ARCHER Tips and Tricks

A few notes from the CSE team
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Outline

- Using Intel MKL
- Impact of HyperThreads
- Showing process/thread placement
- Performance analysis: hardware counters on ARCHER
- Debugging: Disabling autotuning in Cray BLAS
- Enabling and using ATP
Intel MKL

- MKL can be used as an alternative for LibSci
  - We have seen cases where either is better
  - Worth experimenting
- Not interfaced through modules
- Linking using GNU
  
  ```
  -L$(MKLROOT)/lib/intel64/ -Wl,--start-group -lmkl_gnu_thread \\
  -lmkl_gf_lp64 -lmkl_core -Wl,--end-group -ldl
  ```

- Linking using Intel
  
  ```
  -L$(MKLROOT)/lib/intel64/ -Wl,--start-group -lmkl_intel_lp64 \\
  -lmkl_core -lmkl_sequential -Wl,--end-group -ldl
  ```
Intel MKL (cont.)

• The link line is reasonably complicated.
• Use the MKL Link Line Advisor:


• For ARCHER select:
  • Product: Intel Composer XE 2013 SP1
  • OS: Linux
  • Architecture: Intel(R) 64
  • Linking: Static
  • Interface Layer: LP64 (32-bit Integer)
  • (MPI: MPICH2 if required)
Impact of HyperThreads

• HyperThreads allow up to 2 processes/threads to run concurrently on a single physical core
  • Managed in hardware so context switch is fast
  • Use CPU resource while one thread is stalled

• Very program dependent
  • Even a small improvement is worth it (as it is free)
  • Worth testing if it is useful for your program

• aprun syntax (2 nodes):

  aprun -j 2 -n 96 -N 48 ...
Hyperthreading example performance

- XC30: Sandy Bridge (8 cores), fully populated nodes

- VASP

- NAMD

Effects of Hyper-Threading on the NERSC workload on Edison
http://www.nersc.gov/assets/CUG13HTpaper.pdf
Show Process/Thread Placement

• Process/thread placement can have a large impact on performance
  • Particularly when underpopulating nodes or running mixed-mode (MPI/OpenMP) code.
• Add the following lines to your job submission script:
  
  export MPICH_CPUMASK_DISPLAY=1
  export MPICH_RANK_REORDERDISPLAY=1
Placement (cont.)

[PE_0]: MPI rank order: Using default aprun rank ordering.
[PE_0]: rank 0 is on nid02421
[PE_0]: rank 1 is on nid02421
[PE_0]: rank 2 is on nid02421
...
[PE_0]: rank 24 is on nid02505
[PE_0]: rank 25 is on nid02505
[PE_0]: rank 26 is on nid02505
...
Placement (cont.)

[PE_0]: cpumask set to 1 cpu on nid02421, cpumask = 00000000000000000000000000000000000000000000000001
[PE_34]: cpumask set to 1 cpu on nid02505, cpumask = 0000000000000000000000000000000000000010000000000
[PE_33]: cpumask set to 1 cpu on nid02505, cpumask = 0000000000000000000000000000000000000010000000000
[PE_35]: cpumask set to 1 cpu on nid02505, cpumask = 0000000000000000000000000000000000000010000000000
[PE_47]: cpumask set to 1 cpu on nid02505, cpumask = 0000000000000000000000000000000000000100000000000
...
Hardware Counters on ARCHER

• CrayPAT allows you to monitor performance at the hardware level

• Specify set of performance counters using the PAT_RT_PERFCTR environment variable in script that is running instrumented code:

\[
\text{PAT_RT_PERFCTR}=1
\]

(Group = 1 shows a summary with floating-point and cache metrics.)
<table>
<thead>
<tr>
<th>Metric</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PERF_COUNT_HW_CACHE_L1D:ACCESS</td>
<td>458227922309</td>
</tr>
<tr>
<td>PERF_COUNT_HW_CACHE_L1D:PREFETCH</td>
<td>7837418131</td>
</tr>
<tr>
<td>PERF_COUNT_HW_CACHE_L1D:MISS</td>
<td>25703134212</td>
</tr>
<tr>
<td>CPU_CLK_UNHALTED:THREAD_P</td>
<td>884128952294</td>
</tr>
<tr>
<td>CPU_CLK_UNHALTED:REF_P</td>
<td>29852948968</td>
</tr>
<tr>
<td>DTLB_LOAD_MISSES:MISS_CAUSES_A_WALK</td>
<td>219955467</td>
</tr>
<tr>
<td>DTLB_STORE_MISSES:MISS_CAUSES_A_WALK</td>
<td>54655340</td>
</tr>
<tr>
<td>L2_RQSTS:ALL_DEMAND_DATA_RD</td>
<td>17968418083</td>
</tr>
<tr>
<td>L2_RQSTS:DEMAND_DATA_RD_HIT</td>
<td>14820163740</td>
</tr>
<tr>
<td>User time (approx)</td>
<td>304.533 secs</td>
</tr>
<tr>
<td></td>
<td>822542437366 cycles</td>
</tr>
<tr>
<td>CPU_CLK</td>
<td>2.962GHz</td>
</tr>
<tr>
<td>TLB utilization</td>
<td>1790.78 refs/miss</td>
</tr>
<tr>
<td></td>
<td>3.498 avg uses</td>
</tr>
<tr>
<td>D1 cache hit,miss ratios</td>
<td>94.8% hits</td>
</tr>
<tr>
<td></td>
<td>5.2% misses</td>
</tr>
<tr>
<td>D1 cache utilization (misses)</td>
<td>19.13 refs/miss</td>
</tr>
<tr>
<td></td>
<td>2.392 avg hits</td>
</tr>
<tr>
<td>D2 cache hit,miss ratio</td>
<td>87.8% hits</td>
</tr>
<tr>
<td></td>
<td>12.2% misses</td>
</tr>
<tr>
<td>D1+D2 cache hit,miss ratio</td>
<td>99.4% hits</td>
</tr>
<tr>
<td></td>
<td>0.6% misses</td>
</tr>
<tr>
<td>D1+D2 cache utilization</td>
<td>156.20 refs/miss</td>
</tr>
<tr>
<td></td>
<td>19.525 avg hits</td>
</tr>
<tr>
<td>D2 to D1 bandwidth</td>
<td>3601.274MB/sec</td>
</tr>
<tr>
<td></td>
<td>1149978757281 bytes</td>
</tr>
</tbody>
</table>
Disable Cray BLAS autotuning

• If you are debugging and use the Cray LibSci library then you may want to disable autotuning.
  • Ensures autotuning is not causing the error.
• Add:

  CRAYBLAS_AUTOTUNING_OFF=1

to your job scripts.
Using ATP

- ATP (Abnormal Termination Processing) catches dying applications and produces a merged stack backtrace
- Useful for getting more information on crashes
- Set:

  ATP_ENABLED=1

  in your job submission script.
- There is no need to recompile to use ATP
Using ATP (cont.)

- When your program crashes, ATP will:
  - Produce a stack trace of the first failing process
  - Produce a visualisation of every process's stack trace
  - Generate a selection of relevant core files

- Visualise the merged stack trace using `statview`:

  module add stat
  statview atpMergedBT.dot

- Very simple way to start the debugging process
statview (thanks to Cray)