Performance Profiling on KNL with Cray perftools-lite

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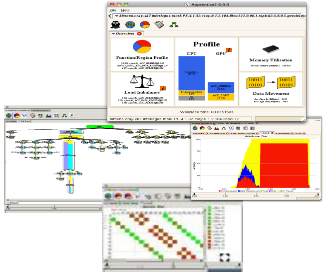
Agenda

- Overview of Cray Performance Tools
- Identifying slowest areas of a program
- Tips for analyzing program performance

Overview of Cray Performance Tools

Load modules to access software



Choose experiment to target your goal

Visualize application bottlenecks

Goals

- Reduce the time investment associated with porting and tuning applications on Cray systems
- Analyze whole-program behavior across many nodes to identify critical performance bottlenecks within a program
- Improve your profiling experience by using simple (lite mode) and/or advanced interfaces for a wealth of capability that targets analyzing large HPC jobs

Functional Highlights

- **Whole program performance analysis with**
  - Novice and advanced user interfaces
  - Support for MPI, SHMEM, OpenMP, PGAS, OpenACC, CUDA
  - Load imbalance detection
  - HW counter metrics (hit rates, computational intensity, etc.)
  - Observations on inefficiencies
  - Data correlation to user source
  - Minimal program perturbation

- **Sampling, tracing with runtime summarization (RTS), full trace (timeline) modes available**

- **Supports CCE, Intel and GCC compilers on Cray XC systems**
- **Supports CCE on Cray CS systems**

Components

- **CrayPat and CrayPat-lite**
  - Identifies top time consuming routines, work load imbalance, MPI rank placement strategies, etc.
- **PAPI**
  - Performance counters (used by CrayPat or directly by user)
- **Cray Apprentice2**
  - Visualize load imbalance, excessive communication, network contention, excessive serialization
- **Reveal**
  - View CCE optimization messages, key loops in program, high bandwidth memory traffic, add OpenMP to program

Cray Performance Tools Status

- **perftools-base/7.0.0 released in Dec 2017**
- **What's new?**
  - Perftools-lite performance improvements (execution, scaling)
  - Performance data experiment directory
  - Memory and vector sensitivity metrics

How to Access Cray Performance Tools

perftools-base module

- Provides access to performance tools instrumentation modules, documentation, Reveal and Apprentice2
- Doesn't impact program build
- If not loaded by default on a system, you can load in your .profile or .login and leave it loaded
- Once loaded, do a '`module avail perftools`' to see available instrumentation modules

Program Instrumentation Modules

- Instrumentation modules prepare an application for performance data collection

```
> module avail perftools

---------- /opt/cray/pe/perftools/7.0.0/modulefiles ----------
perftools
perftools-lite
perftools-lite-events
perftools-lite-gpu
perftools-lite-hbm
perftools-lite-loops
perftools-nwpc
```

Use first to get basic program performance profile

Interfaces Available

- **CrayPat-lite: simple interface for convenience**

- **CrayPat: advanced interface for in-depth performance investigation and tuning assistance as well as data collection control**

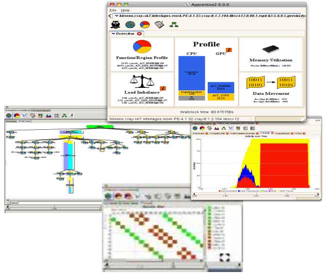
- **Both offer:**
  - Whole program analysis across many nodes
  - Indication of causes of problems
  - Ability to easily switch between the two interfaces

Simple vs Advanced Interface

- Has fewer steps
- Is easier to use if you rarely profile applications (don’t have to remember how to use the tools)
- Provides a condensed text report
- Performs performance data processing and report generation at end of job on compute nodes
- Allows you to mix with advanced interface
  - Run pat_report to get full report with simple interface

Identifying Slowest Areas of a Program

Load perftools-lite



Build and run program

Interpret results

Example: Using perftools-lite

- `$ module load perftools-lite`
- **Build program**
  - Should see message at end of build from CrayPat saying that it created an instrumented executable
  - Add `–hlist=a` to build with CCE listing for optimization feedback
- `$ aprun/srun –n … ./my_program`
- **Performance data sent to `STDOUT` and to directory with unique name**
  - Refer to CCE listing with sampling by line data in Table 2

Example: Cray loopmark Messages

cc/ftn/CC –hlist=a …

```
b-------<  do i3=2,n3-1
b b-----<     do i2=2,n2-1
b b Vr--<        do i1=1,n1
b b Vr            u1(i1) = u(i1,i2-1,i3) + u(i1,i2+1,i3)
b b Vr     *          + u(i1,i2,i3-1) + u(i1,i2,i3+1)
b b Vr            u2(i1) = u(i1,i2-1,i3-1) + u(i1,i2+1,i3-1)
b b Vr     *          + u(i1,i2-1,i3+1) + u(i1,i2+1,i3+1)
b b Vr-->        enddo
b b Vr--<        do i1=2,n1-1
b b Vr            r(i1,i2,i3) = v(i1,i2,i3)
b b Vr     *       - a(0) * u(i1,i2,i3)
b b Vr     *       - a(2) * ( u2(i1) + u1(i1-1) + u1(i1+1) )
b b Vr     *       - a(3) * ( u2(i1-1) + u2(i1+1) )
b b Vr-->        enddo
b b----->     enddo
b------->  enddo
```

Outer loops were blocked (b)

Inner-loops were vectorized and unrolled (Vr)

Example: Cray loopmark Messages (cont)

```
ftn-6289 ftn: VECTOR File = resid.f, Line = 29
  A loop starting at line 29 was not vectorized because a recurrence was found on "U1" between lines 32 and 38.
ftn-6049 ftn: SCALAR File = resid.f, Line = 29
  A loop starting at line 29 was blocked with block size 4.
ftn-6289 ftn: VECTOR File = resid.f, Line = 30
  A loop starting at line 30 was not vectorized because a recurrence was found on "U1" between lines 32 and 38.
ftn-6049 ftn: SCALAR File = resid.f, Line = 30
  A loop starting at line 30 was blocked with block size 4.
ftn-6005 ftn: SCALAR File = resid.f, Line = 31
  A loop starting at line 31 was unrolled 4 times.
ftn-6204 ftn: VECTOR File = resid.f, Line = 31
  A loop starting at line 31 was vectorized.
ftn-6005 ftn: SCALAR File = resid.f, Line = 37
  A loop starting at line 37 was unrolled 4 times.
ftn-6204 ftn: VECTOR File = resid.f, Line = 37
  A loop starting at line 37 was vectorized.
```

Example of Explain Utility

users/ldr> explain ftn-6289

VECTOR: A loop starting at line %s was not vectorized because a recurrence was found on "var" between lines num and num.

Scalar code was generated for the loop because it contains a linear recurrence. The following loop would cause this message to be issued:

```
DO I = 2,100
   B(I) = A(I-1)
   A(I) = B(I)
ENDDO
```

Example: perftools-lite Job Summary

```
#################################################################
#                                                               #
#            CrayPat-lite Performance Statistics                #
#                                                               #
#################################################################
CrayPat/X:  Version 7.0.0.45 Revision 11f412d  11/08/17 09:36:36
Experiment:                  lite  lite/sample_profile
Number of PEs (MPI ranks):     96
Numbers of PEs per Node:       16  PEs on each of  6  Nodes
Numbers of Threads per PE:      1
Number of Cores per Socket:    68
Execution start time:  Tue Nov 14 11:44:06 2017
System name and speed:  nid00037  1401 MHz (approx)
Intel Knights Landing CPU  Family:  6  Model: 87  Stepping:  1
MCDRAM: 7.2 GHz, 16 GiB available as quad, cache (100% cache)

Avg Process Time:   612.10 secs
High Memory:      16,053.7 MBytes     167.2 MBytes per PE
I/O Read Rate:    1.764988 MBytes/sec
I/O Write Rate:   4.349897 MBytes/sec
```

Example: perftools-lite Top Time Consumers

```
Table 1:  Profile by Function Group and Function (top 10 functions shown)

  Samp% |      Samp |    Imb. |  Imb. |Group
        |           |    Samp | Samp% | Function
        |           |         |       |  PE=HIDE

 100.0% | 55,605.7 |      -- |    -- |Total
|-----------------------------------------------------------------------
|  56.5% | 31,412.8 |      -- |    -- |USER
||----------------------------------------------------------------------
||  19.7% | 10,944.1 |   290.9 |  2.6% |create_boundary$boundary_
||  10.7% |  5,937.8 |   214.2 |  3.5% |get_block$blocks_
||   3.9% |  2,194.4 |     7.6 |  0.3% |create_distrb_balanced$distribution_
||   2.0% |  1,135.5 |   137.5 | 10.8% |impvmixt$vertical_mix_
||   1.9% |  1,064.8 |   124.2 | 10.5% |impvmixt_correct$vertical_mix_
||======================================================================
|  22.5% | 12,513.4 |      -- |    -- |ETC
||----------------------------------------------------------------------
||  20.1% | 11,151.4 | 2,758.6 | 19.9% |__cray_memcpy_KNL
||======================================================================
|  20.7% | 11,503.5 |      -- |    -- |MPI
||----------------------------------------------------------------------
||  11.1% |  6,171.6 | 1,785.4 | 22.5% |MPI_ALLREDUCE
||   7.9% |  4,377.8 | 3,254.2 | 42.7% |mpi_waitall
```

Example: perftools-lite Observations

```
MPI Grid Detection:
    There appears to be point-to-point MPI communication in a 32 X 32
    grid pattern. The 20.7% of the total execution time spent in MPI
    functions might be reduced with a rank order that maximizes
    communication between ranks on the same node. The effect of several
    rank orders is estimated below.

    A file named MPICH_RANK_ORDER.Grid was generated along with this
    report and contains usage instructions and the Hilbert rank order
    from the following table.

    Rank Order    On-Node    On-Node  MPICH_RANK_REORDER_METHOD
                 Bytes/PE  Bytes/PE%
                              of Total
                              Bytes/PE

       Hilbert  1.413e+12     81.94%  3
           SMP  1.053e+12     61.04%  1
          Fold  9.405e+11     54.53%  2
    RoundRobin  8.962e+11     51.96%  0
```

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Example: perftools-lite Hot Spots by Line

```
Table 3:  Profile by Group, Function, and Line

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

 100.0% | 60,665.8 |       -- |    -- | Total
|-----------------------------------------------------------------------------
|  94.6% | 57,390.6 |       -- |    -- | USER
||----------------------------------------------------------------------------
||  82.1% | 49,835.3 |       -- |    -- | LAMMPS_NS::PairLJCut::compute
|||---------------------------------------------------------------------------
3||  80.7% | 48,970.1 |       -- |    -- | src/Obj_xc30intel/../pair_lj_cut.cpp
||||--------------------------------------------------------------------------
4|||   3.9% |  2,359.8 |   100.2 |  4.1% | line.102
4|||   1.0% |    596.2 |    61.8 |  9.5% | line.105
4|||   8.3% |  5,022.4 |   683.6 | 12.1% | line.107
4|||   2.9% |  1,744.2 |   966.8 | 36.0% | line.108
```

Get Additional Information Without Re-running

- Run pat_report after collecting data with lite mode
  - `pat_report my_programXXXs/ > full_rpt`

  - `pat_report –O callers` or `pat_report –O callers+src`
  - `pat_report –O calltree` or `pat_report –O calltree+src`
  - **Check out load balance table**

- Learn about related tables in “Table Notes”
  - We try to suggest reports that dive deeper on a related topic
  - Provide data aggregation method

Example: Load Balance by Max Time

```
Table 2:  Profile of maximum function times (limited entries shown)
  Samp% |      Samp |     Imb. |  Imb. | Function
        |           |     Samp | Samp% |  PE=[max,min]
|------------------------------------------------------------------------
| 100.0% | 51,891.0 | 2,055.7 |   4.0% | LAMMPS_NS::PairLJCut::compute
||-----------------------------------------------------------------------
|| 100.0% | 51,891.0 |      -- |     -- | pe.32
||  93.0% | 48,263.0 |      -- |     -- | pe.93
||=======================================================================
|  11.3% |  5,871.0 |   193.1 |   3.3% | LAMMPS_NS::Neighbor::half_bin_newton
||-----------------------------------------------------------------------
||  11.3% |  5,871.0 |      -- |     -- | pe.66
||  10.7% |  5,535.0 |      -- |     -- | pe.94
||=======================================================================
|   8.6% |  4,480.0 | 2,418.6 |  54.6% | MPI_Send
||-----------------------------------------------------------------------
||   8.6% |  4,480.0 |      -- |     -- | pe.45
||   0.9% |    443.0 |      -- |     -- | pe.32
```

Recognizing OpenMP in a Report

- **CrayPat can collect the most detail from OpenMP using the Cray compiler**

- **OpenMP regions and loops are identified in report with the following syntax:**
  - function.REGION@li.49
  - function.LOOP@li.53

- **OpenMP statistics are collected by default (no need to enable anything in the tools)**
  - Most information is available with Cray compiler

How Do I See per-Rank or per-Thread Data?

- `$ pat_report –s pe=ALL`
- `$ pat_report –s th=ALL`

Don’t See an Expected Function?

- To make the profile easier to interpret, samples are attributed to a caller that is either a user defined function, or a library function called directly by a user defined function
- To disable this adjustment, and show functions actually sampled, use the ‘`pat_report –P`’ option to disable pruning
- You should be able to see the caller/callee relationship with ‘`pat_report -P -O callers`’

Don’t See an Expected Function? (cont’d)

- **Why don’t I see a particular function in the report?**
- **Cray tools filter out data that may distract you**
  - Use **`pat_report –T`** to see functions that didn’t take much time
- **Still don’t see it?**
  - Check the compiler listing to see if the function was inlined

What is ETC Group in the Report?

- When a function is called that cannot be attributed to a user-defined parent function, it gets placed in ETC
- Try '`pat_report –P`'
- **Note:** pat_report depends on the accuracy of the DWARF issued by the compiler

Documentation Available

- Release Notes
  - `> module help perftools-base/`*`version_number`*

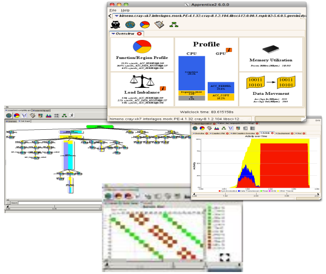
- User manual "Using the Cray Performance Measurement and Analysis Tools" available at http://pubs.cray.com

- pat_help – interactive help utility on the Cray Performance toolset

- Man pages

Tips for Analyzing Program Performance

Load perftools-lite



Build and run program

Interpret results

Where Do I Start?

- Determine problem size / job size that you ultimately want to run
- Get high level program profile at scale to locate key bottlenecks
- Work from high-level (inter-node) to low-level (intra-node) bottlenecks

Helpful Experiments

- **Identify slowest areas and notable bottlenecks of a program**
  - Use `perftools-lite`
  - Good for examining performance characteristics of a program and for scaling analysis
- **Focus on loop optimization, including adding OpenMP with Reveal**
  - Use `perftools-lite-loops`
  - Use `perftools-lite-hbm` for memory bandwidth sensitivity study
- **Focus on MPI communication**
  - Use `perftools-lite` first to determine if MPI time is dominant or if there is a load imbalance between ranks
  - Use `perftools (pat_build –g mpi)` to collect more detailed MPI-specific information
  - Good for scaling analysis at targeted final job size

Focus on Loop Optimization – Find Top Loops

- **`$ module load PrgEnv-cray perftools-lite-loops`**
  - Needs Cray compiler
- **Build program (build from scratch – we add compiler flags)**
  - Should see message at end of build from CrayPat saying that it created an instrumented executable
  - Remember to add `–hlist=a` to build with CCE listing
  - Add `–hpl=/path_to_program_library/my_program.pl` if you want to use Reveal
- **`$ aprun –n … ./my_program`**
- **Performance data sent to `STDOUT` and to experiment data directory with unique name**

Focus on MPI Communication

- `$ module load perftools`
- **Build program**
  - Remember to add `–hlist=a` to build with CCE listing
  - Can relink or use “a.out+orig” if created with perftools-lite
- **Instrument program**
  - `$ pat_build –g mpi ./my_program`
- **Run application**
  - `$ aprun/srun -n …  my_program+pat`
- **Create report**
  - `$ pat_report my_programXXX/ > my_report`

Summary

- Cray performance tools offer functionality that **reduces the time investment** associated with porting and tuning applications on new and existing Cray systems

- Cray performance tools come with a **simple interface plus a wealth of capability** when you need it for analyzing those most critical production codes

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Questions?

Thank You!