Single Node Optimisation

Profiling

Reusing this material

What is profiling?

- Analysing your code to find out the proportion of execution time spent in different routines.
- Essential to know this if we are going to target optimisation.
- No point optimising routines that don't significantly contribute to the overall execution time.
  - can just make your code less readable/maintainable

Code profiling

- Code profiling is the first step for anyone interested in performance optimisation
- Profiling works by instrumenting code at compile time
  - Thus it's (usually) controlled by compiler flags
  - Can reduce performance
- Standard profiles return data on:
  - Number of function calls
  - Amount of time spent in sections of code
- Also tools that will return hardware specific data
  - Cache misses, TLB misses, cache re-use, flop rate, etc…
  - Useful for in-depth performance optimisation

Sampling and tracing

- Many profilers work by sampling the program counter at regular intervals (normally 100 times per second).
  - low overhead, little effect on execution time
- Builds a statistical picture of which routines the code is spending time in.
  - if the run time is too small (< ~10 seconds) there aren't enough samples for good statistics
- Tracing can get more detailed information by recording some data (e.g. time stamp) at entry/exit to functions
  - higher overhead, more effect on runtime
  - unrestrained use can result in huge output files

Standard Unix profilers

- Standard Unix profilers are prof and gprof
- Many other profiling tools use same formats
- Usual compiler flags are **`-p`** and **`-pg`**:
  - **`ftn -p mycode.F90 -o myprog`** for prof
  - **`cc -pg mycode.c -o myprog`** for gprof
- When code is run it produces instrumentation log
  - **`mon.out`** for prof
  - **`gmon.out`** for gprof
- Then run prof/gprof *on your executable program*
  - eg. **`gprof myprog`** (*not* **`gprof gmon.out`**)

Standard profilers

- **`prof myprog`** reads **`mon.out`** and produces this:

```
%Time Seconds Cumsecs  #Calls   msec/call  Name
 32.4    0.71    0.71      14     50.7     relax_
 28.3    0.62    1.33      14     44.3     resid_
 11.4    0.25    1.58       3     83.      __f90_close
  5.9    0.13    1.71 1629419      0.0001  _mcount
  5.0    0.11    1.82  339044      0.0003  __f90_slr_i4
  5.0    0.11    1.93  167045      0.0007  __inrange_single
  2.7    0.06    1.99     507      0.12    _read
  2.7    0.06    2.05       1     60.      MAIN_
```

Standard profilers

- **`gprof myprog`** reads **`gmon.out`** and produces something very similar
- **`gprof`** also produces a program calltree sorted by inclusive times
- Both profilers list all routines, including obscure system ones
    - Of note: **`mcount`**(), **`_mcount`**(), **`moncontrol`**(), **`_moncontrol`**() **`monitor`**() and **`_monitor`**() are all overheads of the profiling implementation itself
    - **`_mcount`**() is called every time your code calls a function; if it's high in the profile, it can indicate high function-call overhead
    - **`gprof`** assumes calls to a routine from different parents take the same amount of time – may not be true

The Golden Rules of profiling

- **Profile your code**
  - The compiler/runtime will NOT do all the optimisation for you.
- **Profile your code yourself**
  - Don't believe what anyone tells you. They're wrong.
- **Profile on the hardware you want to run on**
  - Don't profile on your laptop if you plan to run on ARCHER2.
- **Profile your code running the full-sized problem**
  - The profile will almost certainly be qualitatively different for a test case.
- **Keep profiling your code as you optimise**
  - Concentrate your efforts on the thing that slows your code down.
  - This will change as you optimise.
  - So keep on profiling.

CrayPAT

- Can do both statistic sampling and function/loop level tracing.

Recommended usage:

1. Build and instrument code
2. Run code and get statistic profile
3. Re-instrument based on profile
4. Re-run code to get more detailed tracing

Example with CrayPAT

- Load performance tools software
  ~~`module load perftools-base`~~ (automatically loaded on ARCHER2)

  `module load perftools-lite`

- Re-build application (keep .o files)
  ```
  make clean
  make
  ```

- Application automatically instrumented for you

- Run the instrumented application to get top time consuming routines
  - You should get performance profiling in your Slurm output file
  - You should get a performance file <executable_name+93500-1088s>

Example with CrayPAT

epcc

CrayPat/X: Version 20.10.0 Revision 7ec62de47 09/16/20 16:57:54
Experiment: lite lite-samples
……

```
Table 1:  Profile by Function

  Samp% |  Samp | Imb. |  Imb. | Group
        |       | Samp | Samp% |  Function=[MAX10]
        |       |      |       |   PE=HIDE

 100.0% | 305.8 |   -- |    -- | Total
|-----------------------------------------------
|  54.4% | 166.4 |   -- |    -- | MPI
||----------------------------------------------
||  51.6% | 157.8 | 24.2 | 13.4% | MPI_ALLTOALL
||   1.4% |   4.4 |  5.6 | 56.4% | MPI_ALLREDUCE
||==============================================
|  41.7% | 127.5 |   -- |    -- | USER
||----------------------------------------------
||  10.5% |  32.2 | 17.8 | 36.0% | riemann_
||   9.9% |  30.4 | 20.6 | 40.7% | parabola_
||   4.8% |  14.8 | 11.2 | 43.5% | sweepz_
||   4.6% |  13.9 | 10.1 | 42.3% | remap_
||   3.5% |  10.7 |  9.3 | 46.7% | sweepy_
||   2.3% |   7.0 |  9.0 | 56.4% | paraset_
||   1.8% |   5.4 |  9.6 | 64.4% | evolve_
||   1.4% |   4.2 |  5.8 | 58.0% | states_
||==============================================
|   3.0% |   9.1 |   -- |    -- | ETC
|==============================================
```

……

Program invocation:
 /lus/cls01095/work/z19/z19/adrianj/DistributedStream/src/./distributed_streams

For a complete report with expanded tables and notes, run:
 pat_report /lus/cls01095/work/z19/z19/adrianj/DistributedStream/src/distributed_streams+93500-1088s

For help identifying callers of particular functions:
 pat_report -O callers+src /lus/cls01095/work/z19/z19/adrianj/DistributedStream/src/distributed_streams+93500-1088s
To see the entire call tree:
 pat_report -O calltree+src /lus/cls01095/work/z19/z19/adrianj/DistributedStream/src/distributed_streams+93500-1088s

For interactive, graphical performance analysis, run:
 app2 /lus/cls01095/work/z19/z19/adrianj/DistributedStream/src/distributed_streams+93500-1088s

```
Notes for table 2:

  This table shows functions, and line numbers within functions, that
    have significant exclusive sample hits, averaged across ranks.
  For further explanation, see the "General table notes" below,
    or use:  pat_report -v -O samp_profile+src ...

Table 2:  Profile by Group, Function, and Line

  Samp% |  Samp | Imb. |  Imb. | Group
        |       | Samp | Samp% |  Function=[MAX10]
        |       |      |       |   Source
        |       |      |       |    Line
        |       |      |       |     PE=HIDE

 100.0% | 305.8 |   -- |    -- | Total
|-------------------------------------------------------------
|  54.4% | 166.4 |   -- |    -- | MPI
||------------------------------------------------------------
||  51.6% | 157.8 | 24.2 | 13.4% | MPI_ALLTOALL
||   1.4% |   4.4 |  5.6 | 56.4% | MPI_ALLREDUCE
||============================================================
|  41.7% | 127.5 |   -- |    -- | USER
||------------------------------------------------------------
||  10.5% |  32.2 |   -- |    -- | riemann_
3|        |       |      |       |  Archer2Opt/VH1/src/riemann.f90
||||----------------------------------------------------------
4|||   3.4% |  10.5 |  9.5 | 47.6% | line.77
4|||   3.5% |  10.6 |  8.4 | 44.4% | line.78
||||==========================================================
||   9.9% |  30.4 |   -- |    -- | parabola_
3|        |       |      |       |  Archer2Opt/VH1/src/parabola.f90
||||----------------------------------------------------------
4|||   2.5% |   7.7 |  8.3 | 52.0% | line.45
4|||   1.9% |   6.0 |  6.0 | 50.8% | line.86
||||==========================================================
||   4.8% |  14.8 |   -- |    -- | sweepz_
3|        |       |      |       |  Archer2Opt/VH1/src/sweepz.f90
||||----------------------------------------------------------
4|||   1.3% |   4.0 |  6.0 | 60.5% | line.27
4|||   1.1% |   3.5 |  4.5 | 57.1% | line.33
||||==========================================================
||   4.6% |  13.9 |   -- |    -- | remap_
3|        |       |      |       |  Archer2Opt/VH1/src/remap.f90
||   3.5% |  10.7 |   -- |    -- | sweepy_
3|        |       |      |       |  Archer2Opt/VH1/src/sweepy.f90
||   2.3% |   7.0 |   -- |    -- | paraset_
3|        |       |      |       |  Archer2Opt/VH1/src/parabola.f90
||   1.8% |   5.4 |   -- |    -- | evolve_
3|        |       |      |       |  Archer2Opt/VH1/src/evolve.f90
||   1.4% |   4.2 |   -- |    -- | states_
3|        |       |      |       |  Archer2Opt/VH1/src/states.f90
||============================================================
|   3.0% |   9.1 |   -- |    -- | ETC
|=============================================================
```

archer2

Example with CrayPAT

- Load performance tools software
  ~~`module load perftools-base`~~ (automatically loaded on ARCHER2)
  `module load perftools`

- Re-build application (keep .o files)
  ```
  make clean
  make
  ```

- Instrument application for automatic profiling analysis
  - You should get an instrumented program `a.out+pat`
    `pat_build –O apa a.out`

- Run the instrumented application (...+pat) to get top time consuming routines
  - You should get a performance file (“`<sdatafile>.xf`”) or multiple files in a directory `<sdatadir>`

Example with CrayPAT (2/2)

epcc

- Generate text report and an `.apa` instrumentation file
  pat_report [<sdatafile>.xf | <sdatadir>]
  - Inspect the `.apa` file and sampling report whether additional instrumentation is needed
    - See especially sites “Libraries to trace” and “HWPC group to collect”
- Instrument application for further analysis (a.out+apa)
  pat_build –O <apafile>.apa
- Run application (…+apa)
- Generate text report and visualization file (.ap2)
  pat_report –o *my_text_report.txt* <data>
- View report in text and/or with Cray Apprentice[2]
  app2 <*datafile*>.ap2

archer2

Finding single-core hotspots

- Remember: pay attention only to user routines that consume significant portion of the total time
- View the key hardware counters, for example
  - L1 and L2 cache metrics
  - use of vector (SSE/AVX) instructions

- CrayPAT has mechanisms for finding “the” hotspot in a routine (e.g. in case the routine contains several and/or long loops)
  - CrayPAT API
    - Possibility to give labels to “PAT regions”
  - Loop statistics (works only with Cray compiler)
    - Compile & link with CCE using -h profile_generate
    - pat_report will generate loop statistics if the flag is enabled

```
USER / remap_
-----------------------------------------------------------------------------
  Time%                                                     25.2%
  Time                                                  15.801180 secs
  Imb. Time                                              2.582609 secs
  Imb. Time%                                                14.7%
  Calls                             0.026M/sec          460,800.0 calls
  CPU_CLK_UNHALTED:THREAD_P                        77,964,376,624
  CPU_CLK_UNHALTED:REF_P                            2,689,572,161
  DTLB_LOAD_MISSES:MISS_CAUSES_A_WALK                  20,626,569
  DTLB_STORE_MISSES:MISS_CAUSES_A_WALK                 17,745,058
  L1D:REPLACEMENT                                   2,753,483,367
  L2_RQSTS:ALL_DEMAND_DATA_RD                       1,912,839,218
  L2_RQSTS:DEMAND_DATA_RD_HIT                       1,757,495,428
  FP_COMP_OPS_EXE:SSE_SCALAR_DOUBLE                         1,597
  FP_COMP_OPS_EXE:SSE_FP_SCALAR_SINGLE              1,556,036,610
  FP_COMP_OPS_EXE:X87                               1,878,388,524
  FP_COMP_OPS_EXE:SSE_PACKED_SINGLE                   302,976,589
  SIMD_FP_256:PACKED_SINGLE                         5,003,127,724
  User time (approx)               17.476 secs     47,202,147,918 cycles  100.0% Time
  CPU_CLK                           2.90GHz
  HW FP Ops / User time         2,556.183M/sec     44,671,354,883 ops    11.8%peak(DP)
  Total SP ops                  2,448.698M/sec     42,792,964,761 ops
  Total DP ops                    107.485M/sec      1,878,390,122 ops
  MFLOPS (aggregate)           61,348.39M/sec
  D2 cache hit,miss ratio           94.4% hits               5.6% misses
  D2 to D1 bandwidth            6,680.690MiB/sec  122,421,709,963 bytes
  Average Time per Call                                  0.000034 secs
  CrayPat Overhead : Time           11.4%
```

Flat profile data

HW counter values

Derived metrics

Hardware performance counters

- CrayPAT can interface with HWPCs
  - Gives extra information on how hardware is behaving
  - Very useful for understanding (& optimising) application performance
- Provides information on
  - hardware features, e.g. caches, vectorisation and memory bandwidth
- Available on per-program and per-function basis
  - Per-function information only available through tracing
- Number of simultaneous counters limited by hardware
  - 2 counters available with AMD Rome processors
  - If you need more, you'll need multiple runs
- Most counters accessed through the PAPI interface
  - Either native counters or derived metrics constructed from these

Hardware counters selection

- HWPCs collected using CrayPAT
  - Compile and instrument code for profiling as before
- Set PAT_RT_PERFCTR environment variable at runtime
  - e.g. in the job script
    - Hardware counter events are not collected by default (except with APA)
- `export PAT_RT_PERFCTR=...`
  - either a list of named PAPI counters
  - or `<set number>` = a pre-defined (and useful) set of counters
    - recommended way to use HWPCs
    - there are 8 groups to choose from
      - To see them:
        - `pat_help -> counters -> rome -> groups`
        - `man hwpc`
        - More `/opt/cray/pe/perftools/20.10.0/share/counters/CounterGroups.amd_fam23mod49`

Technical term for AMD Rome

Predefined AMD Rome HW Counter Groups

0: Summary with translation lookaside buffer activity

1: Summary with branch activity

default: mem_bw

default_samp: default

mem_bw: memory bandwidth

mem_bw_1: memory load bandwidth, stalls

mem_bw_2: memory load bandwidth, cycles

stalls: Dispatch stalls for load, store, fp

Example: mem_bw

```
 USER / sweepy_
-----------------------------------------------------------------------------
  Time%                                                       14.6%
  Time                                                     8.738150 secs
  Imb. Time                                                3.077320 secs
  Imb. Time%                                                  27.2%
  Calls                     11.547 /sec                       100.0 calls
  CPU_CLK_UNHALTED:THREAD_P                          92,754,888,918
  CPU_CLK_UNHALTED:REF_P                              2,759,876,135
  L1D:REPLACEMENT                                     1,813,741,166
  L2_RQSTS:ALL_DEMAND_DATA_RD                         1,891,459,700
  L2_RQSTS:DEMAND_DATA_RD_HIT                         1,644,133,800
  LLC_MISSES                                             98,952,928
  LLC_REFERENCES                                        690,626,471
  User time (approx)         8.660 secs              23,390,899,520 cycles  100.0% Time
  CPU_CLK                     3.36GHz
  D2 cache hit,miss ratio    86.4% hits                       13.6% misses
  L3 cache hit,miss ratio    85.7% hits                       14.3% misses
  D2 to D1 bandwidth    13,330.757MiB/sec           121,053,420,792 bytes
  Average Time per Call                                    0.087381 secs
  CrayPat Overhead : Time     0.0% ….
```

Interpreting the performance numbers

- Performance numbers are an average over all ranks
  - explains non-integer values
- This does not always make sense
  - e.g. if ranks are not all doing the same thing:
    - Leader-worker schemes
    - MPMD apruns combining multiple, different programs
- Want them to only process data for certain ranks
  - `pat_report -sfilter_input='condition' ...`
  - `condition` should be an expression involving pe, e.g.
    - `pe<1024` for the first 1024 ranks only
    - `pe%2==0` for every second rank

OpenMP data collection and reporting

- Give finer-grained profiling of threaded routines
  - Measure overhead incurred entering and leaving
    - Parallel regions
      - #pragma omp parallel
    - Work-sharing constructs within parallel regions
      - #pragma omp for

- Timings and other data now shown per-thread
  - rather than per-rank

- OpenMP tracing enabled with `pat_build -gomp ...`
  - CCE: insert tracing points around parallel regions automatically
  - AMD, Gnu: need to use CrayPAT API manually

OpenMP data collection and reporting

- Load imbalance for hybrid MPI/OpenMP programs
  - now calculated across all threads in all ranks
  - imbalances for MPI and OpenMP combined
    - Can choose to see imbalance in each programming model separately
    - See next slide for details

- Data displayed by default in pat_report
  - no additional options needed
  - Report focuses on where program is spending its time
  - Assumes all requested resources should be used
    - you may have reasons not to want to do this, of course

Memory usage

- Knowing how much memory each rank uses is important:
  - What is the minimum number of cores I can run this problem on?
    - given there is 256GB (~254GB usable) of memory per node (128 cores)
  - Does memory usage scale well in the application?
  - Is memory usage balanced across the ranks in the application?
  - Is my application spending too much time allocating and freeing?

Heap statistics

Memory per rank
~254GB usable memory per node

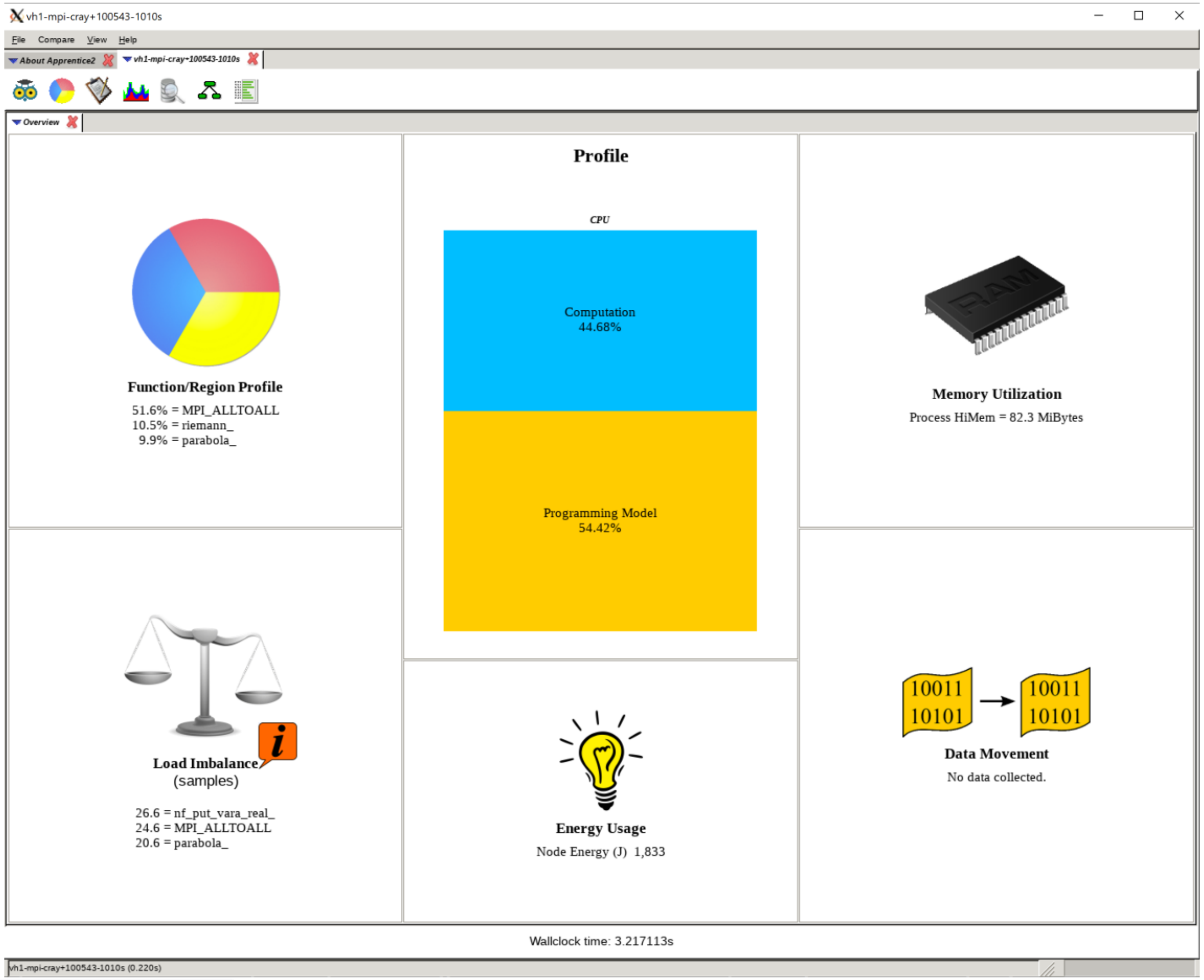
Too many allocs/frees?
Would show up as ETC time in CrayPAT report

Memory leaks
Not usually a problem in HPC

```
Notes for table 5:

  Table option:
    -O heap_hiwater
  Options implied by table option:
    -d am@,ub,ta,ua,tf,nf,ac,ab -b pe=[mmm]

  This table shows only lines with Tracked Heap HiWater MBytes > 0.


Table 5:  Heap Stats during Main Program

 Tracked |  Total |  Total | Tracked | Tracked |PE[mmm]
    Heap | Allocs |  Frees | Objects |  MBytes |
 HiWater |        |        |     Not |     Not |
  MBytes |        |        |   Freed |   Freed |

   9.794 |    915 |    910 |       4 |   1.011 |Total
|-----------------------------------------------------
|   9.943 |   1170 |   1103 |      68 |   1.046 |pe.0
|   9.909 |    715 |    712 |       3 |   1.010 |pe.22
|   9.446 |   1278 |   1275 |       3 |   1.010 |pe.43
|=====================================================
```

Viewing data

- Apprentice 2 tool
  - GUI for exploring code/data
  - Insight summaries
- Can install desktop version
- **/opt/cray/pe/perftools /$(current_version)/share /desktop_installers/**



Summary

- Profiling is essential to identify performance bottlenecks
  - even at single core level
- CrayPAT has some very useful extra features
  - can pinpoint and characterise the hotspot loops (not just routines)
  - hardware performance counters give extra insight into performance
  - well-integrated view of hybrid programming models
    - most commonly MPI/OpenMP
    - also CAF, UPC, SHMEM, pthreads, OpenACC, CUDA
  - information on memory usage
- And remember the Golden Rules
  - including the one about not believing what anyone tells you