BLUE WATERS SUSTAINED PETASCALE COMPUTING

Performance Tools on Blue Waters

Manisha Gajbe + others























Performance Tools

- Cray Performance Tools
- Perfsuite (NCSA)
- TAU













Topics

- Cray performance tools overview
- Steps to using the tools
- Performance measurement on the Cray XE system
- Using HW performance counters
 - Access to Northbridge: L3 and memory
- Profiling applications
- Visualization of performance data through pat_report
- Visualization of performance data through Cray Apprentice2
- MPI Rank Order
- PerfSuite (NCSA)
- TAU: Tuning and Analysis Utilities
- Congestion Protection and Balanced Injection













Overview













Design Goals

Assist the user with application performance analysis and optimization

- Help user identify important and meaningful information from potentially massive data sets
- Help user identify problem areas instead of just reporting data
- Bring optimization knowledge to a wider set of users













Design Goals

Focus on ease of use and intuitive user interfaces

- Automatic program instrumentation
- Automatic analysis

Target scalability issues in all areas of tool development

- Data management
 - Storage, movement, presentation













Strengths

solution from instrumentation to measurement to analysis to visualization of data

- Performance measurement and analysis on large systems
 - Automatic Profiling Analysis
 - Load Imbalance
 - HW counter derived metrics
 - Predefined trace groups provide performance statistics for libraries called by program (blas, lapack, pgas runtime, netcdf, hdf5, etc.)
 - Observations of inefficient performance
 - Data collection and presentation filtering
 - Data correlates to user source (line number info, etc.)
 - Support MPI, SHMEM, OpenMP, UPC, CAF, OpenACC
 - Access to network counters
 - Minimal program perturbation













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
- To access software:
 - module load perftools













The Cray Performance Analysis Framework

CrayPat

- Instrumentation of optimized code
- No source code modification required
- Data collection transparent to the user
- Text-based performance reports
- Derived metrics
- Performance analysis

Cray Apprentice2

- Performance data visualization tool
- Call tree view
- Source code mappings













Steps To Using Tools













Application Instrumentation with pat_build

- pat_build is a stand-alone utility that instruments the application for performance collection
- Requires no source code or makefile modification
- Automatic instrumentation at group (function) level
 - o Groups: mpi, io, heap, math SW, ...
- Performs link-time instrumentation
- Requires object files
- Instruments optimized code
- Generates stand-alone instrumented program
- Preserves original binary





Application Instrumentation with pat_build (2)

- Supports two categories of experiments
 - asynchronous experiments (sampling) which capture values from the call stack or the program counter at specified intervals or when a specified counter overflows
 - Event-based experiments (tracing) which count some events such as the number of times a specific system call is executed
- While tracing provides most useful information, it can be very heavy if the application runs on a large number of cores for a long period of time
- Sampling can be useful as a starting point, to provide a first overview of the work distribution









Sampling with Line Number information

```
heidi@limited: /h/heidi - ssh - 81×26
Table 2: Profile by Group, Function, and Line
 Samp% | Samp
               | Imb. | Imb. | Group
               I Samp | Samp% | Function
                                 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
31
    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
4111
    1.0% | 84.5 | 17.5 | 17.6% | line.95
4||| 1.0% | 86.8 | 33.2 | 28.2% |line.96
4||| 1.3% | 105.0 | 23.0 | 18.4% |line.97
                             17.7% | line.98
    1.4% | 116.5 | 24.5 |
4111
                                                          144,1
                                                                      38%
```







Where to Run Instrumented Application

- By default, data files are written to the execution directory
- Default behavior requires file system that supports record locking, such as Lustre (/mnt/snx3/..., /lus/..., /scratch/...,etc.)
 - Can use PAT_RT_EXPFILE_DIR to point to existing directory that resides on a high-performance file system if not execution directory
- Number of files used to store raw data
 - − 1 file created for program with 1 256 processes
 - – √n files created for program with 257 n processes
 - Ability to customize with PAT_RT_EXPFILE_MAX
- See intro_craypat(1) man page













CrayPat Runtime Options

- Runtime controlled through PAT_RT_XXX environment variables
- Examples of control
 - Enable full trace
 - Change number of data files created
 - Enable collection of HW counters
 - Enable collection of network counters
 - Enable tracing filters to control trace file size (max threads, max call stack depth, etc.)













Example Runtime Environment Variables

- Optional timeline view of program available
 - export PAT_RT_SUMMARY=0 (Collect data in detail than aggregate)
 - View trace file with Cray Apprentice²
- Request hardware performance counter information:
 - export PAT_RT_HWPC=<HWPC Group>
 - export PAT_RT_ACCPC=<HWPC Group>
 - Can specify events or predefined groups













Predefined Trace Wrappers (-g tracegroup)

- blas Basic Linear Algebra subprograms
- caf Co-Array Fortran (Cray CCE compiler only)
- hdf5 manages extremely large data collection
- heap dynamic heap
- io includes stdio and sysio groups
- lapack Linear Algebra Package
- math ANSI math
- mpi MPI
- omp OpenMP API
- pthreads POSIX threads
- shmem SHMEM
- sysio I/O system calls
- system system calls
- upc Unified Parallel C (Cray CCE compiler only)

For a full list, please see pat_build(1) man page











Example Experiments

- > pat_build –O apa
 - Gets you top time consuming routines
 - Lightest-weight sampling
- > pat_build -u -g mpi ./my_program
 - Collects information about user functions and MPI
- > pat_build –w ./my_program
 - Collections information for MAIN
 - Lightest-weight tracing
- > pat_build –g netcdf,mpi ./my_program
 - Collects information about netcdf routines and MPI













pat_report

- Combines information from binary with raw performance data
- Performs analysis on data
- Generates text report of performance results
- Generates customized instrumentation template for automatic profiling analysis
- Formats data for input into Cray Apprentice²













Automatic Profiling Analysis













Why Should I generate a ".ap2" file?

- The ".ap2" file is a self contained compressed performance file
- Normally it is about 5 times smaller than the ".xf" file
- Contains the information needed from the application binary
 - Can be reused, even if the application binary is no longer available or if it was rebuilt
- It is the only input format accepted by Cray Apprentice²













Program Instrumentation - Automatic Profiling Analysis

- Automatic profiling analysis (APA)
 - Provides simple procedure to instrument and collect performance data for novice users
 - Identifies top time consuming routines
 - Automatically creates instrumentation template customized to application for future in-depth measurement and analysis











Steps to Collecting Performance Data

Access performance tools software

```
% module load perftools
```

Build application keeping .o files (CCE: -h keepfiles)

```
% 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 application to get top time consuming routines

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











Steps to Collecting Performance Data (2)

- You should get a performance file ("<sdatafile>.xf") or multiple files in a directory <sdatadir>
- Generate report and .apa instrumentation file

```
% pat_report <sdatafile>.xf > sampling_report
% pat_report -o sampling_report
[<sdatafile>.xf | <sdatadir>]
```

- Inspect .apa file and sampling report
- Verify if additional instrumentation is needed











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
```













CPU HW Performance Counters











PAPI Predefined Events

- Common set of events deemed relevant and useful for application performance tuning
 - Accesses to the memory hierarchy, cycle and instruction counts, functional units, pipeline status, etc.
 - The "papi_avail" utility shows which predefined events are available on the system – execute on compute node
- PAPI also provides access to native events
 - The "papi_native_avail" utility lists all AMD native events available on the system – execute on compute node
- PAPI uses perf events Linux subsystem
- Information on PAPI and AMD native events
 - pat_help counters
 - man intro_papi (points to PAPI documentation: http://icl.cs.utk.edu/papi/)
 - http://lists.eecs.utk.edu/pipermail/perfapi-devel/2011-January/004078.html











Hardware Counters Selection

- HW counter collection enabled with PAT_RT_HWPC environment variable
- PAT_RT_HWPC <set number> | <event list>
 - A set number can be used to select a group of predefined hardware counters events (recommended)
 - CrayPat provides 23 groups on the Cray XT/XE systems
 - See pat_help(1) or the hwpc(5) man page for a list of groups
 - Alternatively a list of hardware performance counter event names can be used
 - Hardware counter events are not collected by default













Predefined Interlagos HW Counter Groups

See pat_help -> counters -> amd_fam15h -> groups

- 0: Summary with instructions metrics
- 1: Summary with TLB metrics
- 2: L1 and L2 Metrics
- 3: Bandwidth information
- 4: <Unused>
- 5: Floating operations dispatched
- 6: Cycles stalled, resources idle
- 7: Cycles stalled, resources full
- 8: Instructions and branches
- 9: Instruction cache
- 10: Cache Hierarchy (unsupported for IL)













Predefined Interlagos HW Counter Groups (cont'd)

- 11: Floating point operations dispatched
- 12: Dual pipe floating point operations dispatched
- 13: Floating point operations SP
- 14: Floating point operations DP
- 19: Prefetchs
- 20: FP, D1, TLB, MIPS
- 21: FP, D1, TLB, Stalls
- 22: D1, TLB, MemBW
- 23: FP, D1, D2, TLB
- default: group 23

Support for L3 cache counters now available.











New HW counter groups for Interlagos (6 counters)

Group 20: FP, D1, TLB, MIPS

```
PAPI_FP_OPS
PAPI_L1_DCA
PAPI_L1_DCM
PAPI_TLB_DM
DATA_CACHE_REFILLS_FROM_NORTHBRIDGE
PAPI_TOT_INS
```

Group 21: FP, D1, TLB, Stalls

```
PAPI_FP_OPS
PAPI_L1_DCA
PAPI_L1_DCM
PAPI_TLB_DM
DATA_CACHE_REFILLS_FROM_NORTHBRIDGE
PAPI_RES_STL
```













AMD North-Bridge events

L3_CACHE_MISSES:type:core

READ_BLOCK_EXCLUSIVE, READ_BLOCK_SHARED, READ_BLOCK_MODIFY, PREFETCH, ALL

CORE_0, CORE_1 ... CORE_7, ALL_CORES

DRAM_ACCESSES:type

DCT0_PAGE_HIT, DCT0_PAGE_MISS, DCT0_PAGE_CONFLICT same for DCT1, ALL

To see all NB events (start with craynb:::)

> aprun papi native avail









Example: HW counter data & Derived Metrics

PAPI TLB DM Data translation lookaside buffer misses PAPI L1 DCA Level 1 data cache accesses PAT RT HWPC=1 PAPI FP OPS Floating point operations DC MISS Data Cache Miss Flat profile data User Cycles Virtual Cycles **Raw counts Derived metrics** USER 98.3% Time% Time 4.434402 secs Imb. Time -- secs Imb. Time% 0.001M/sec 4500.0 calls Calls PAPI L1 DCM 14.820M/sec 65712197 misses PAPI TLB DM 0.902M/sec3998928 misses PAPI L1 DCA 333.331M/sec 1477996162 refs PAPI FP OPS 445.571M/sec 1975672594 ops 11971868993 cycles 100.0%Time User time (approx) 4.434 secs Average Time per Call 0.000985 sec CrayPat Overhead : Time 0.1% HW FP Ops / User time 445.571M/sec 1975672594 ops 4.1%peak(DP) 445.533M/sec HW FP Ops / WCT Computational intensity 1.34 ops/ref 0.17 ops/cycle MFLOPS (aggregate) 1782.28M/sec 369.60 refs/miss TLB utilization 0.722 avg uses 4.4% misses D1 cache hit, miss ratios 95.6% hits D1 cache utilization (misses) 22.49 refs/miss 2.811 avg hits











USER						
Time%				98.3%		
Time			4.4	36808	secs	
Imb.Time					secs	
Imb.Time%						
Calls	0.001 M/sec		4500.0		calls	
DATA_CACHE_REFILLS:						
L2_MODIFIED:L2_OWNED:						
L2_EXCLUSIVE:L2_SHARED		1/sec	435	67825	fills	
DATA_CACHE_REFILLS_FROM_SYSTE						
ALL			1097			
	14.824					
	332.9601					
	4.436	secs				100.0%Time
Average Time per Call			0.0	00986	sec	
CrayPat Overhead : Time						
D1 cache hit, miss ratios						
D1 cache utilization (misses)					_	
D1 cache utilization (refills						3
D2 cache hit, miss ratio						
D1+D2 cache hit, miss ratio						
D1+D2 cache utilization						3
System to D1 refill						
System to D1 bandwidth	L510.217N	MB/sec	70253	86144	bytes	
D2 to D1 bandwidth	599.3981	/B/sec	27883	40816	bytes	













Profile Visualization with pat_report











pat_report: Job Execution Information

```
CrayPat/X: Version 5.2.3.8078 Revision 8078 (xf 8063) 08/25/11 ...
Number of PEs (MPI ranks):
                             16
Numbers of PEs per Node: 16
Numbers of Threads per PE:
Number of Cores per Socket:
                             12
Execution start time: Thu Aug 25 14:16:51 2011
System type and speed: x86 64 2000 MHz
Current path to data file:
  /lus/scratch/heidi/ted swim/mpi-openmp/run/swim+pat+27472-34t.ap2
Notes for table 1:
```











pat_report: Table Notes

```
Notes for table 1:
  Table option:
    -O profile
  Options implied by table option:
    -d ti%@0.95,ti,imb ti,imb ti%,tr -b gr,fu,pe=HIDE
  Other options:
    -\mathbf{T}
  Options for related tables:
    -O profile pe.th
                               -O profile th pe
                              -O load baTance
    -O profile Farc
    -O callers
                               -0 callers+src
    -O calltree
                                -O calltree+src
  The Total value for Time, Calls is the sum for the Group values.
  The Group value for Time, Calls is the sum for the Function values.
  The Function value for Time, Calls is the avg for the PE values.
    (To specify different aggregations, see: pat help report options s1)
  This table shows only lines with Time  > 0.
  Percentages at each level are of the Total for the program.
    (For percentages relative to next level up, specify:
      -s percent=r[elative])
```











pat_report: Additional Information

```
Instrumented with:
   pat_build -gmpi -u himenoBMTxpr.x
```

Program invocation:

../bin/himenoBMTxpr+pat.x

Exit Status: 0 for 256 PEs

CPU Family: 15h Model: 01h Stepping: 2

Core Performance Boost: Configured for 0 PEs

Capable for 256 PEs

Memory pagesize: 4096

Accelerator Model: Nvidia X2090 Memory: 6.00 GB Frequency: 1.15 GHz

Programming environment: CRAY

Runtime environment variables:

OMP NUM THREADS=1









Sampling Output (Table 1)

					- /							
N	otes for t	table 1:										
•	• •											
T	Table 1: Profile by Function											
	Samp % S	Samp	Imb. G	. Group								
			Imb. Samp S		Function							
	j	j	• i	· i	PE='HIDE'							
	100.0%	775 I	1	IT	otal							
1			<u>'</u>									
	94.2%	730			USER							
	13 18	336	 Ω 75	 2 6%	mlwxyz							
	43.4% 16.1%	336 125	8.75 6.25 1.88	%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%	half —							
İ	8.0 %	62	6.25 1.88	j 9.5%	full_							
	0.8%	53 30		1 3.5%	artv <u> </u>							
	8.0%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%	28	1.34	93.69 3.69	currenf							
j	2.2%	17 i	1.50	8.6%	bndsf -							
		13	1.97 1.53	13.5% 12.2%	model— cfl —							
	1.4% 1.3%	62388731088 11118			cur <u>r</u> enh							
	1.0%	l Š	0.75 5.28 8.28	7.0% 41.9%	bndbo -							
	1.0%	8	8.28	<u> 53.4%</u>	bndto							
	5.4% 42		 	MPI								
		- -		<u>-</u>								
ĺ	1.9%	15 14	4.62 16.53	23.9%	mpi_sendrecv_							
	1.9% 1.8% 1.7%	13	5.66	23.9% 55.0% 30.7%	mpi=bcast = mpi=barrier							
			J. 00	- 30.7°								











pat_report: Flat Profile

```
Table 1: Profile by Function Group and Function
Time % | Time | Imb. | Calls | Group
                           | Time % | | Function
                                         | PE='HIDE'
100.0% | 104.593634 | -- | -- | 22649 | Total
 71.0% | 74.230520 | -- | -- | 10473 |MPI
|| 69.7% | 72.905208 | 0.508369 | 0.7% | 125 |mpi allreduce
  1.0% | 1.050931 | 0.030042 | 2.8% | 94 |mpi_alltoall_
 25.3% | 26.514029 | -- | -- | 73 | USER
|| 16.7% | 17.461110 | 0.329532 | 1.9% | 23 |selfgravity
   7.7% | 8.078474 | 0.114913 | 1.4% | 48 |ffte4
   2.5% | 2.659429 | -- | -- | 435 |MPI SYNC
   2.1% | 2.207467 | 0.768347 | 26.2% | 172 | mpi barrier (sync)
   1.1% | 1.188998 | -- | -- | 11608 | HEAP
    1.1% | 1.166707 | 0.142473 | 11.1% | 5235 | free
```









pat_report: Message Stats by Caller

```
Table 4: MPI Message Stats by Caller
   MPI Msg | MPI Msg | MsgSz | 4KB<= | Function
     Bytes | Count | <16B | MsgSz | Caller
                      Count | <64KB | PE[mmm]
                             | Count |
 15138076.0 | 4099.4 | 411.6 | 3687.8 | Total
 15138028.0 | 4093.4 | 405.6 | 3687.8 | MPI ISEND
   8080500.0 | 2062.5 | 93.8 | 1968.8 | calc2
3 I
                                | MAIN
4||| 8216000.0 | 3000.0 | 1000.0 | 2000.0 |pe.0
4||| 8208000.0 | 2000.0 | -- | 2000.0 |pe.9
     6160000.0 | 2000.0 | 500.0 | 1500.0 |pe.15
|| 6285250.0 | 1656.2 | 125.0 | 1531.2 |calc1
3|
                                       | MAIN
4||| 8216000.0 | 3000.0 | 1000.0 | 2000.0 |pe.0
4||| 6156000.0 | 1500.0 | -- | 1500.0 |pe.3
     6156000.0 | 1500.0 | -- | 1500.0 |pe.5
```













Using L3 NB counters with CrayPat

Load CrayPat module

\$ module load perftools

Compile and Instrument as usual:

```
$ cc -o stream stream.c
```

\$ pat build stream

Define counters (up to 4)

\$ export PAT RT PERFCTR=L3 CACHE MISSES,...

Run

\$ aprun -ss -cc 0 stream+pat

Generate the report

\$ pat_report -0 hwpc stream+pat+2313073-25560s.xf











pat_report excerpts for L3

Limited derived metrics at the moment. Can be used to calculate bandwidth to main memory.

Table 3: Program HW Performance Counter Data

L3_CACHE_MISSES:ALL:CORE_0 | L3_CACHE_MISSES | Total 207185723 | 207502576 | Total

Table 2:













Profile Visualization with Cray Apprentice2













Cray Apprentice²

- Call graph profile
- Communication statistics
- Time-line view
 - Communication
 - o I/O
- Activity view
- Pair-wise communication statistics
- Text reports
- Source code mapping
- Runs on login node
- Supported on Mac OS and Windows also

- Cray Apprentice² helps identify:
 - Load imbalance
 - Excessive communication
 - Network contention
 - Excessive serialization
 - o I/O Problems











Application Performance Summary







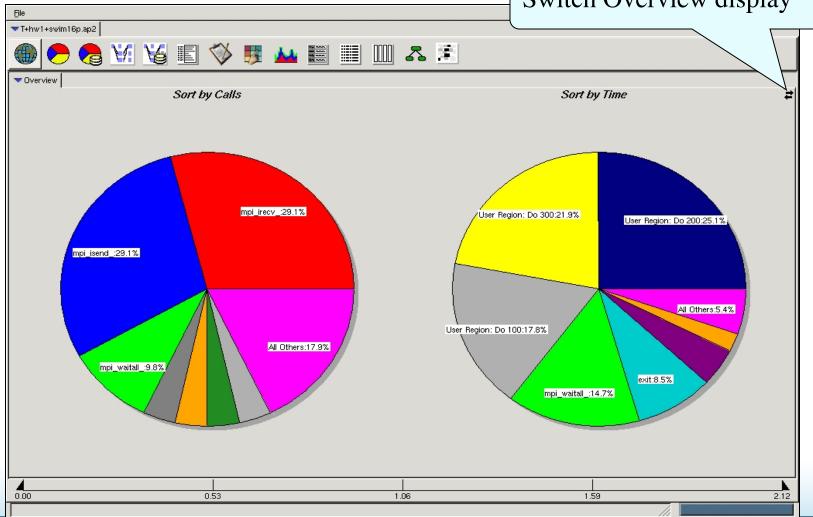






Statistics Overview

Switch Overview display





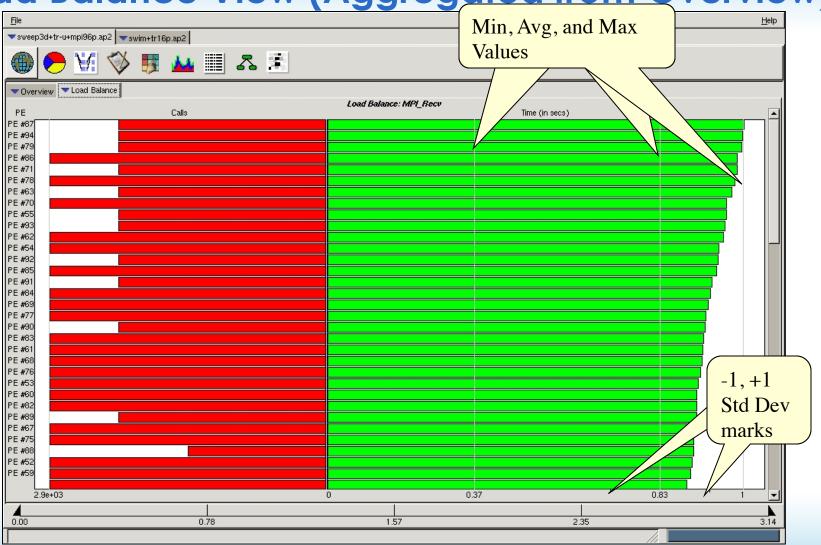








Load Balance View (Aggregated from Overview)















pat_report Tables in Cray Apprentice2

- Complimentary performance data available in one place
- Drop down menu provides quick access to most common reports
- Ability to easily generate different views of performance data
- Provides mechanism for more in depth explanation of data presented

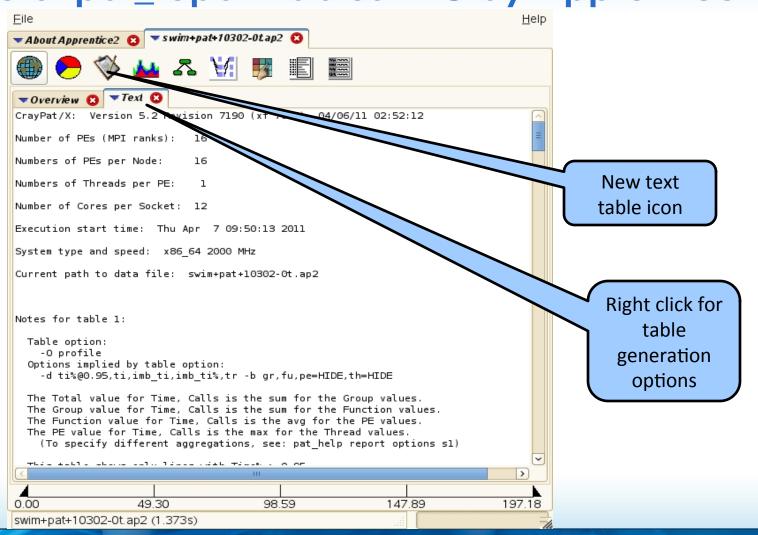








Example of pat_report Tables in Cray Apprentice2















Generating New pat_report Tables

_	_		
✓	Р	rof	ile

- Custom...
- Source
- Calltree
- Callers
- ✓ Show Notes
- ☐ Show All PE's
- ✓ Show HWPC
- ✓ Use Thresholds

Select All

Select None

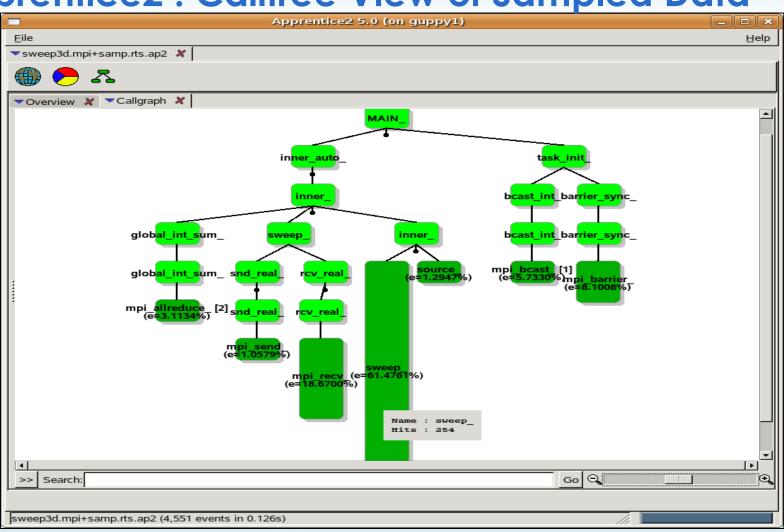
Panel Actions

Panel Help





Apprentice2: Calltree View of Sampled Data





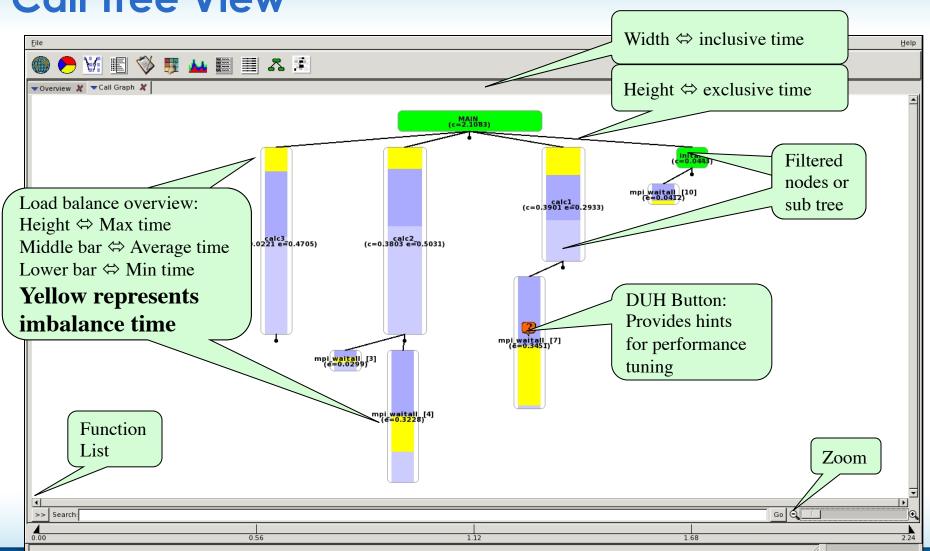














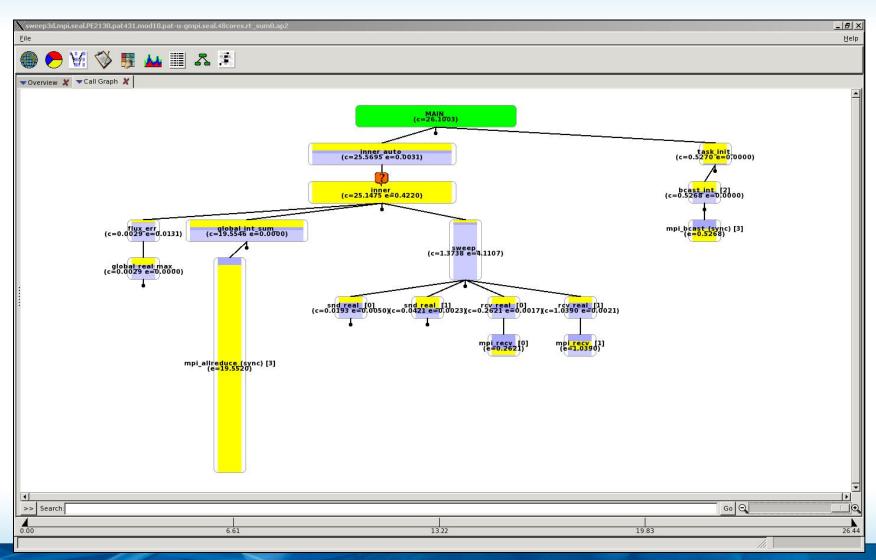








Call Tree Visualization





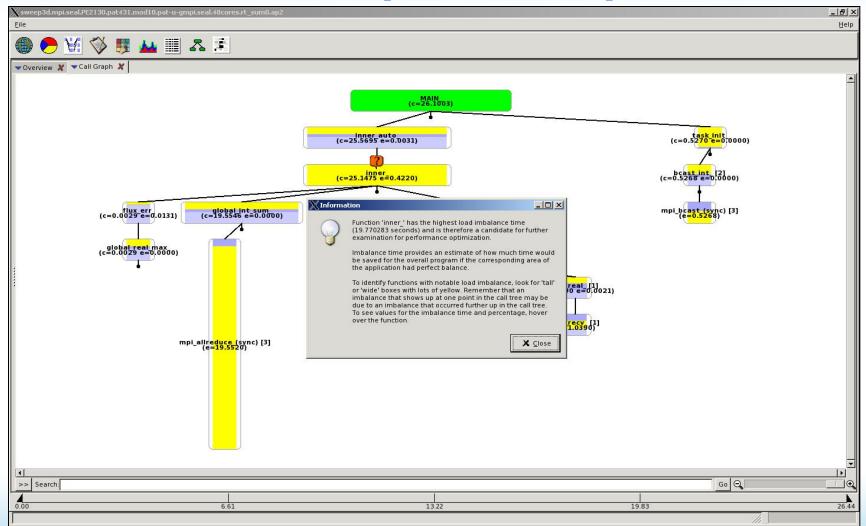








Discrete Unit of Help (DUH Button)





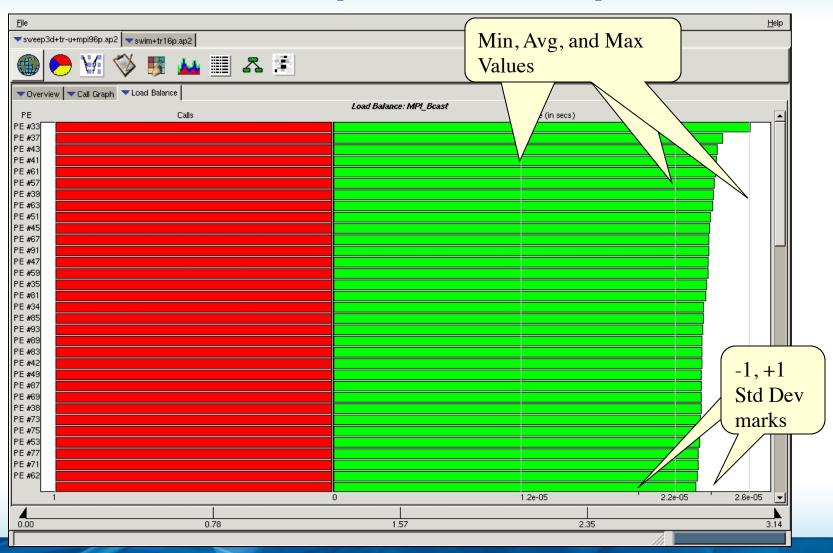








Load Balance View (from Call Tree)





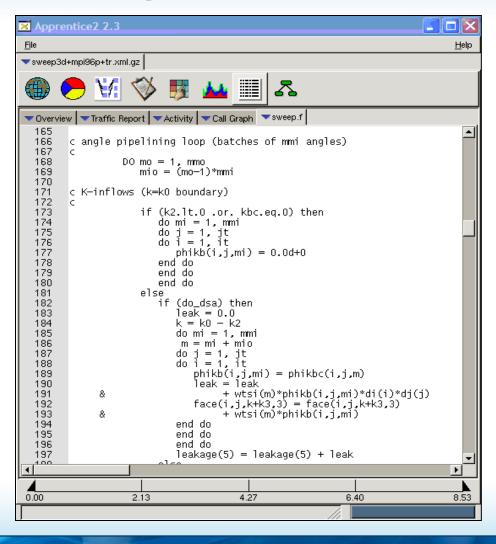








Source Mapping from Call Tree















Full Trace Visualization with Cray Apprentice2

BLUE WATERS





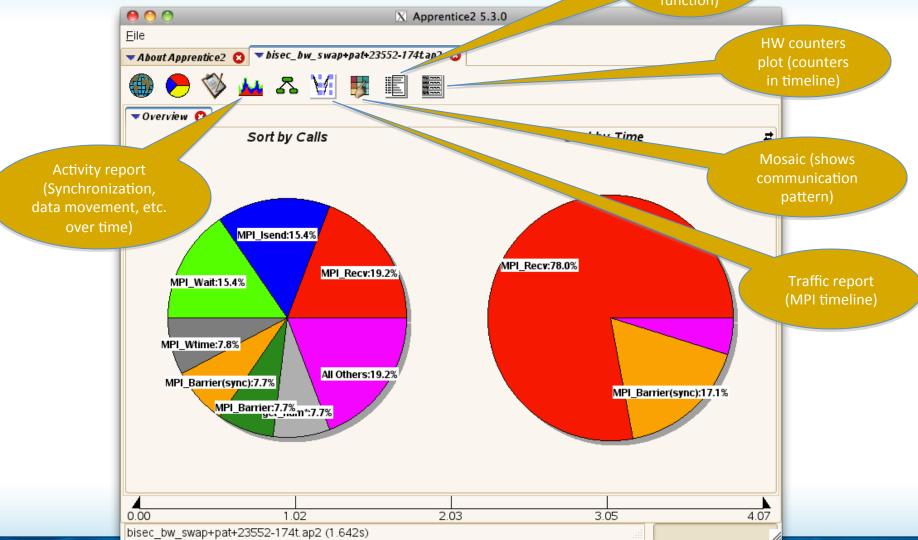


GREAT LAKES CONSORTIUM



HW counters overview (counter histogram by function)

Trace Overview – Additional V





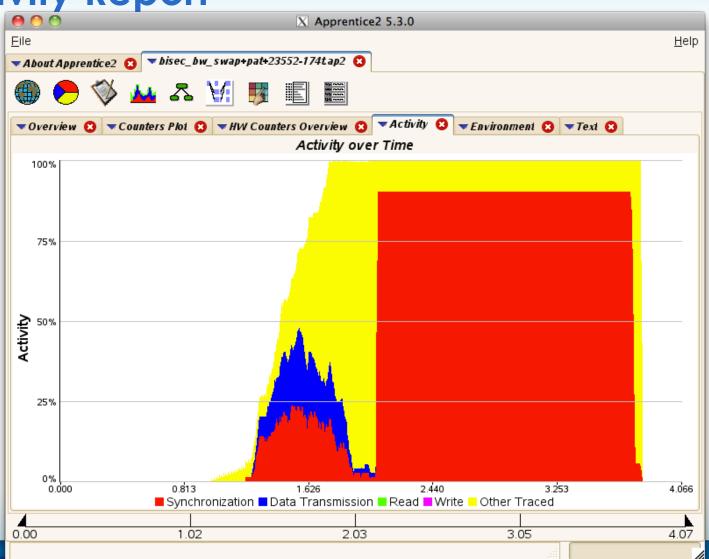








Activity Report



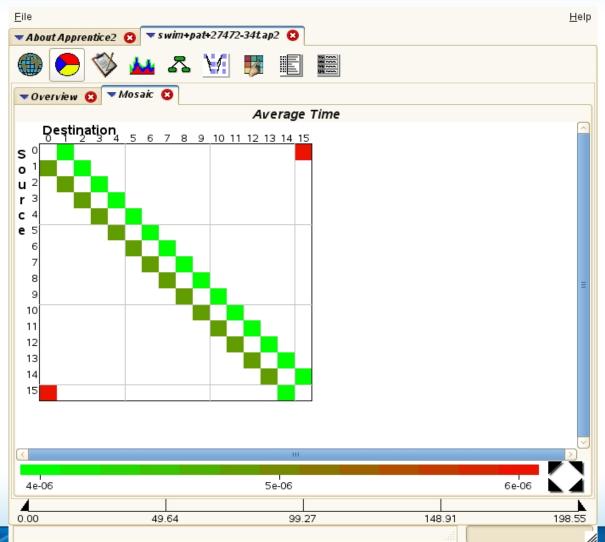








Mosaic View - Shows Communication Pattern





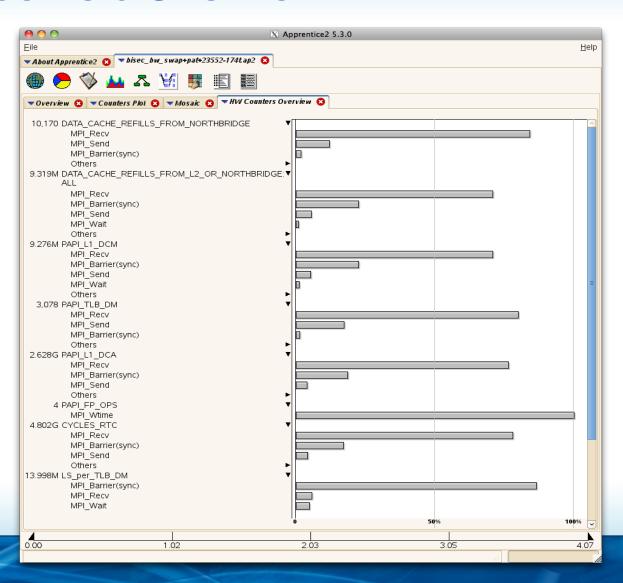








HW Counters Overview





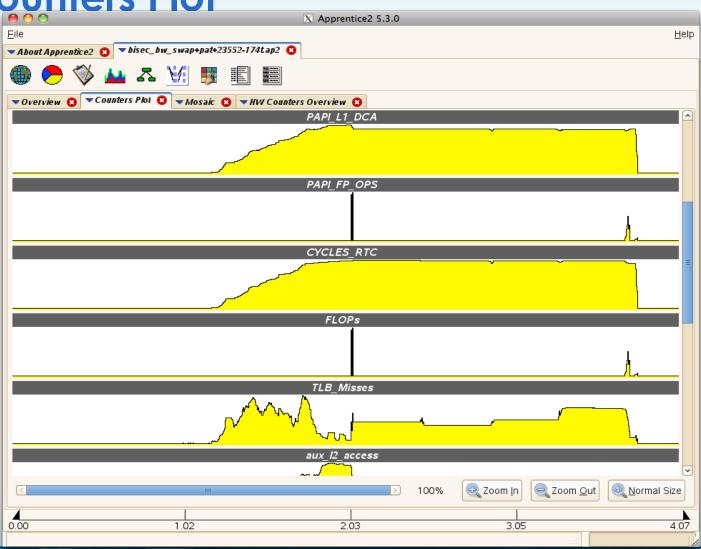




GREAT LAKES CONSORTIUM



HW Counters Plot



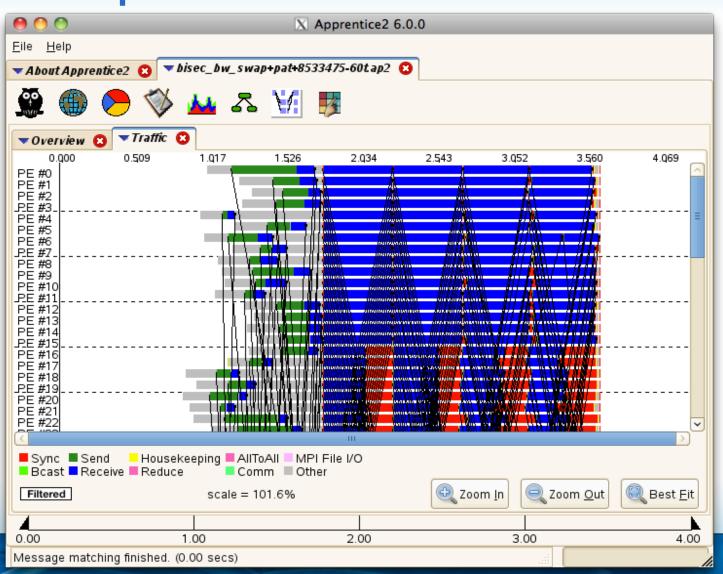








Traffic Report – MPI Communication Timeline













Man pages

- intro_craypat(1)
 Introduces the craypat performance tool
- pat_build(1)
 Instrument a program for performance analysis
- pat_help(1)
 Interactive online help utility
- pat_report(1)
 Generate performance report in both text and for use with GUI
- app2 (1)
 Describes how to launch Cray Apprentice2 to visualize performance data













Man pages (2)

- **hwpc**(5)
 - describes predefined hardware performance counter groups
- nwpc(5)
 - Describes predefined network performance counter groups
- accpc(5) / accpc_k20(5)
 - Describes predefined GPU performance counter groups
- intro_papi(3)
 - Lists PAPI event counters
 - Use papi_avail or papi_native_avail utilities to get list of events when running on a specific architecture













MPI Rank Order













MPI Rank Order

Is your nearest neighbor really your nearest neighbor?

And do you want them to be your nearest neighbor?











MPI Rank Placement

- Change default rank ordering with:
 - MPICH_RANK_REORDER_METHOD
- Settings:
 - 0: Round-robin placement Sequential ranks are placed on the next node in the list. Placement starts over with the first node upon reaching the end of the list.
 - 1: SMP-style placement Sequential ranks fill up each node before moving to the next. - DEFAULT
 - 2: Folded rank placement Similar to round-robin placement except that each pass over the node list is in the opposite direction of the previous pass.
 - 3: Custom ordering The ordering is specified in a file named MPICH RANK ORDER.













When Is Rank Re-ordering Useful?
Maximize on-node communication between MPI ranks

 Grid detection and rank re-ordering is helpful for programs with significant point-to-point communication

 Relieve on-node shared resource contention by pairing threads or processes that perform different work (for example computation with off-node communication) on the same node













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

					3111 0 1		
Т	able 1:	Profile by	Function Group	and Func	tion		
	Time% 	Time		Imb. Time%	Calls	Group Function PE=HIDE	
ı	100.0%	463.147240			21621.0	Total	
	52.0%	240.974379			21523.0	MPI	
	•	the state of the s	6 36.214468 1 25.849906		•	· - —	
	43.3%	200.474690			32.0	USER	
	•	•	0 58.716197 6 1.899097		•		
	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			27.0	SYSCALL	











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











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:
#
            /lus/nid00030/heidi/sweep3d/mod/sweep3d.mpi
# Program:
# 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

AUIO OC	HUIGIGIC	ALL INGLINA	
# The 'USER Time hybrid'	,475	5,439,37,407,69,447,101,4	,124,615 722,731,763,658,642,755,7
rank order in this file	73,395,81,427,57,459,17,4	15,13,471,45,503,29,479,7	3,440,35,432,67,400,99,40 39,675,707,650,682,715,69
targets nodes with multi-	19,113,491,49,387,89,451,	7,511	8,11,464,43,496,27,472,51 8,666,690,747
core	121,483	53,399,85,431,21,463,61,3	
<pre># processors, based on</pre>	6,436,102,468,70,404,38,4	91,109,423,93,455,117,495	19,392,75,424,59,456,83,373,337,609,369,577,377,61
Sent Msg Total Bytes	12,14,444,46,476,110,508,	,125,487	84,107,416,91,488,115,448 7,329,513,529
collected for:	78,500	2,530,34,562,66,538,98,52	
#			132,401,196,441,164,409,2 85,537,601,289,553,353,59
# Program: /lus/	92,118,420,22,452,94,388,	,602	28,433,236,465,204,473,24 3,521,569,561
nid00023/malice/craypat/	126,484	18,514,74,586,58,626,82,5	
WORKSHOP/bh2o-demo/Rank/			252,505,140,425,212,457,180,317,272,381,269,309,28
sweep3d/src/sweep3d	25,539,241,595,233,523,24		56,385,172,417,180,449,14 5,333,277,365
# Ap2 File:	9,603,185,555	135,315,167,339,199,347,2	
sweep3d.gmpi-u.ap2	153,587,169,627,137,635,2	59,307,231,371,239,379,19	131,534,195,542,163,566,2 28,304,360,312,376,293,29
# Number PEs: 768	01,619,177,515,145,579,20	1,331,247,299	27,526,235,574,203,598,24 6,368,336,344
# Max PEs/Node: 16	9,547,217,611	175,363,159,323,143,355,2	
#	7,405,71,469,39,437,103,4	55,291,207,275,183,283,15	251,590,211,630,179,638,174,370,766,306,710,378,74
# To use this file, make	13,47,445,15,509,79,477,3		39,622,155,550,171,518,21 2,330,678,362
a copy named	1,501	133,406,197,438,165,470,2	
MPICH_RANK_ORDER, and set	111,397,63,461,55,429,87,		761,660,737,652,705,668,7 58,290,734,662,686,670,72
the	121/25/155/115/505/55/155		45,692,673,700,641,684,71 6,702,694,654
<pre># environment variable</pre>	,127,485	157,510,189,462,173,430,2	
MPICH_RANK_REORDER_METHOD	134,402,198,434,166,410,2	1 494 221 486	729,732,681,756,721,716,771,351,286,319,278,342,28
to 3 prior to	30,442,238,466,174,506,15		64,676,697,748,689,657,74 7,350,279,374
<pre># executing the program.</pre>	8,394,246,474	130,316,260,340,194,372,1	
#	190,498,254,426,142,458,1 50,386,182,418,206,490,21	2 332 250 300	760,528,736,536,704,560,7 95,382,326,303,327,367,36 44,520,672,568,712,592,75 6,335,302,334
0,532,64,564,32,572,96,54	4,450,222,482	202,364,186,324,154,356,1	2,552,640,600 765,661,709,663,741,653,7
0,8,596,72,524,40,604,24,			728,584,680,624,720,512,6 11,669,767,655,743,671,74
588	32,525,224,573,240,597,18	0,218,268,146	96,632,688,616,664,544,60 9,695,679,703
104,556,16,628,80,636,56,	4,557,248,605	4,535,36,543,68,567,100,5	
620,48,516,112,580,88,548			762,659,738,651,706,667,7 17,687,757,685,733,725,71
,120,612	36,549,176,637,144,621,20		46,643,714,691,674,699,75 9,735,645,759
1,403,65,435,33,411,97,44	8,581,216,613	52,591,20,631,60,639,84,5	4.683.730.723
3,9,467,25,499,105,507,41	-,,-2-,,	19,108,623,92,551,116,583	













grid_order Utility

- 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











Reorder Example for Bisection Bandwidth

- Assume 32 ranks
- Decide on row or column ordering:
- \$ grid_order -R -g 2,16

• \$ 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





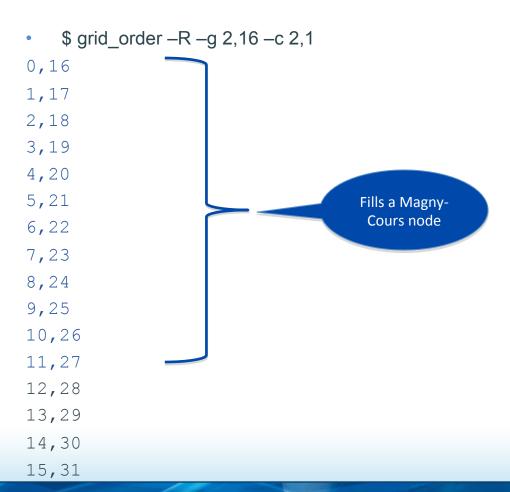






Reorder Example for Bisection Bandwidth (2)

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















Using New Rank Order

- Save grid_order output to file called MPICH_RANK_ORDER
- Export MPICH RANK REORDER METHOD=3

 Run non-instrumented binary with and without new rank order to check overall wallclock time for improvement













Example Performance Results

- Default thread ordering
 - Application 8538980 resources: utime ~126s, stime ~108s

- Maximized on-node data movement with reordering
 - Application 8538982 resources: utime ~38s, stime
 ~106s

BLUE WATERS SUSTAINED PETASCALE COMPUTING

PerfSuite























PerfSuite Background

- Active development at NCSA since 2001
- UI/NCSA Open Source license
- Targeted to users of all levels of expertise
 - The intent is to provide an easy-to-use mechanism for measuring application performance, and to expose problem areas for further exploration
- Low measurement overhead













Features

- Counting and profiling using hardware performance event counters on CPUs, GPUs, networks, and using interval timers
- Executes un-modified dynamically-linked applications
- Easy to use XML files for configuration and output
 - Easy to change the events to count/profile, just change the XML file
- Metadata (such as processor information, pid, memory and time usage) stored in the output
- Functionality available through both command-line tools and library API











Provides

- Three performance counter-related utilities:
 - psrun generate raw counter or statistical profiling data from an unmodified binary
 - o psprocess pre- and post-process data
 - o psinv query events and machine information
- Three libraries
 - libpshwpc HardWare Performance Counter library
 - This is the one that you are most likely to use, if you ever need to
 - Insert API calls in the source code for finer control of start/ end locations
 - libperfsuite the "core" library
 - libpshwpc_mpi a convenience library to capture MPI calls











Using PerfSuite on BW

- # First, load the perfsuite module
- % module load perfsuite
- # By default, psrun does event counting on the given program,
- # then use psprocess to produce psrun's output XML files
- % aprun -n <num> psrun -f -p myprog myprog args
- % psprocess myprog.0.12345.nid01234.xml
- # Use a profiling config file to do profiling instead of counting
- % aprun -n <num> psrun -C -c papi_profile_cycles.xml -f -p
 myprog myprog args
- % psprocess myprog.1.67890.nid12345.xml













psinv: Processor Inventory

- Lists information about the characteristics of the computer
- This same information is also stored in PerfSuite XML output and is useful for later generating derived
- Lists available hardware performance events

```
titan:~3% psinv -v
System Information -
```

Processors: 2

Total Memory: 2007.16 MB System Page Size: 16.00 KB

Processor Information -

Vendor: Intel
Processor family: IPF
Model (Type): Itanium

Revision: 6

Clock Speed: 800.136 MHz

Cache and TLB Information - Cache levels: 3
Caches/TLBs: 7

Cache Details -

Level 1:

Type: Data
Size: 16 KB
Line size: 32 bytes

Associativity: 4-way set associative

Type: Instruction

Size: 16 KB Line size: 32 bytes

Associativity: 4-way set associative













psrun: Performance Measurement

- Hardware performance counting and profiling with unmodified dynamically-linked executables
- Supports:
 - x86, x86-64, and powerpc
 - MPI and OpenMP
 - resource usage (memory, CPU time) collection
 - Both PAPI standard and CPU/GPU native events
- Configuration = XML, Output = XML or text
- Use "-p" for OpenMP programs, "-f" for MPI, and "-f -p" for MPI+OpenMP programs









Example Configuration

- For counting: set "ps_hwpc_eventlist" as the XML root element
- For profiling: set "ps_hwpc_profile" as the XML root element











psprocess: Text Mode (default)

PerfSuite Hardware Performance Summary Report

Version : 1.0

Created : Mon Dec 30 11:31:53 AM Central Standard Time 2002

Generator : psprocess 0.5

XML Source : /u/ncsa/anyuser/performance/psrun-ia64.xml

Execution Information

Date : Sun Dec 15 21:01:20 2002

Host : user01

Processor and System Information

Node CPUs : 2

Vendor : Intel Family : IPF

Model : Itanium

CPU Revision: 6

Clock (MHz) : 800.136 Memory (MB) : 2007.16

Pagesize (KB): 16













psprocess: Text Mode, cont'd

Cache Information

Cache levels : 3

Level 1

Type : data

Size (KB) : 16

Linesize (B) : 32

Assoc : 4

Type : instruction

Size (KB) : 16

Linesize (B): 32

Assoc : 4

Level 2

Type : unified

Size (KB) : 96 Linesize (B) : 64 Assoc : 6 The reports (text or HTML) generated by psprocess have several sections, covering:

- Report creation details
- Run details
- Machine information
- Raw counter listings
- Counter explanations and index
- Derived metrics
- Run annotation defined by you

Derived metrics are evaluated at run-time and can be extended (text mode only)











psprocess: Text Mode, cont'd

Index Description	Counter Value
1 Conditional branch instructions mispredicted 4 Floating point instructions	4831072449 86124489172 594547754568 1049339828741
Statistics ====================================	========
Graduated instructions per cycle	1.765 0.145 0.957 385.087 10.410 43.139 115.905 114.441











psprocess Text-Based Profiles

```
Profile Information
Class
                             : PAPI
Version
                             : 3.6.2
                             : PAPI TOT CYC (Total cycles)
Event
                             : 1000<del>0</del>0
Period
                             : 200471
Samples
Domain
                             : user
Run Time
                             : 27.19 (seconds)
Min Self %
                             : (all)
Module Summary
 Samples
          Self % Total % Module
                     92.82%
                             /home/rkufrin/apps/aspcg/aspcg
            92.82%
   186068
           7.07% 99.89% /opt/intel/cc/9.0/lib/libguide.so
    14182
             0.09% 99.98% /lib/ld-2.3.6.so
      187
             0.01% 99.99% /lib/tls/libc-2.3.6.so
       18
             0.01% 100.00% /lib/tls/libpthread-2.3.6.so
             0.00% 100.00% /tmp/perfsuite/lib/libpsrun r.so.0.0.1
File Summary
           Self % Total % File
 Samples
                             /home/rkufrin/apps/aspcg/pc jac2d blk3.f
   154346
            76.99%
                     76.99%
                             /home/rkufrin/apps/aspcg/cg3 blk.f
    14506
             7.24%
                     84.23%
    14505
             7.24%
                     91.46%
    10185
             5.08%
                    96.54%
                             /home/rkufrin/apps/aspcg/matxvec2d blk3.f
     3042
             1.52%
                    98.06% /home/rkufrin/apps/aspcg/dot prod2d blk3.f
                   99.24%
                             /home/rkufrin/apps/aspcg/add exchange2d blk3.f
             1.18%
     2366
                             /home/rkufrin/apps/aspcg/main3.f
      834
             0.42%
                     99.66%
                             /home/rkufrin/apps/aspcg/cs jac2d blk3.f
      687
                    100.00%
```











Text-based profiles, cont'd

```
Function Summary
Samples
          Self % Total % Function
           76.99%
                    76.99% pc jac2d blk3
   154346
   14506
           7.24%
                    84.23%
                            cg3 blk
   10185
            5.08%
                    89.31%
                            matxvec2d blk3
    6937
            3.46%
                    92.77%
                              kmp x86 pause
                            kmp wait sleep
    4711
            2.35%
                    95.12%
                            dot prod2d blk3
    3042
            1.52%
                    96.64%
                            add exchange2d blk3
    2366
                    97.82%
            1.18%
Function: File: Line Summary
Samples Self % Total % Function: File: Line
                            pc jac2d blk3:/home/rkufrin/apps/aspcg/pc jac2d blk3.f:20
           19.49%
                    19.49%
    39063
                            pc jac2d blk3:/home/rkufrin/apps/aspcg/pc jac2d blk3.f:19
   24134
           12.04%
                    31.52%
   15626
           7.79%
                    39.32%
                            pc jac2d blk3:/home/rkufrin/apps/aspcg/pc jac2d blk3.f:21
   15028
           7.50%
                    46.82%
                            pc jac2d blk3:/home/rkufrin/apps/aspcg/pc jac2d blk3.f:33
   13878
            6.92%
                    53.74%
                            pc jac2d blk3:/home/rkufrin/apps/aspcg/pc jac2d blk3.f:24
   11880
            5.93%
                    59.66%
                            pc jac2d blk3:/home/rkufrin/apps/aspcg/pc jac2d blk3.f:31
            4.44%
                            pc jac2d blk3:/home/rkufrin/apps/aspcg/pc jac2d blk3.f:22
    8896
                    64.10%
    7863
            3.92%
                    68.02%
                            matxvec2d blk3:/home/rkufrin/apps/aspcg/matxvec2d blk3.f:19
                    71.59%
                            pc jac2d blk3:/home/rkufrin/apps/aspcg/pc jac2d blk3.f:32
     7145
             3.56%
```



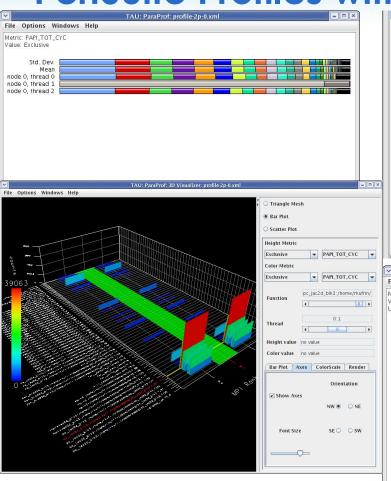


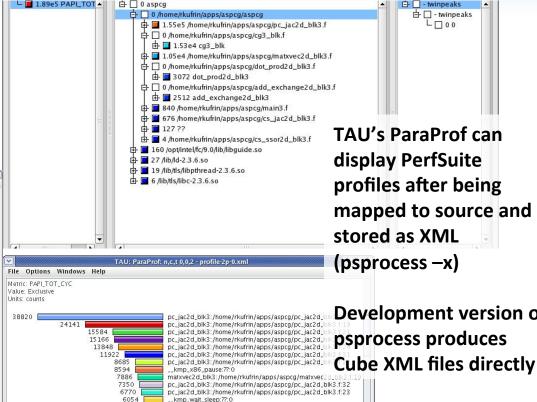






PerfSuite Profiles with ParaProf and Cube3





pc_iac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:27 pc_jac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:34 cg3_blk:/home/rkufrin/apps/aspcg/cg3_blk.f:207 cg3_blk:/home/rkufrin/apps/aspcg/cg3_blk.f:206 2182 g3_blk:/home/rkufrin/apps/aspcg/cg3_blk.t/s46 1843 dot.prod2d_blk3:/home/rkufrin/apps/aspcg/dot.prod2d_blk3:f2 add_exchange2d_blk3:/home/rkufrin/apps/aspcg/add_exchange2

matxvec2d_blk3:/home/rkufrin/apps/aspcg/matxvec2d_blk3.f:25 dot_prod2d_blk3:/home/rkufrin/apps/aspcg/dot_prod2d_blk3.f:2 matxvec2d_blk3:/home/rkufrin/apps/aspcg/matxvec2d_blk3.f:17 cg3_blk:/home/rkufrin/apps/aspcg/cg3_blk.f:279 cg3_blk:/home/rkufrin/apps/aspcg/cg3_blk.f:293 585 | matxvec2d blk3:/home/rkufrin/apps/aspcg/matxvec2d blk3.f:23 | **

_kmp_check_stack_overlap:??:0 1429 gcg3_blk:/home/rkufrin/apps/aspcg/cg3_blk.f:347

__kmp_yield:77:0

1035

(psprocess -x) **Development version of** psprocess produces

L 🗆 0 0











libpshwpc: Performance Collection API

C / C++

```
ps_hwpc_init (void)
ps_hwpc_start (void)
ps_hwpc_read (long long *values)
ps_hwpc_suspend (void)
ps_hwpc_stop (char *prefix)
ps hwpc shutdown (void)
```

Fortran

```
call psf_hwpc_init (ierr)
call psf_hwpc_start (ierr)
call psf_hwpc_read (integer*8
    values,ierr)
call psf_hwpc_suspend (ierr)
call psf_hwpc_stop (prefix, ierr)
call psf_hwpc_shutdown (ierr)
```

- Call "init" once, call "start", "read" and "suspend" as many times as you like. Call "stop" (supplying a file name prefix of your choice) to get the performance data XML document
- Optionally, call "shutdown"
- Example programs demonstrating use are installed in PerfSuite "examples" subdirectory
 - Additional routines

 ps hwpc numevents()

ps_hwpc_numevents() and ps_hwpc_eventnames() allow querying current configuration









FORTRAN API Example

```
include 'fperfsuite.h'
call PSF_hwpc_init(ierr)
call PSF_hwpc_start(ierr)
do j = 1, n
    do i = 1, m
    do k = 1, 1
        c(i,j) = c(i,j) + a(i,k)*b(k,j)
    end do
    end do
end do
call PSF_hwpc_stop('perf', ierr)
call PSF_hwpc_shutdown(ierr)
```

```
% ftn -c matmult.f -I /sw/xe/perfsuite/1.1.2/
cnl4.1_gnu4.7.2_papi5.1.0.2/include
% ftn matmult.o -L /sw/xe/perfsuite/1.1.2/cnl4.1_gnu4.7.2_papi5.1.0.2/
lib -L /opt/cray/papi/5.1.0.2/perf_events/no-cuda/lib -lpshwpc -
lperfsuite -lpapi
```













Java-based Performance Measurement

- PerfSuite 1.0.0+ supports measuring unmodified Java applications using PAPI similar to psrun
- Implemented using JVMTI (Java Virtual Machine Tool Interface)
- Usage:
 - java -agentlib:psjrun MyClass
- Results are contained in XML documents that can be post-processed using psprocess













For More Information

- PerfSuite web sites:
 - https://bluewaters.ncsa.illinois.edu/perfsuite
 - http://perfsuite.ncsa.illinois.edu



BLUE WATERS SUSTAINED PETASCALE COMPUTING

TAU: <u>Tuning</u> and <u>Analysis</u> <u>Utilities</u>













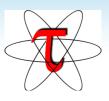












- <u>Tuning and Analysis Utilities</u> (18+ year project)
- Developed at University of Oregon, Eugene
- Performance problem solving framework for HPC
 - Integrated, scalable, flexible, portable
 - Target all parallel programming / execution paradigms
- Integrated performance toolkit (open source)
 - Instrumentation, measurement, analysis, visualization
 - Widely-ported performance profiling / tracing system
 - Performance data management and data mining
- Broad application use (NSF, DOE, DOD, ...)













Instrumentation and Sampling

- Supports both instrumentation (direct performance observation) and sampling (indirect perf observation)
- Instrumentation can be:
 - Manually insert into the source code
 - Automatically by compiler (use the "-optCompInst" option)
 - Automatically by TAU's PDT tool (by choosing a TAU makefile containing the "-pdt" string)
- Supports selective instrumentation:
 - Selects the files, functions/routines, loops
 - Supports patterns: "*", "?" (for file names), "#" (for loops)



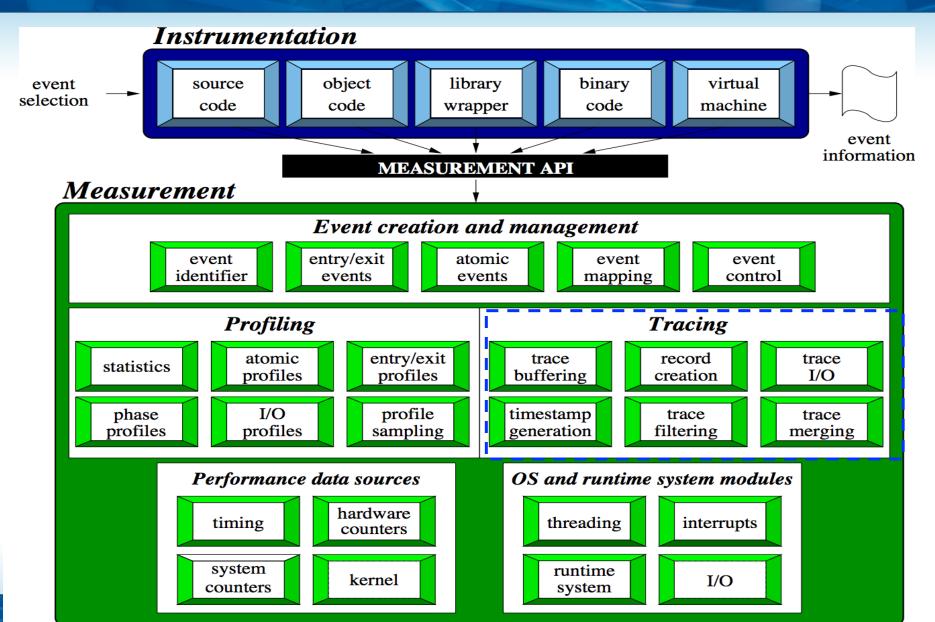






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Using TAU on BW

- First, load the tau module
- Two methods to run to generate TAU profile or trace files
 - Choose a TAU makefile or use a TAU compiler script, to instrument the source code, build an instrumented executable, then execute it
 - Use "tau_exec" to run an uninstrumented executable
- Analyze the generated files, using "pprof" for quick text output, or "paraprof" for richer visualization











TAU Makefiles on BW

- To see all installed TAU versions
 module avail tau
- To load the tau module, use one of the following: module load tau

module load tau/<specific version>

- The TAU makefiles are located at: /sw/xe/tau/<tau_version>/<build>/craycnl/lib/Makefile.tau-* For example, for TAU 2.21.4 using PrgEnv-cray, they are: /sw/xe/tau/2.21.4/cnl4.1_cray8.1.1/craycnl/lib/Makefile.tau-*
- For an MPI+F90 application, you may want to start with Makefile.tau-cray-mpi-pdt, which supports MPI instrumentation & PDT for automatic source instrumentation

```
setenv TAU MAKEFILE
/sw/xe/tau72.21.4/cnl4.1 cray8.1.1/craycnl/lib/
Makefile.tau-cray-mpi-pdt
```

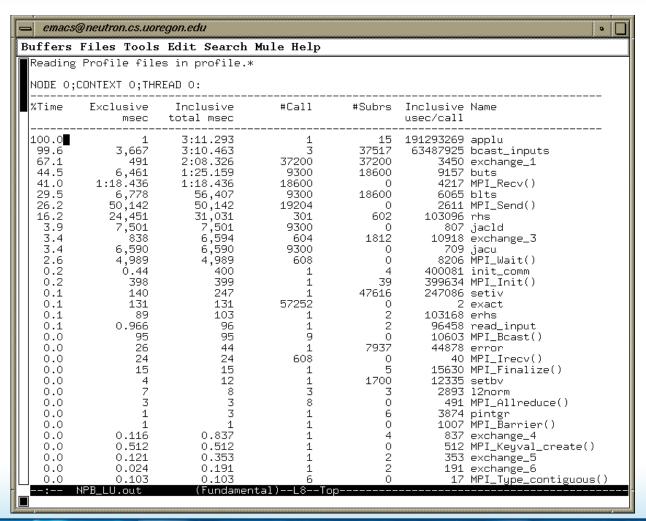








Parallel Profile Analysis – pprof







GREAT LAKES CONSORTIUM



. . X



PerfDMF managed

(database)

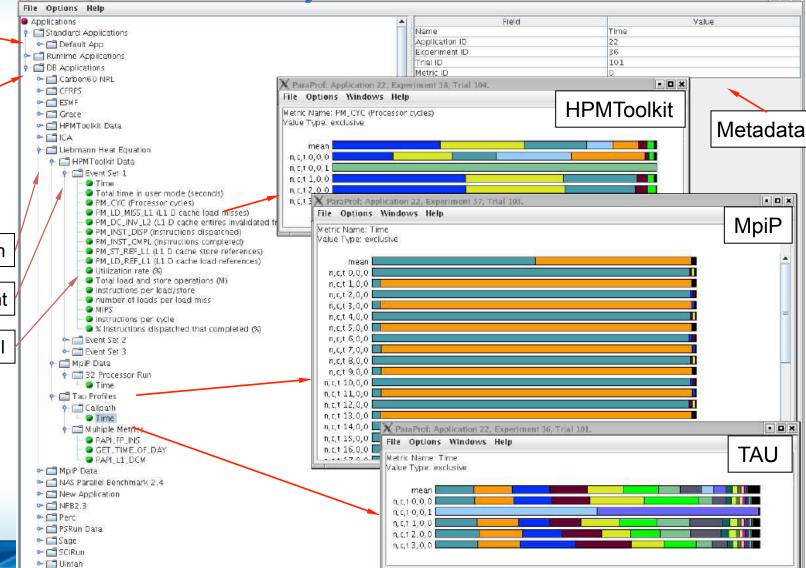
Raw files

Application

Experiment

Trial

CHUTE





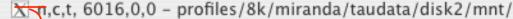


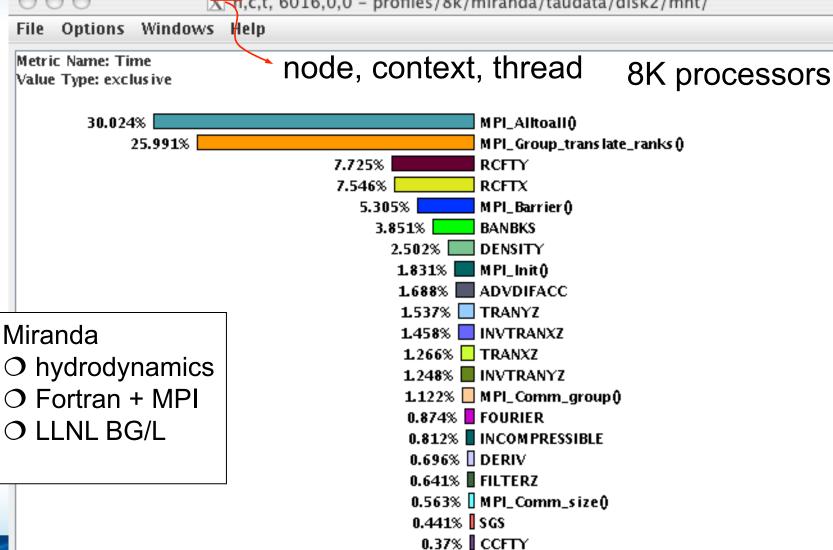






ParaProf – Flat Profile











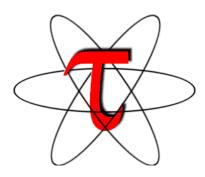






For More Information

- TAU web sites:
 - https://bluewaters.ncsa.illinois.edu/tau
 - http://tau.uoregon.edu



BLUE WATERS SUSTAINED PETASCALE COMPUTING

Congestion Protection and Balanced Injection





















What is Congestion Protection?

- Network congestion is a condition that occurs when the volume of traffic on the high-speed network (HSN) exceeds the capacity to handle it.
- To "protect" the network from data loss, congestion protection (CP) globally "throttles" injection bandwidth per-node.
- If CP happens often, application performance degrades.



http://lh5.google.ca/abramsv/R9WYOKtl.e1l/AAAAAAAAI.O4/FLefbnOg5rO/s1600-h/495711679_52f8d76d11_o.jpg

- At job completion you might see the following message reported to stdout:
- Application 61435 network throttled: 4459 nodes throttled, 25:31:21 node-seconds Application 61435 balanced injection 100, after throttle 63
- The throttling event lasts for 20 seconds each time CP is triggered.













Types of congestion events

- There are two main forms of congestion: many-to-one and long-path.
 The former is easy to detect and correct. The latter is harder to detect and may not be correctable.
- Many-to-one congestion occurs in some algorithms and can be corrected. uGNI and DMAPP based codes doing All-to-one operations are common case. See "Modifying Your Application to Avoid Gemini Network Congestion Errors" on balanced injection section on the portal.
- Long-path congestion is typically due to a combination of communication pattern and node allocation. It can also be due to a combination of jobs running on the system.
- We monitor for cases of congestion protection and try to determine the most likely cause.





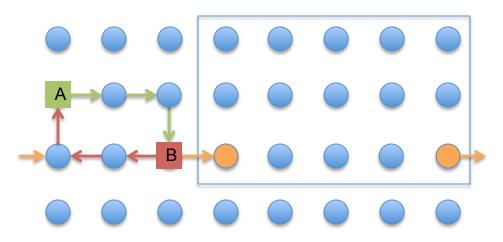






Congestion on a Shared, Torus Network

- HSN uses dimension ordered routing: x-then-y-then-z between two locations on the torus. Note that A→B≠B→A.
- Shortest route can sometimes cause traffic to pass through geminis used by other jobs.



- Non-convex node allocations can have traffic that passes through geminis used by other jobs.
- Non-local I/O traffic and Lustre striping can lead to network hot-spots.
- We are working with Adaptive and Cray on eliminating some of the above causes of congestion with better node allocation: shape, location, etc.











Balanced Injection

- Balanced Injection (BI) is a mechanism that attempts to reduce compute node injection bandwidth in order to prevent throttling and which may have the effect of improving application performance for certain communication patterns.
- BI can be applied "per-job" using an environment variable or with user accessible API.
- export APRUN BALANCED INJECTION=64
- Can be set from 1-100 (100 = no BI).
- There isn't a linear relation of BI to application performance.
- MPI-based applications have "balanced injection" enabled in collective MPI calls that locally "throttle" injection bandwidth.













Thank You