinea MAP, Intel TAC, Scalasca, TAU ...
 - + Works 'out of the box'
 - + Various levels of detail
 - + Extreme customisability for expert users
 - Only on Cray Platforms
 - GUI not as powerful as e.g. MAP



Overview of CrayPAT

- Tools

- `pat_build`
 - Instruments existing binaries for profiling
- `pat_report`
 - Report generator, analyses data from profiling runs
- Apprentice2
 - GUI for analysing profiling data
- Reveal
 - GUI for code-level analysis, compile-time optimization feedback
 - NB. For Cray compiler only.

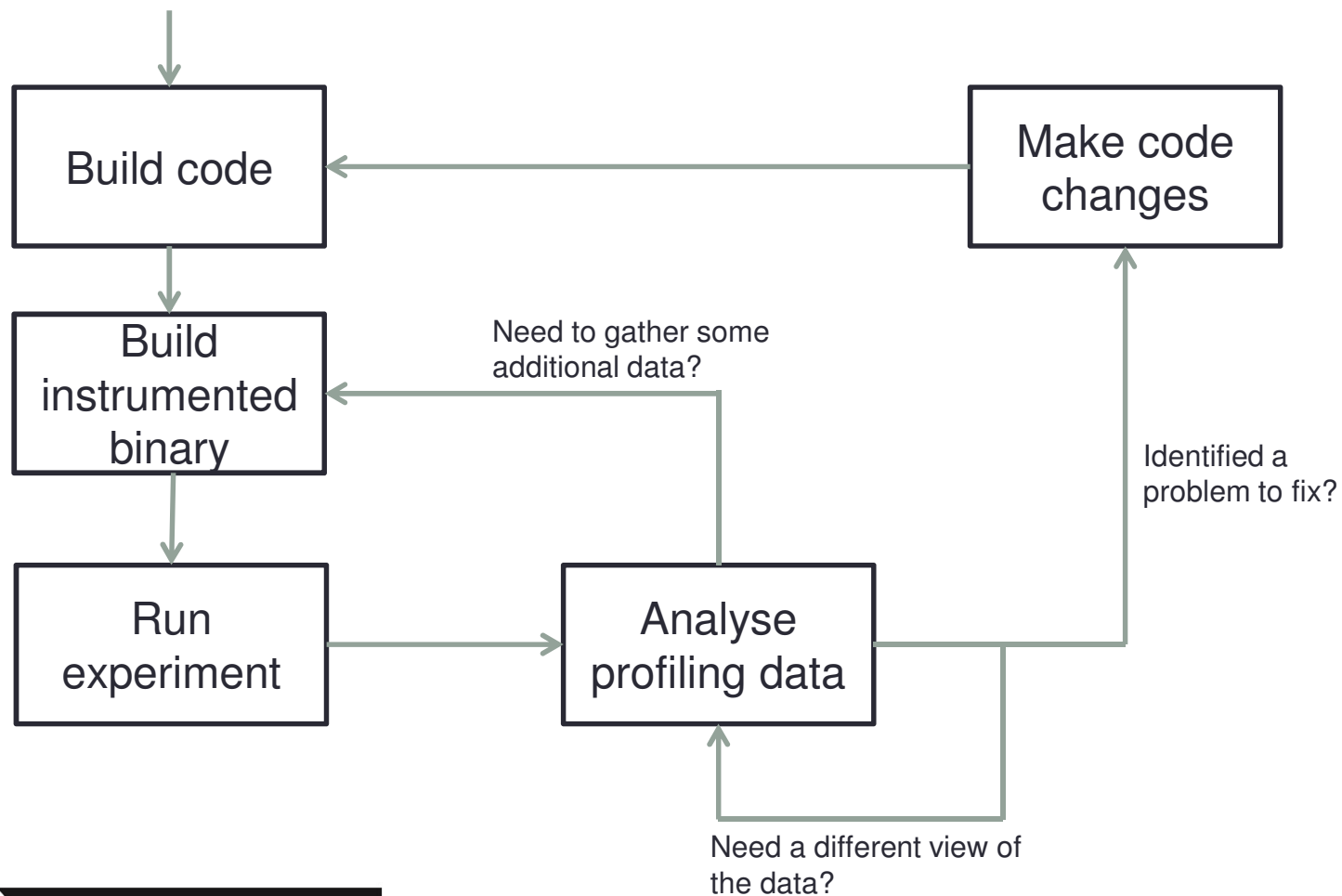


Overview of CrayPAT

- Choosing a suitable job for profiling
 - Program execution should be representative of real production job
 - Must be reasonably short, to avoid generating large data, waste AUs
 - Must be long (enough) to hide start-up, finalisation parts
 - Should include all the I/O of a normal job
- Example
 - Using CP2K - www.cp2k.org
 - H2O-64 benchmark - <http://www.cp2k.org/performance#h20-64>
 - Takes ~80s using 24 MPI processes, single node of ARCHER



Overview of CrayPAT



Perftools-lite

- Extremely easy introduction to profiling tools
 - Automatically gather profiling data during program execution
 - Basic reporting dumped into standard output at end of run
 - Generate CrayPAT data files for further analysis (if needed)



Perftools-lite

1. Load the **perftools-lite** module

```
module load perftools-lite
```

2. Build your program as normal

- Use your configure, Makefile, build scripts etc.
- Look for message at end:

```
INFO: creating the CrayPat-instrumented executable  
' /home/z01/z01/ibethune/cp2k/exe/ARCHER/cp2k.psmpp '  
(sample_profile) ...OK
```



Perftools-lite

3. Run your program
 - Usual PBS job submission script

4. Basic profiling data appears at the end of job output
 - Overall job info
 - Top 10 most time-consuming functions
 - I/O, memory information
 - Report also saved in `*.rpt` file
 - A CrayPAT performance data file `*.ap2` also created for further analysis



Perftools-lite

See example files.



Sampling Experiments

- What is sampling?
 - Every so often (100 Hz default), look at the call stack of the program
 - Record which function is being executed (+ callers etc.)
- A good starting point if you know nothing about the behaviour of a program
- Low overhead (~1%)
- Very easy to set up & run



Sampling Experiments

1. Load the **perftools** module

```
module load perftools
```

2. Build your program as normal

- Use your configure, Makefile, build scripts etc.
- NB. Compile and link stages must be separated

3. Build a sampling-instrumented program

```
pat_build -o cp2k.psmtp+samp cp2k.psmtp
```



Sampling Experiments

3. Run your program
 - Usual PBS job submission script
 - Change the name of the executable!
4. Once job has completed, CrayPAT will dump data file(s) into the run directory
 - * .xf file
 - Or, if running on large numbers of PEs, a directory containing several * .xf files



Sampling Experiments

5. Generate a report on the data

```
pat_report *.xf > report
```

- Produces a text report file
- Produces a portable performance data file *.ap2
- Produces a *.apa Automated Profiling Analysis file



Sampling Experiments

See example files.



Tracing Experiments

- What is tracing?
 - ‘Trace intercept routines’ inserted at entry and exit of routines
 - Records amount of time spend in each call of a function
 - Exact sequence of events in a program execution
 - Allows for checking state of hardware counters
 - Possible to generate endless detail about program execution
 - Moderate overhead (~5-10%), depending on what you choose to trace
 - Balance between detailed measurement and disturbing the experiment



Tracing Experiments

1. Load the **perftools** module

```
module load perftools
```

2. Build your program as normal

- Use your configure, Makefile, build scripts etc.
- NB. Compile and link stages must be separated

3. Build a tracing-instrumented program

```
pat_build [options] -o cp2k.psmpt+trace cp2k.psmpt
```



Tracing Experiments

- Pat_build options:
 - For full list see `man pat_build`
 - Tracegroups (`-g`)
 - e.g. `mpi`, `lapack`, `omp`
 - Tracing user functions
 - `-w` enables tracing user functions
 - `-T` trace specific functions
 - `-u` trace all visible user functions (use with extreme caution!)
- Complex to set up
 - Except if you only want to trace e.g. MPI library calls
 - This is where APA helps



Tracing Experiments

- Automated Profiling Analysis (APA)
 - From the sampling experiment report generation, a *.apa file was generated containing recommended options for pat_build to set up a tracing experiment

```
pat_build -O *.apa
```

- Defaults:
 - Trace MPI calls
 - Gather default hardware counter group
 - Trace user functions with > 1% of samples, up to limit of 200
 - Very small functions (< 200 bytes) not traced to limit overhead



Tracing Experiments

3. Run your program
 - Usual PBS job submission script
 - Change the name of the executable!
4. Once job has completed, CrayPAT will dump data file(s) into the run directory
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Tracing Experiments

5. Generate a report on the data

```
pat_report *.xf > report
```

- Produces a text report file
- Produces a portable performance data file *.ap2



Tracing Experiments

- `pat_report` options
 - Report generation is (almost) endlessly customisable
 - There are several pre-defined reports that are a good place to start:
 - `-O profile` (default) – list of most expensive functions
 - `-O calltree / callers` – top-up / bottom up function calls
 - `-O ca+src` – as above, with line numbers
 - `-O load balance` – displays min/mean/max across Pes
 - Each table in the report lists which options are needed to generate it:
 - e.g. Table option:
`-O profile`
- Options implied by table option:
- ```
-d ti%@0.95,ti,imb_ti,imb_ti%,tr -b gr,fu,pe=HIDE
```



# Tracing Experiments

- Implied options are a good starting point for customisation
  - See `man pat_report` for full list of options
- Each table also suggests options for related tables, and additional `pat_report` flags
- Also, check the ‘Observations and suggestions’ section



# Tracing Experiments

See example files.



# CrayPAT GUI

- CrayPAT includes a GUI called Apprentice2
  - Reads the portable \* .ap2 file format
  - Graphical view of the calltree
  - Chart views of selected data
  - Hardware counters, activity graphs
  - Application trace available by setting `PAT_RT_SUMMARY=0` before running your application
  - **Warning** – v. large trace files (MBs -> GBs!)
- Can be run directly from ARCHER via X-windows  
`app2 &`
- Or binaries available for Mac & Windows  
`/opt/cray/perftools/6.2.2/share/desktop_installers/`



# CrayPAT GUI

See example files.



# Using the CrayPAT API

- For even finer-graining tracing, CrayPAT provides an API to control tracing

- Start/stop tracing at certain points
- Define regions within (or spanning) subroutine calls

```
PAT_region_begin(1, "region name")
```

```
PAT_region_end(1)
```

- Also a Fortran API

- Build application, then instrument binary with

```
pat_build -w -o cp2k.psm+api cp2k.psm
```

- May also include `-g mpi` etc.





# Using the CrayPAT API

- Application code with CrayPAT API calls now depends on CrayPAT library
  - Will not build without perftools module loaded
- If including in production code, protect CrayPAT calls with preprocessor defines.



That's all folks!

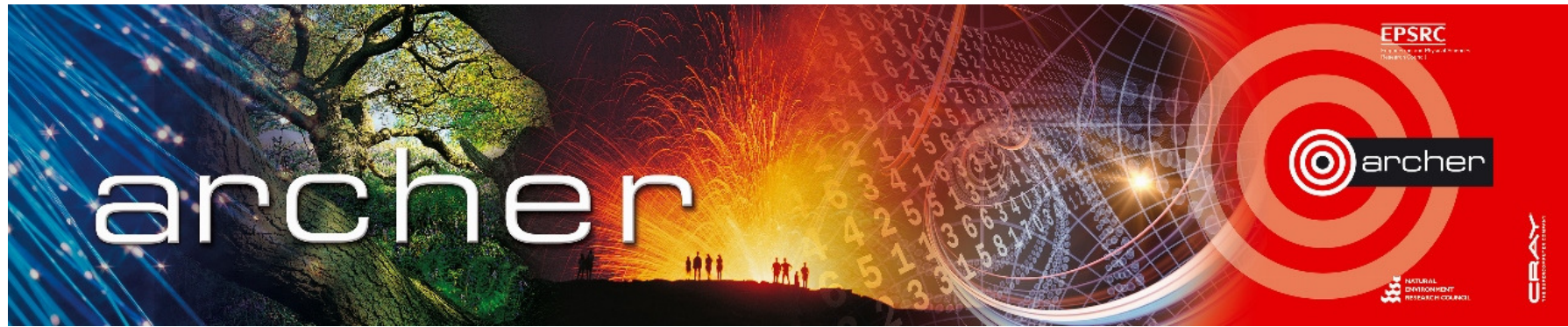
Questions?



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