Cray XC Series Application Programming and Optimization Student Guide

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TR-CPO NERSC

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Cray delivers an integrated set of performance tools that provide automatic program instrumentation, without requiring source code or file modifications. Before you can use these tools, ensure that your code compiles cleanly, runs to completion, and produces expected results.



Trace-based or synchronous experiments count every entry into and out of each function that is called in the application. Build (pat_build) options can reduce the number of functions to include in the experiment. Further experimentation on a fine-grained portion of the application can occur through source code modifications, where a user uses CrayPat pat_region API in the source code. Normally this is not required.

CrayPat

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Consists of three major components

pat_build	Used to instrument the program to be analyzed
pat_report	A report generator
pat_help	An online help system, faq is on the front page
Additional man pages ar	e hwpc, papi_counters, and intro_craypat

- CrayPat (pat_build) supports two types of experiments: sampling and tracing
 - Sampling experiments capture values from the call stack or the program counter at specified intervals or when a specified counter overflows
 - Tracing counts an event, such as the number of times an MPI call is executed

• CrayPat uses PAPI to read the performance counters of the processor

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pat_build Sampling If tracing options are not included on the pat_build command line, pat_build defaults to sampling Sampling is controlled by the environment variable PAT_RT_EXPERIMENT Supported sampling functions are: samp_pc_time, samp_pc_ovfl, samp_cs_time, or samp_cs_ovfl Caution: Do not collect hardware counter information when you sample by overflow (for example< samp_pc_ovfl) Use sampling to obtain a profile and then trace functions of interest

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In the example above, %pat_build program1 examines the program program1 and relinks its object and library files with files from the CrayPat run-time library to produce program1+pat. This operation requires the continued availability of the object files that were used to link program1 (either in their locations at the time program1 was linked or in a directory specified by the PAT_BUILD_LINK_DIR environment variable).

Using pat_build Run pat_build to instrument the program rns/samp264% pat_build samp264 rns/samp264% ls -l samp264* -rwxr-xr-x 1 rns hwpt 12067872 Feb 12 17:41 samp264 -rwxr-xr-x 1 rns hwpt 19306104 Feb 12 17:45 samp264+pat Execute the instrumented program If your using a workload manager submit the job from the job-script rns/samp264% cat samp264.slm #! /bin/bash #SBATCH -n 16 # srun ./samp264 # Job profiling phases srun ./samp264+pat # srun ./samp264+apa rns/samp264% sbatch samp264.slm Submitted batch job 141769 rns/samp264% rns/samp264% squeue TIME TIME_LEFT NODES CPUS JOBID USER ACCOUNT NAME ST REASON START_TIME 141769 rns (null) samp264.slm R None 2019-02-12T21:48:43 1:28 58:32 1 16 rns/samp264% 2/11/2019 6

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Experiment Output The instrumented program generates a subdirectory For example the run on the previous page created a directory named samp264+pat+26031-24s • The directory name contains the following information: name of the instrumented program: samp264+pat the process ID: 26031 the physical node—the application started on: 24 and the type of experiment performed: s for sample and t for trace In the subdirectory will be a subdirectory named xf-files In there will be a .xf file for each of the nodes The .xf files are the experiment output files 2/11/2019 Cray, Inc. Private

By default, for jobs with 255 PEs or less, a single .xf file is created. If the job uses 256 PEs or more, the square root number of PEs .xf files are created.

The user had to instrument their program with pat_build –O apa in order for pat_report to generate the .apa file.

Using pat_report



Use the pat_report command to read the experiment file

- pat_report will generate an ap2-files sub-directory, build-options.apa file, an index.ap2 file, and a report to stdout
 - The .ap2 is used to generate additional text reports or is used by Apprentice2
 - The .ap2 files are portable; it does not require the source or .xf files
 - Prior to generating the ap2 files pat_report requires the .o, source, and .xf files be maintained.
 - The ap2 file is portable and can be archived for later use
 - The build-options.apa (Automatic Profiling Analysis) file is used (optionally) to assist you in creating a trace based experiment file

```
rns/samp264% ll samp264+pat+26031-24s
total 72
drwxr-xr-x 2 rns hwpt 4096 Feb 12 22:17 ap2-files
-rw-r--r-- 1 rns hwpt 1832 Feb 12 22:17 build-options.apa
-rw-r--r-- 1 rns hwpt 59392 Feb 12 22:17 index.ap2
drwxr-x--- 2 rns hwpt 4096 Feb 12 22:02 xf-files
rns/samp264%
```

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The top time-consuming routines comes from the initial pat_build –O apa, which performs a form of sampling to get an initial profile. Then further information can be obtained for those top time consuming routines (identified in the .apa file) with the program instrumented using the .apa, and rerun.

Use pat_report to process the .xf file, not view the .xf file. View the text report generated to stdout or through Apprentice2.



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Use pat_report to process the .xf file, not view the .xf file. View the text report generated to stdout or through Apprentice2.

pat_build Trace Options

• To trace functions and create the instrumented executable, use the following pat_build options:

- -g traces non-user library functions for one of the predefined groups, like [caf|cuda|gni|...|upc]
 - Refer to the pat_build man page for a complete list
- -t tracefile to specify a file containing a lists of functions to trace
- -T tracefunc where tracefunc is a comma-separated list of function names to trace; !tracefunc excludes function
- -u trace user functions
- -w is used to trace MAIN. There are only trace points to collect performance data inserted at the beginning and end of MAIN.
 - This is helpful if the user wants to collect some data that has high collection overhead and wants to minimize additional tracing overhead.
- -o allows you to specify the name of resulting instrumented program or the name can be the final argument. If neither are specified, the program name is appended with +pat
- -f is used overwrite existing output file instr_program
- Note: pat_build does not enable you to instrument a program that is also using the PAPI interface directly (via libhwpc)

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Environment Variables

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PAT_RT_SUMMARY 0 Turn off summary 1 Enable summary (default) PAT_RT_PERFCTR Specify the performance counter group collected PAT_RT_EXPFILE_PER_PROCESS 0 Write experiment data to a single file Requires a file system capable of 1 Write a separate file for each process • An application may abort if the n processes exceeds the number of the permitted	up to be file of locking
PAT_RT_PERFCTR Specify the performance counter group collected PAT_RT_EXPFILE_PER_PROCESS 0 Write experiment data to a single file Requires a file system capable of 1 Write a separate file for each process • An application may abort if the n processes exceeds the number of the permitted • An application may abort if the n processes exceeds the number of the permitted	file of locking
PAT_RT_EXPFILE_PER_PROCESS 0 Write experiment data to a single file Requires a file system capable of 1 Write a separate file for each process • An application may abort if the n processes exceeds the number	file of locking
permited	ess number of er of open files
PAT_RT_EXPFILE_NAME The experiment file name	
PAT_RT_EXPFILE_DIR The directory that contains the experim • Specify a Lustre directory when single experiment output file	riment output file n you create a

There are a number of environmental variables that define/modify the way CrayPat operates. See the intro_craypat man page for more information.

A Sequence of Commands

```
rns/samp264% module load perftools
                                      # Loaded the CrayPat module
rns/samp264% ftn -o samp264 samp264.f # compiled the code - simple application
                                 # Created the experiment executable
rns/samp264% pat_build samp264
rns/samp264% vi samp264.slm
                                    # modify the job script to run samp64+pat
                                   # run the job
rns/samp264% sbatch samp264.slm
rns/samp264% cat samp264.slm.o141770 🛛 # Made sure the job ran 😊
rns/samp264% pat_report samp264+pat+26031-24s> samp264+pat+26031-24s.report
rns/samp264% view samp264+pat+26031-24s.report
rns/samp264% pat_build -0 samp264+pat+26031-24s/build-options.apa
rns/samp264% ls -ltr
total 59184
-rwxr-xr-x 1 rns hwpt
                       5488 Oct 26 2014 samp264.f
-rwxr-xr-x 1 rns hwpt 15696888 Feb 12 22:00 samp264
-rwxr-xr-x 1 rns hwpt 22433392 Feb 12 22:00 samp264+pat
-rw-r--r-- 1 rns hwpt
                        127 Feb 12 22:06 samp264.slm.o141770
                        147 Feb 12 22:06 samp264.slm.e141770
-rw-r--r-- 1 rns hwpt
                      4096 Feb 12 22:17 samp264+pat+26031-24s
drwxr-x--- 4 rns hwpt
-rw-r--r-- 1 rns hwpt 214 Feb 12 22:39 samp264.slm
rns/samp264% vi samp264.slm
                                     # modify the job script to run samp64+apa
rns/samp264% sbatch samp264.slm  # run the job
rns/samp264% pat_report samp264+apa+27643-24t > samp264+apa+27643-24t.report
rns/samp264% view samp264+apa+27643-24t.report
```

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Table 1: Profile by Samp% Samp	y Function	This is the report from the first "sample" experiment.
	Samp Samp% Funct: PE=H: Total	Ion Table 1 shows the highest used functions,
99.8% 25,854.3	27.7 0.1% USER	Table 2 show more detail about the function ghost_ and in this example the high and low
Table 2: Profile of Samp% Samp 100 0% 25 882 0	E maximum function times Imb. Imb. Function Samp Samp% PE=[ma 27.7 0.1% ghost	s on ax,min]
Table 2: Profile of Samp% Samp 	f maximum function time; Imb. Imb. Function Samp Samp% PE=[ma 27.7 0.1% ghost 0 pe.0 0 pe.1	s on ax,min] 2 ======

The table is a portion of the output of program1.rpt1.

The fifth column, labelled *Calls*, contains the count for all 4 PEs.

The second column, *Time*, lists the maximum time used by any PE per function.

The third column, *Imb.* (Imbalance) *Time*, lists the average time required by all PEs per function.

The fourth column, "*Imb. Time %,*, a value of 100% indicates that a single PE executed the function. A value of 0% would indicate that all PEs spent equal time performing the function. (Refer to the man page for information about the math used to calculate the percentage.)

ble 1:	Profile by	/ Functio	m		
Samp% 		Imb. Samp	Imb. Samp%	Group Function PE=HIDE	This is the report generated after pat_build -0 \ samp264+pat+26031-24s/build-options.apa
00.0%	25,917.9			Total	was executed and the executable samp264+apa was
99.8%	25,854.3	27.7	0.1%	USER	run. The APA file suggested PERFCT value 1 be used. This is where the performance counter data
99.8%	25,854.3	3 27.7	0.1	% ghost_	comes from in Table 4
		.========	:======		
ble 2:	Profile of	maximur	funct	ion times	
Samp%	Samp	Imb.	Imb.	Function	
Í		Samp	Samp%	PE=[max,m	lin]
 100 08	25 882 0	 27 7	0 12		
	1 25 002 0)		- pe.0	
100.0%	25,002.0				
100.0% 99.7%	25,882.0)		- pe.12	
100.0% 99.7% ======	25,002.0)		- pe.12	
100.0% 99.7% =======	25,002.0) ==================================	-	- pe.12	
100.0% 99.7% ====================================	Program HW) ======== I Perform	- ====================================	- pe.12 	
100.0% 99.7% ======= ble 4: ======= Total	Program HW) 	- nance Co	- pe.12	
100.0% 99.7% ======= ble 4: ======= Total	Program HW) 	- mance C(- pe.12 ounter Data	250 6/1997 2022
100.0% 99.7% ======= ble 4: ======= Total Thread 7 CPU CLK	Program HW		-	- pe.12 	259.641887 secs 852 323 364 085
100.0% 99.7% ble 4: Total Thread T CPU_CLK_ DTLB LOA	Program HW) V Perform 	hance Co	- pe.12 ounter Data	259.641887 secs 852,323,364,085 223,631,012,363
100.0% 99.7% ======= Total Thread T CPU_CLK_ DTLB_LOZ INST_RET	Program HW Program HW) V Perform 	hance Co	- pe.12	259.641887 secs 852,323,364,085 223,631,012,363 91,684,175,564
100.0% 99.7% ======= Total Thread T CPU_CLK_ DTLB_LOF INST_RET RESOURCE	Program HW Program HW UNHALTED:T AD_MISSES:W IRED:ANY_P STALLS:AN) V Perform VHREAD_P IALK_DURF IY	- mance Co	- pe.12 ounter Data	259.641887 secs 852,323,364,085 223,631,012,363 91,684,175,564 792,419,692,546
100.0% 99.7% Dle 4: Total Thread T CPU_CLK_ DTLB_LOP INST_RET RESOURCE UNHALTEI	Program HW Program HW UNHALTED:T D_MISSES:W IRED:ANY_P STALLS:AN REFERENCE) I Perform 	- ance Co	- pe.12 ounter Data	259.641887 secs 852,323,364,085 223,631,012,363 91,684,175,564 792,419,692,546 774,839,428,386
100.0% 99.7% ======= Total Thread T CPU_CLK_ DTLB_LOP INST_RET RESOURCH UNHALTEI OFFCORE_	Program HW Program HW UNHALTED:T D_MISSES:W IRED:ANY_P STALLS:AN REFERENCE RESPONSE_0	Perform Perform THREAD_P TALK_DURA TY CYCLES	- hance C 	- pe.12 punter Data 	259.641887 secs 852,323,364,085 223,631,012,363 91,684,175,564 792,419,692,546 774,839,428,386 AL 6,912,550,656



An event set is a group of PAPI preset or native events

CrayPat defines 20 groups (sets)

Select a set by using the environment variable PAT_RT_HWPC

Profiling - counting specified events

Used in CrayPat

Overflow - testing events and alerting the application when a count is exceeded Requires modification of the user application

Looking Closer



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In C/C++

#include <pat_api.h> PAT_region_begin(1, "halo_loop"); ... PAT_region_end(1);



ble 3: Profile by Function Group and Fu clip	From Ic	op in code	;
USER / #1.Std_Deviation			
 Time%		4.3%	
Time		11.291691	secs
Imb. Time		0.040904	secs
Imb. Time%		0.4%	
Calls	8.856 /sec	100.0	calls
CPU_CLK_UNHALTED:THREAD_P	37,11	7,179,867	
DTLB_LOAD_MISSES:WALK_DURATION	18	0,919,720	
INST_RETIRED:ANY_P	7,20	0,138,317	
RESOURCE_STALLS: ANY	32,40	9,753,945	
UNHALTED_REFERENCE_CYCLES	33,74	2,890,690	
OFFCORE_RESPONSE_0:ANY_REQUEST:LLC_MISS_	LOCAL 60	1,357,957	
CPU CLK Boost		1.10	Х
Resource stall cycles / Cycles		87.3%	
Memory traffic GBytes	3.408G/sec	38.49	GB
Local Memory traffic GBytes	3.408G/sec	38.49	GB
Memory Traffic / Nominal Peak		5.7%	
Retired Inst per Clock		0.19	
Average Time per Call		0.112917	secs
CrayPat Overhead : Time	0.0%		

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PAPI	-
 PAPI provides a common interface for the performance counters in various processors, including the Opteron 	
 PAPI defines a set of Preset counters that map to a common performance counter in various processors 	X
 The Preset name matches as closely as possible to the Native event Using the Preset name provides portability between processors when user code is modified to collect performance data 	
 A Native event is an actual hardware counter in the processor See the papi_counters, papi_avail, and papi_native_avail man pages 	
 papi_avail, and papi_native_avail are commands that can be executed on the compute node to determine the available counters srun -n 1 /opt/cray/pe/papi/default/bin 	
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Rank Order and CrayPAT	
 One can also use the CrayPat performance measurem tools to generate a suggested custom ordering. 	ent
 Available if MPI functions traced (-g mpi or –O apa) 	
 pat_build –O apa my_program 	
 see Examples section of pat_build man page 	
pat_report options:	
 mpi_sm_rank_order 	
 Uses message data from tracing MPI to generate suggested MPI ra order. Requires the program to be instrumented using the pat_build mpi option. 	nk -g
 mpi_rank_order 	
 Uses time in user functions, or alternatively, any other metric specifi using the -s mro_metric options, to generate suggested MPI rank or 	ed by der.
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ank Order and CrayPAT	
module load perftools	•
Rebuild your code	
• pat_build -0 apa a.out	
Runa.out+pat	
<pre>pat_report -Ompi_sm_rank_order a.out+pat+sdt/ > pat.report</pre>	
 Creates MPICH_RANK_REORDER_METHOD.x file 	
 Then set environment variable MPICH_RANK_REORDER_METHOD=3 and link the file MPICH_RANK_REORDER_METHOD.x to MPICH_RANK_ORDER 	
Rerun your code	
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HSN Network Counters



- HSN Network counters are accessed through CrayPat and environment variables
 - See the intro_craypat and nwpc man pages

PAT_RT_NWPC	Specifies individual Gemini performance counter event names.
PAT_RT_NWPC_CONTROL	Specifies parameters that control various aspects of the Gemini networking performance counters.
PAT_RT_NWPC_FILE	Specifies a file or list of files containing individual Gemini performance counter event names.
PAT_RT_NWPC_FILE_GROUP	Specifies a file or list of files containing specifications of Gemini performance counter groups.
PAT_RT_NWPC_FILE_TILE	Specifies a file or list unset of files containing specifications of Gemini performance counters that use the filtering counters to define new events.
PAT_RT_NWPC_TILE_DISPLAY	If set to nonzero value, writes the filtered tile NWPC event specifications to stdout.

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The left screen appears during data collection; later, the pie charts appear.



Reveal



Performance analysis and code restructuring assistant

- Integrated performance analysis and code optimization tool
- Extends Cray's existing performance measurement, analysis, and visualization technology by combining run-time performance statistics and program source code visualization with Cray Compiling Environment (CCE) compile-time optimization feedback.





Reveal	CRAY
X Reveal	
File Edit View Help	
▼samp264.pl 🐰	
Navigation Program View	Source - Aus/scratch/ms/samp264/samp264.f
 ✓ samp264.f ✓ GHOST Loop@43 Loop@45 Loop@57 ✓ USE_DATA Loop@111 Loop@123 Loop@124 Loop@125 Loop@135 Loop@136 Loop@148 Loop@149 Loop@150 	<pre>104 ! (add the halo to planes 1 and nz 105 subroutine use_data (mype, array, nx, ny, nz, result) 106 integer nx, ny, nz, mype, i, j, k 107 real*8 array(nx, ny, 0:nz+1), total, result 108 real*8 mean, var, stddev 109 110 ! add in the halo (ghost) planes FVr2 111 do i = 1, nx CF 112 do k = 1, ny 113 array(i,k, 1) = array(i,k, 1) + array(i,k, 0) 114 array(i,k,nz) = array(i,k,nz) + array(i,k,nz+1) 115 enddo 116 enddo 117 118 elem = nx*ny*nz 119 120 ! first find the mean 121 ! (valk thru memory as sequentially as possible)</pre>
	Info - Line 111 A loop starting at line 111 is flat (contains no external calls). A loop starting at line 111 was unrolled 2 times. A loop starting at line 111 was vectorized. A loop starting at line 112 is flat (contains no external calls).
samp264.pl loaded	
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Reveal O	penMP Scoping	-
	Keveal OpenMP Scoping	•
	Scope Loops Scoping Results Edit List List of Loops to be Scoped Scope? Line # File or Source Line P /lus/scratch/rns/samp264/samp264.f Apply Filter Time: 0.000 Timps: 2 Threads: 4 Speedup: 0.010	3
	Start Scoping Cancel Close Close	
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X Re	veal OpenMI	P Scoping		0.8
Scop	Loops Sc	oping Results	List of Loops to be Scoped	
Scop	? Line # 9 44 0 44 0 54 0 54 0 54 0 111 0 123 0 124 0 124 0 125 0 136 0 136 0 148 0 146 149 150 Fitter Time	File of Source Line 4 Loop at line 4 Loop at line 4 Loop at line 4 Loop at line 5 Loop at line 7 Loop at line 1 Loop at line Loop at line 1 <th>In this example I reduced the number of loops to just line 111</th> <th></th>	In this example I reduced the number of loops to just line 111	

eal Scop	oing Res	sults		CRAY
X Rev	eal OpenMP Scoping	N		
Scope	Loops Scoping Results	L		
		samp264.f: Loop@111		1
Name	Type Scope In	fo		
i	Scalar Private			
k	Scalar Private			
array	Array Shared			
nx	Scalar Shared			
ny	Scalar Shared			
- First/La	st Private			
🔲 🔲 Ena	ble FirstPrivate	None	[+]	
🗌 Ena	ble LastPrivate			
Find Na	me:			
Insert	Directive Show Directive		Close	
		Cray, Inc. Private		32

Reveal Scoping Results X Reveal 52 <u>File Edit View H</u>elp F 🕶 samp264.pl 🐰 Navigation-Source - /lus/scratch/rns/samp264/samp264.f-Program View • 💠 <u></u> <u>↓</u> <u>U</u>p Jown Save \$ 103 ! Do some useful work on my new halo cell data ٠ ▼ samp264.f 104 (add the halo to planes 1 and nz ▼ GHOST 105 subroutine use data (mype, array, nx, ny, nz, result) Loop@43 106 integer nx, ny, nz, mype, i, j, k Loop@44 107 real*8 array(nx, ny, 0:nz+1), total, result Loop@45 108 real*8 mean, var, stddev Loop@54 109 Loop@57 110 add in the halo (ghost) planes V USE_DATA 111 do 🧾 = 1, nx -FSVr2 - CF 112 do k = 1, ny Loop@112 🔼 Loop@123 113 array(<mark>i</mark>,k, 1) = array(<mark>i</mark>,k, 1) + array(<mark>i</mark>,k, 0) array(1,k,nz) = array(1,k,nz) + array(1,k,nz+1) Loop@124 114 115 enddo Loop@125 Loop@134 116 enddo 117 Loop@135 Loop@136 118 elem = nx*ny*nz 119 Loop@148 Loop@149 120 ! first find the mean Loop@150 Info - Line 111-. A loop starting at line 111 is flat (contains no external calls). A loop starting at line 111 was unrolled 2 times. A loop starting at line 111 was vectorized. A loop starting at line 112 is flat (contains no external calls). samp264.pl loaded 2/11/2019 Cray, Inc. Private 33