

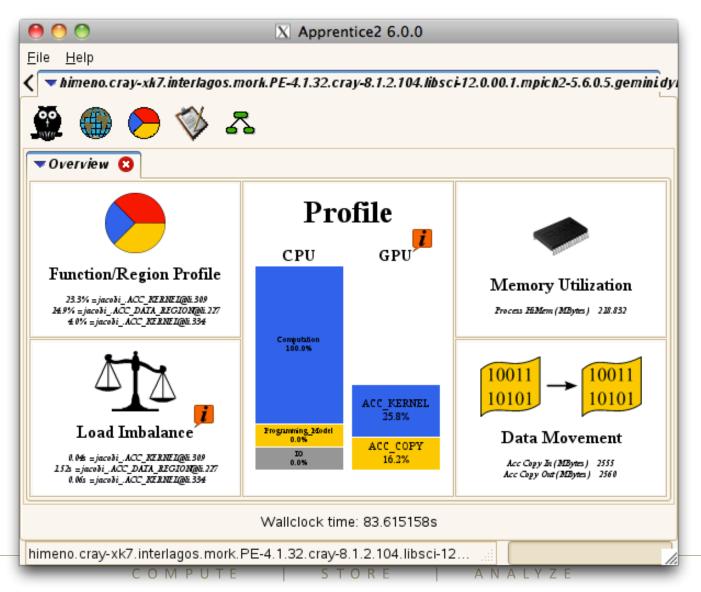
Cray Performance Measurement, Analysis and Porting Tools

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Cray Performance Tools Refresher





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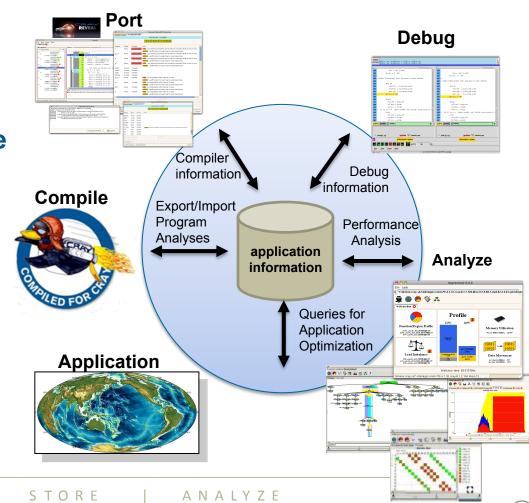
Agenda



- 10:20 10:30 Overview of Cray PE topics for the day
- 10:30 11:15 Cray Performance Tools refresher
- 11:15 12:00 lab (CrayPat-lite, loop stats, Rank reorder)
- 12:00 13:00 Lunch
- 13:00 14:00 Reveal
- 14:00 14:30 CCE and OpenACC update
- 14:30 15:00 lab with Reveal
- 15:00 15:20 Break
- 15:20 16:00 CCDB
- 16:00 17:00 find a bug using CCDB, general lab time

The Programming Environment Mission

- It is the role of the Programming Environment to close the gap between observed performance and achievable performance
- Support the application development life cycle by providing a tightly coupled environment with compilers, libraries, and tools that will hide the complexity of the system
 - Address issues of scale and complexity of HPC systems
 - Target ease of use with extended functionality and increased automation
 - Close interaction with users
 - For feedback targeting functionality enhancements



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Cray Programming Environment Focus



Performance

- Help users maximize the cycles to the application
 - Address issues of scale and complexity of HPC systems

Programmability

- How do you get intuitive behavior and best performance with the least amount of effort
 - Provide the best environment to develop, debug, analyze, and optimize applications for production supercomputing
 - Provide programming environment consistency across Cray platforms

Recent Enhancements



- Cray Apprentice2 available for Linux, Mac and Windows with .dmg and .exe installers
 - Available in \$CRAYPAT ROOT/share/desktop installers
- Router-aware MPI rank placement
- Simplified Interface to performance counters
- Program timeline

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- I/O statistics in CrayPat-lite
- pat build default is now pat build –O apa

Two Interfaces to the Performance Tools



- CrayPat offers a wealth of performance measurement, analysis and presentation options for in-depth performance investigation and tuning assistance
- CrayPat-lite offers easy access to an application performance summary for users not familiar with the Cray performance tools or who may not be familiar with performance analysis
- CrayPat classic and CrayPat-lite are designed to compliment each other
 - Produce files with same format
 - Users familiar with CrayPat can easily switch back and forth between the two interfaces
 - CrayPat-lite users become familiar with reporting style also used with CrayPat

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CrayPat-lite



- Produces application performance statistics at the end of a job
 - Focus is to offer a simplified interface to basic application performance information for users not familiar with the Cray performance tools and perhaps new to application performance analysis
 - Gives sites the option to enable/disable application performance data collection for all users for a period of time
- Compliments "classic" perftools

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 Provides a simple way to transition from perftools-lite to perftools to encourage further tool use for more in-depth performance analysis

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Using CrayPat-lite



Access light version of performance tools software

> module load perftools-lite

Build program

> make



a.out (instrumented program)

Run program (no modification to batch script)

aprun a.out



Condensed report to stdout a.out*.rpt (same as stdout) a.out*.ap2 MPICH RANK XXX files

Performance Statistics Available



- Set of predefined experiments, enabled with the CRAYPAT_LITE environment variable
 - Sample_profile
 - Event profile
 - GPU
- Job information
 - Number of MPI ranks, ranks per node, number of threads
 - Wallclock
 - High memory water mark
 - Aggregate MFLOPS (CPU only)
 - 1/0
- Profile of top time consuming routines with load balance
- **Observations**
- Instructions on how to get more information

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CrayPat-lite Output Example



```
CrayPat/X: Version 6.1.4.12457 Revision 12457 (xf 12277) 02/26/14 13:58:24
Experiment:
                          lite lite/sample profile
Number of PEs (MPI ranks): 8164
Numbers of PEs per Node:
                          16 PEs on each of 510 Nodes
                           4 PEs on 1 Node
Numbers of Threads per PE:
Number of Cores per Socket:
Execution start time: Fri Feb 28 23:06:31 2014
System name and speed: hera2 2100 MHz
Wall Clock Time: 999.595275 secs
High Memory:
                  475.52 MBytes
MFLOPS (aggregate): 806112.33 M/sec
I/O Read Rate: 33.57 MBytes/Sec
I/O Write Rate: 215.40 MBytes/Sec
Table 1: Profile by Function Group and Function (top 7 functions shown)
Time% |
             Time | Imb. | Imb. | Calls | Group
                     Time | Time% |
                                               | Function
100.0% | 101.961423 |
                                  -- | 5315211.9 |Total
|| 75.8% | 77.248585 | 2.356249 | 3.0% | 1001.0 |LAMMPS NS::PairLJCut::compute
|| 6.5% | 6.644545 | 0.105246 | 1.6% | 51.0 | LAMMPS NS::Neighbor::half bin newton
  4.1% | 4.131842 | 0.634032 | 13.5% | 1.0 | LAMMPS NS::Verlet::run
|| 3.8% | 3.841349 | 1.241434 | 24.8% | 5262868.9 |LAMMPS NS::Pair::ev tally
  1.3% | 1.288463 | 0.181268 | 12.5% | 1000.0 | LAMMPS NS::FixNVE::final integrate
                         -- | -- | 42637.0 |MPI
   4.8% | 4.851309 | 3.371093 | 41.6% | 12267.0 |MPI Send
  1.5% | 1.536106 | 2.592504 | 63.8% | 12267.0 | MPI Wait
```

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The Cray Performance Analysis Framework



Supports traditional post-mortem performance analysis

- Automatic identification of performance problems
 - Indication of causes of problems
 - Suggestions of modifications for performance improvement
- pat build: provides automatic instrumentation
- CrayPat run-time library collects measurements (transparent to the user)
- pat report performs analysis and generates text reports
- pat help: online help utility
- Cray Apprentice2: graphical visualization tool

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Steps to Using CrayPat "classic"

Access performance tools software

> module load perftools

Build program, retaining .o files

> make



a.out

Instrument binary

> pat_build -O apa a.out



a.out+pat

Modify batch script and run program

aprun a.out+pat



a.out+pat*.xf

Process raw performance data and create report

> pat_report a.out+pat*.xf



a.out+pat*.ap2
Text report to stdout
a.out+pat*.apa
MPICH_RANK_XXX

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```
0 0
                           heidi@limited: /h/heidi — ssh — 81×26
Table 2:
         Profile by Group, Function, and Line
 Samp% |
          Samp | Imb. | Imb. | Group
                I Samp
                       | Samp% | Function
                                 I Source
                                    Line
                                      PE=HIDE
 100.0% | 8376.9 | -- | -- |Total
  93.2% | 7804.0 | -- | -- | USER
| | 51.7% | 4328.7 | -- | -- |calc3_
| | | | | heidi/DARPA/cache_util/calc3.do300-ijswap.F
     15.7% | 1314.4 | 93.6 | 6.8% | line.78
     13.9% | 1167.7 | 98.3 | 7.9% | line.79
4111
4111
     14.5% | 1211.6 | 97.4 | 7.6% | line.80
4111
     1.2% | 103.1 | 26.9 | 21.2% | line.93
     1.1% | 88.4 | 22.6 | 20.8% | line.94
4111
     1.0% | 84.5 |
                       17.5 | 17.6% | line.95
4111
4111
     1.0% I
             86.8 I
                       33.2 | 28.2% | line.96
4111
     1.3% | 105.0 | 23.0 | 18.4% | line.97
4111
      1.4% | 116.5 | 24.5 | 17.7% | line.98
                                                             144,1
                                                                           38%
```

APA File Example



```
You can edit this file, if desired, and use it
  to reinstrument the program for tracing like this:
         pat build -O standard.crav-
   xt.PE-2.1.56HD.pgi-8.0.amd64.pat-5.0.0.2-Oapa.512.quad.cores.seal.
   090405.1154.mpi.pat rt exp=default.pat rt hwpc=none.14999.xf.xf.apa
 These suggested trace options are based on data from:
   /home/users/malice/pat/Runs/Runs.seal.pat5001.2009Apr04/./pat.quad/
   homme/standard.cray-xt.PE-2.1.56HD.pgi-8.0.amd64.pat-5.0.0.2-Oapa.
   512.quad.cores.seal
   090405.1154.mpi.pat_rt_exp=default.pat_rt_hwpc=none.14999.xf.xf.cdb
      HWPC group to collect by default.
-Drtenv=PAT RT HWPC=1 # Summary with TLB metrics.
      Libraries to trace.
-g mpi
      User-defined functions to trace, sorted by % of samples.
      The way these functions are filtered can be controlled with
      pat report options (values used for this file are shown):
                              No more than 200 functions are listed.
      -s apa max count=200
      -s apa min size=800
                              Commented out if text size < 800 bytes.
      -s apa min pct=1
                              Commented out if it had < 1% of samples.
                             Commented out after cumulative 90%.
      -s apa max cum pct=90
      Local functions are listed for completeness, but cannot be traced.
   # Enable tracing of user-defined functions.
    # Note: -u should NOT be specified as an additional option.
```

```
# 31.29% 38517 bytes
         -T prim advance mod preq advance exp
# 15.07% 14158 bytes
         -T prim si mod prim diffusion
# 9.76% 5474 bytes
         -T derivative mod gradient str nonstag
# 2.95% 3067 bytes
         -T forcing mod apply forcing
# 2.93% 118585 bytes
         -T column model mod applycolumnmodel
# Functions below this point account for less than 10% of samples.
# 0.66% 4575 bytes
          -T bndry mod bndry exchangev thsave time
# 0.10% 46797 bytes
          -T baroclinic inst mod binst init state
# 0.04% 62214 bytes
          -T prim state mod prim printstate
# 0.00% 118 bytes
          -T time mod timelevel update
  -o preqx.cray-xt.PE-2.1.56HD.pgi-8.0.amd64.pat-5.0.0.2.x+apa
     # New instrumented program.
  /.AUTO/cray/css.pe tools/malice/craypat/build/pat/2009Apr03/2.1.56HD/amd64/homme/pgi7pat-5.0.0.2/homme/2005Dec08/build.Linux/preqx.cray
     xt.PE-2.1.56HD.pgi-8.0.amd64.pat-5.0.0.2.x # Original program.
```

CrayPat Runtime Options



- Runtime controlled through PAT_RT_XXX environment variables
- See intro_craypat(1) man page
- Examples of control
 - Enable full trace
 - Change number of data files created
 - Enable collection of HW counters
 - Enable collection of network counters

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 Enable tracing filters to control trace file size (max threads, max call stack depth, etc.)

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Example Runtime Environment Variables



- Optional timeline view of program available
 - export PAT_RT_SUMMARY=0
 - View trace file with Cray Apprentice²
- Write 1 file per node:
 - export PAT_RT_EXPFILE_MAX=0
- Request hardware performance counter information:
 - export PAT_RT_PERFCTR=<HW counter group or event(s)>
 - Can specify individual events or predefined groups

Generating Profile from APA



Instrument application for further analysis (a.out+apa)

```
% pat_build -O <apafile>.apa
```

Run application

```
% aprun ... a.out+apa (or qsub <apa script>)
```

Generate text report and visualization file (.ap2)

View report in text and/or with Cray Apprentice²

```
% app2 < datafile > .ap2
```

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File Suffix	Description
a.out+pat	Program instrumented for data collection
a.outs.xf	Raw data for sampling experiment, available after application execution
a.outt.xf	Raw data for trace (summarized or full) experiment, available after application execution
a.outst.ap2	Processed data, generated by pat_report, contains application symbol information
a.outs.apa	Automatic profiling pnalysis template, generated by pat_report (based on pat_build –O apa experiment)
a.out+apa	Program instrumented using .apa file
MPICH_RANK_ORDER.Custom	Rank reorder file generated by pat_report from automatic grid detection an reorder suggestions

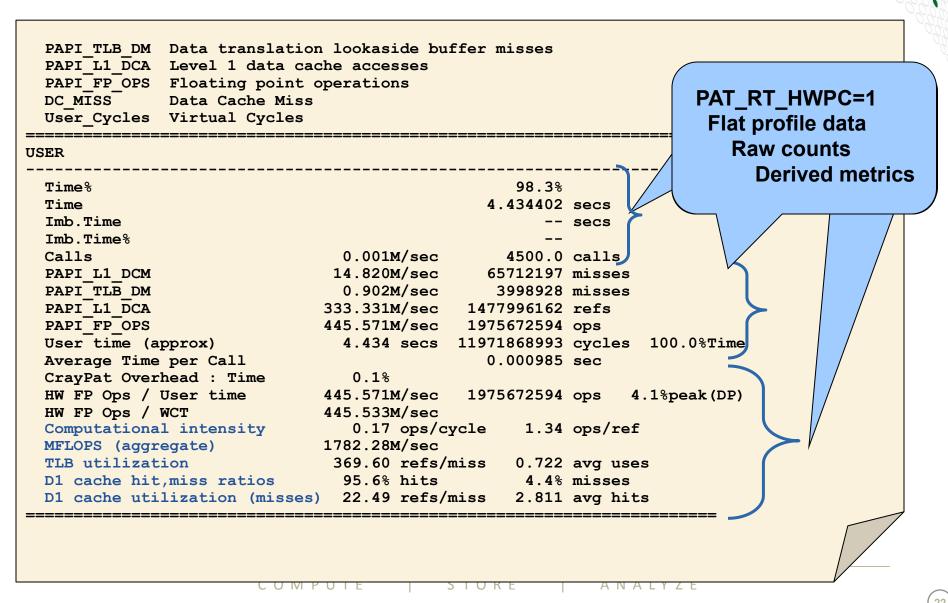
Performance Counters



- Cray supports raw counters, derived metrics and thresholds for:
 - Processor
 - Network
 - Accelerator
 - Power
- Predefined groups
 - Groups together suggested counters for experiments
- Single interface to access counters (PAT RT PERFCTR environment variable)
- PAPI with Cray custom components for network, uncore, power (available to 3rd party tool developers)

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Example: HW counter data and Derived Metrics

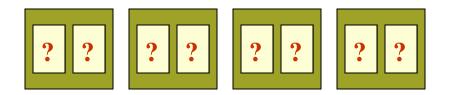


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MPI Rank Reorder



MPI rank placement with environment variable



- Distributed placement
- SMP style placement
- Folded rank placement
- User provided rank file

MPI Rank Reorder (cont'd)



- Non-default MPI rank placements are useful when point-to-point communication consumes significant fraction of the program time, and there is a significant load imbalance
- Performance report contains a prioritized list of placement scenarios and includes instructions on how to choose one of the placements for subsequent program execution
- Custom placement files automatically generated, user just chooses one
- Utilities available to create MPI rank placements for applications with grid or lattice topologies.

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Automatic Communication Grid Detection



 Cray performance tools produce a custom rank order if it's beneficial based on grid size, grid order and cost metric

- Heuristics available for:
 - MPI sent message statistics
 - User time (time spent in user functions) can be used for PGAS codes
 - Hybrid of sent message and user time)
- Summarized findings in report
- Available with sampling or tracing
- Describe how to re-run with custom rank order

MPI Rank Order Observations



Time%	Time	Imb. Time	Imb. Time%	Calls	Group Function PE=HIDE
100.0%	463.147240			21621.0	Total
52.0%	240.974379			21523.0	MPI
47.7%	221.142266 19.829001	36.214468 25.849906			mpi_recv MPI_SEND
43.3%	200.474690			32.0	USER
41.0%	1	58.716197 1.899097	23.6% 20.1%	12.0	sweep_ source_
4.7%	21.698147			39.0	MPI_SYNC
4.3%	20.091165	20.005424	99.6%	32.0	mpi_allreduce_(sync)
0.0%	0.000024	I		27.0	SYSCALL

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MPI Rank Order Observations (2)



MPI Grid Detection:

There appears to be point-to-point MPI communication in a 96 X 8 grid pattern. The 52% 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 Custom rank order from the following table.

Rank Order	On-Node Bytes/PE	On-Node Bytes/PE% of Total Bytes/PE	MPICH_RANK_REORDER_METHOD
Custom	2.385e+09	95.55%	3
SMP	1.880e+09	75.30%	1
Fold	1.373e+06	0.06%	2
RoundRobin	0.000e+00	0.00%	0

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MPICH_RANK_ORDER File



```
# The 'Custom' rank order in this file targets nodes with multi-core
# processors, based on Sent Msg Total Bytes collected for:
#
# Program: /lus/nid00030/heidi/sweep3d/mod/sweep3d.mpi
# Ap2 File: sweep3d.mpi+pat+27054-89t.ap2
# Number PEs: 48
# Max PEs/Node: 4
#
# To use this file, make a copy named MPICH_RANK_ORDER, and set the
# environment variable MPICH_RANK_REORDER_METHOD to 3 prior to
# executing the program.
#
# The following table lists rank order alternatives and the grid_order
# command-line options that can be used to generate a new order.
```

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Auto-Generated MPI Rank Order File



```
# The
                      1,403,65,435,33,411,97 5,439,37,407,69,447,10 3,440,35,432,67,400,99 257,345,265,313,281,30
'USER Time hybrid'
                       ,443,9,467,25,499,105,1,415,13,471,45,503,29,408,11,464,43,496,27,5,273,337,609,369,577,
rank order in this
                      507,41,475
                                             ,479,77,511
                                                                    472,51,504
                                                                                           377,617,329,513,529
file targets nodes
                      73,395,81,427,57,459,153,399,85,431,21,463,619,392,75,424,59,456,8545,297,633,361,625,32
with multi-core
                      7,419,113,491,49,387,81,391,109,423,93,455,13,384,107,416,91,488,11,585,537,601,289,553,
# processors, based on 9,451,121,483
                                                                    15,448,123,480
                                             17,495,125,487
                                                                                           353,593,521,569,561
Sent Msg Total Bytes
                      6,436,102,468,70,404,32,530,34,562,66,538,98 132,401,196,441,164,40 256,373,261,341,264,34
collected for:
                      8,412,14,444,46,476,11,522,10,570,42,554,26,9,228,433,236,465,204,9,280,317,272,381,269,
                      0,508,78,500
                                             594,50,602
                                                                    473,244,393,188,497
                                                                                           309,285,333,277,365
# Program:
                /lus/ 86,396,30,428,62,460,518,514,74,586,58,626,8252,505,140,425,212,45352,301,320,325,288,35
nid00023/malice/
                      4,492,118,420,22,452,9 2,546,106,634,90,578,1 7,156,385,172,417,180, 7,328,304,360,312,376,
craypat/WORKSHOP/bh2o- 4,388,126,484
                                                                    449,148,489,220,481
                                             14,618,122,610
                                                                                           293, 296, 368, 336, 344
demo/Rank/sweep3d/src/<sub>129,563,193,531,161,57,135,315,167,339,199,34,131,534,195,542,163,56,258,338,266,346,282,31</sub>
sweep3d
                      1,225,539,241,595,233,7,259,307,231,371,239,6,227,526,235,574,203,4,274,370,766,306,710,
# Ap2 File:
                      523,249,603,185,555
                                             379,191,331,247,299
                                                                    598,243,558,187,606
                                                                                           378,742,330,678,362
sweep3d.gmpi-u.ap2
                      153,587,169,627,137,63 175,363,159,323,143,35 251,590,211,630,179,63 646,298,750,322,718,35
                      5,201,619,177,515,145,5,255,291,207,275,183,8,139,622,155,550,171,4,758,290,734,662,686,
# Number PEs:
                768
                      579,209,547,217,611
                                             283, 151, 267, 215, 223
                                                                    518,219,582,147,614
                                                                                           670,726,702,694,654
# Max PEs/Node: 16
                      7,405,71,469,39,437,10 133,406,197,438,165,47 761,660,737,652,705,66 262,375,263,343,270,31
                      3,413,47,445,15,509,790,229,414,245,446,141,8,745,692,673,700,641,1,271,351,286,319,278,
# To use this file,
                      ,477,31,501
                                             478,237,502,253,398
                                                                    684,713,644,753,724
                                                                                           342,287,350,279,374
make a copy named
                      111,397,63,461,55,429, 157,510,189,462,173,43 729,732,681,756,721,71 294,318,358,383,359,31
MPICH RANK ORDER, and
                      87,421,23,493,119,389,0,205,390,149,422,213,6,764,676,697,748,689,0,295,382,326,303,327,
set the
                      95,453,127,485
                                             454,181,494,221,486 657,740,665,649,708
                                                                                           367,366,335,302,334
# environment variable
MPICH RANK REORDER MET 134,402,198,434,166,41 130,316,260,340,194,37 760,528,736,536,704,56 765,661,709,663,741,65
                      0,230,442,238,466,174,2,162,348,226,308,234,0,744,520,672,568,712,3,711,669,767,655,743,
HOD to 3 prior to
                      506, 158, 394, 246, 474
                                             380,242,332,250,300
                                                                    592,752,552,640,600
                                                                                           671,749,695,679,703
# executing the
                      190,498,254,426,142,45 202,364,186,324,154,35 728,584,680,624,720,51 677,727,751,693,647,70
program.
                      8,150,386,182,418,206,6,138,292,170,276,178,2,696,632,688,616,664,1,717,687,757,685,733,
                      490,214,450,222,482
                                             284,210,218,268,146
                                                                    544,608,656,648,576
                                                                                        725,719,735,645,759
0,532,64,564,32,572,96
                      128,533,192,541,160,564,535,36,543,68,567,10762,659,738,651,706,66
,540,8,596,72,524,40,6
                      5,232,525,224,573,240,0,527,12,599,44,575,287,746,643,714,691,674,
04,24,588
                      597,184,557,248,605
                                             ,559,76,607
                                                                    699,754,683,730,723
104,556,16,628,80,636,
                      168.589.200,517,152,62 52,591,20,631,60,639,8 722,731,763,658,642,75
56,620,48,516,112,580,
                      9,136,549,176,637,144,4,519,108,623,92,551,15,739,675,707,650,682,
88,548,120,612
                      621,208,581,216,613 16,583,124,615
                                                                    715,698,666,690,747
                             CUMPULE
```

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grid_order Utility

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- Can use grid_order utility without first running the application with the Cray performance tools if you know a program's data movement pattern
- Originally designed for MPI programs, but since reordering is done by PMI, it can be used by other programming models (since PMI is used by MPI, SHMEM and PGAS programming models)
- Utility available if perftools modulefile is loaded
- See grid_order(1) man page or run grid_order with no arguments to see usage information

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Reorder Example for Bisection Bandwidth

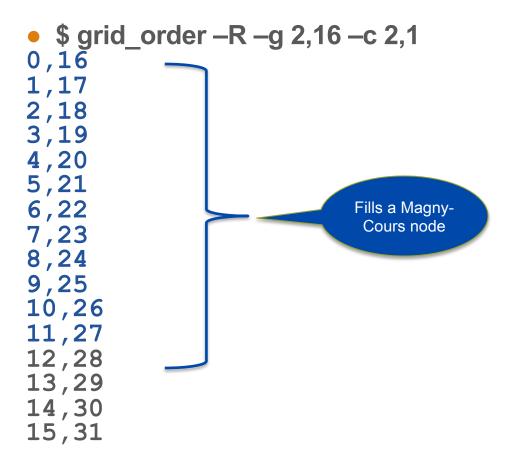


- Assume 32 ranks
- Decide on row or column ordering:
- \$ grid_order -R -g 2,16
 0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15
 16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31
- \$ grid_order -C -g 2,16
 0,2,4,6,8,10,12,14,16,18,20,22,24,26,28,30
 1,3,5,7,9,11,13,15,17,19,21,23,25,27,29,31
- Since rank 0 talks to rank 16, and not with rank 1, we choose Row ordering

Reorder Example for Bisection Bandwidth (2)



 Specify cell (or chunk) to make sure rank pairs live on same node (but don't care how many pairs live on a node)



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Using New Rank Order



 Save grid_order output to file called MPICH_RANK_ORDER

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- Export MPICH_RANK_REORDER_METHOD=3
- Run non-instrumented binary with and without new rank order to check overall wallclock time for improvements

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Collecting Loop Work Estimates



- Load PrgEnv-cray module (must use CCE)
- Load perftools module
- Compile AND link with –h profile_generate
 - cc –h profile_generate –o my_program my_program.c
- Instrument binary for tracing
 - pat_build –w my_program
- Run application
- Create report with loop statistics
 - pat_report my_program.xf > loops_report

pat_report produces report plus .ap2 file that can be used with Reveal

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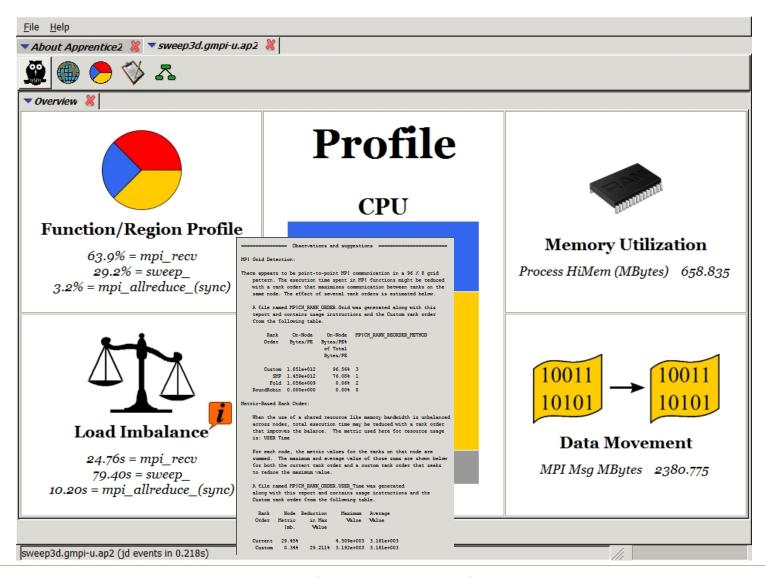
Table 2: Loop Stats by Function (from -hprofile_generate)						
Loop	Loop	Loop	Loop	Loop	Function=/.LOOP[.]	
Incl	Hit	Trips	Trips	Trips	PE=HIDE	
Time		Avg	Min	Max		
Total	I		I			
8.995914	100	25	0	25	sweepyLOOP.1.li.33	
8.995604	2500	25	0	25	sweepyLOOP.2.li.34	
8.894750	50	25	0	25	sweepzLOOP.05.1i.49	
8.894637	1250	25	0	25	sweepzLOOP.06.li.50	
4.420629	50	25	0	25	sweepx2LOOP.1.li.29	
4.420536	1250	25	0	25	sweepx2LOOP.2.1i.30	
4.387534	50	25	0	25	sweepx1LOOP.1.1i.29	
4.387457	1250	25	0	25	sweepx1LOOP.2.li.30	
2.523214	187500	107	0	107	riemannLOOP.2.li.63	
1.541299	20062500	12	0	12	riemannLOOP.3.li.64	
0.863656	1687500	104	0	108	parabolaLOOP.6.li.67	

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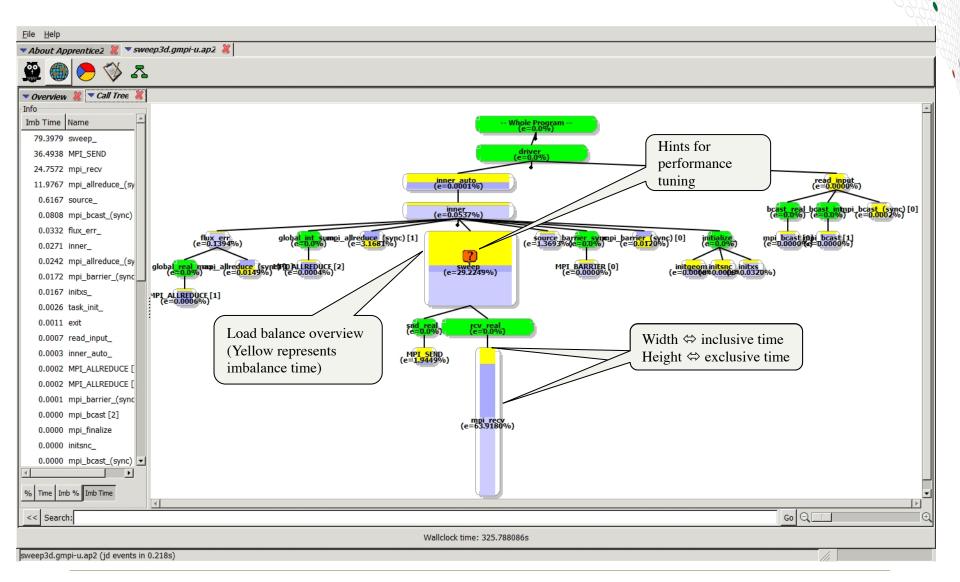
Cray Apprentice2 Overview



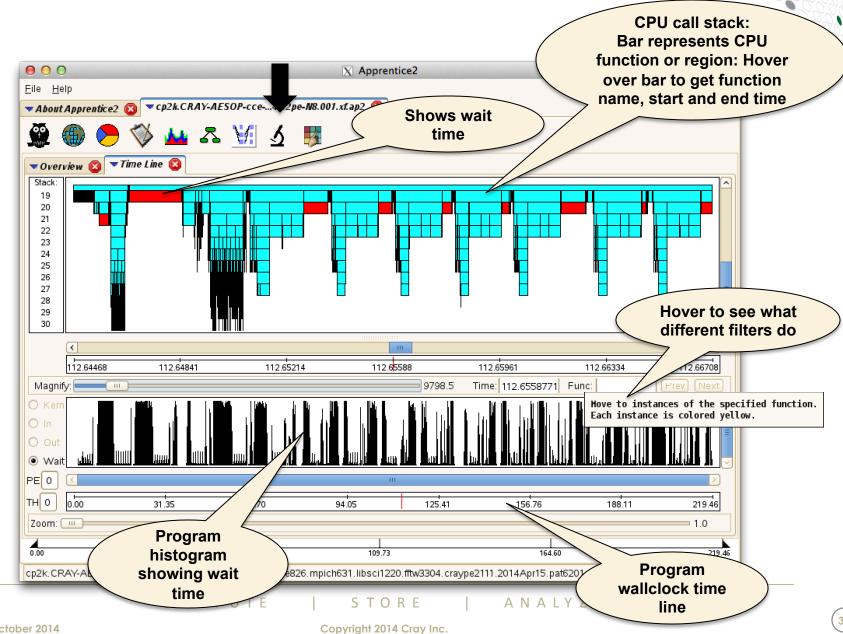


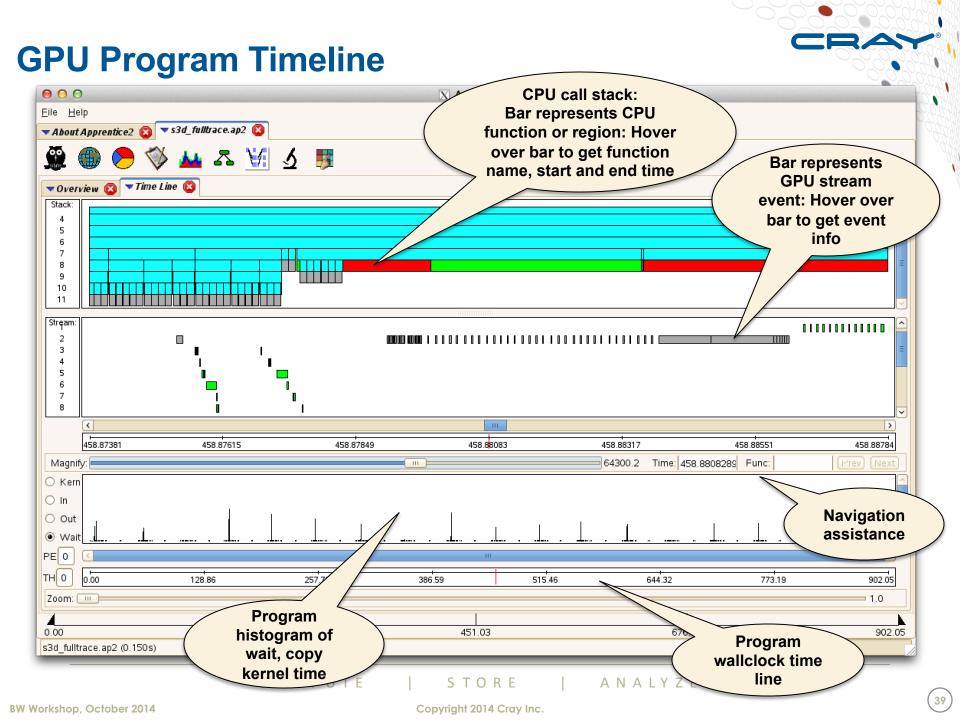
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Call Tree View with Load Imbalance Information



CPU Program Timeline: 36GB CP2K Full Trace









```
Table 1: Time and Bytes Transferred for Accelerator Regions
 Host | Host | Acc | Acc Copy | Acc Copy | Calls | Calltree
Time% | Time | Time | In | Out | | PE=HIDE
 | | (MBytes) | (MBytes) |
100.0% | 2.750 | 2.015 | 2812.760 | 13.568 | 103 | Total
| 100.0% | 2.750 | 2.015 | 2812.760 | 13.568 | 103 | lbm3d2p d
3|| 63.5% | 1.747 | 1.747 | 2799.192 | -- | 1 |lbm3d2p_d_.ACC_COPY@li.104
3|| 22.1% | 0.609 | 0.088 | 12.304 | 12.304 | 36 |streaming_
6||| 1.1% | 0.031 | -- | -- | 1 | streaming .ACC REGION@li.909(exclusive)
```

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Lab Time



- bw.ncsa.illinois.edu:~heidi/scratch/lab/
 - CrayPat-lite
 - pr01
 - Loop statistics
 - pr05
 - MPI rank reorder
 - pr03
 - Apprentice2
 - pr04
 - Reveal
 - pr05, pr01
- CCDB



Questions

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