TAU

August 11, 2021, 3:40pm – 4:15pm CT
ATPESC workshop via Zoom

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http://tau.uoregon.edu/tau_atpesc21.pdf

Tuning and Analysis Utilities

E4S

EXASCALE COMPUTING PROJECT

National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY | Office of Science

TAU: Quickstart Guide

Setup:

- `% module load tau  [ on Theta, use aprun instead of mpirun, and on ThetaGPU please use:]`
- `% module use /soft/perftools/tau/modulefiles/thetagpu; module load tau`

Profiling with an un-instrumented application:

- MPI: `% mpirun -np 64 tau_exec -ebs ./a.out`
- MPI+OpenMP with Intel 19+:
  ```
  % export TAU_OMPT_SUPPORT_LEVEL=full;
  % mpirun -np 64 tau_exec -T ompt,v5 -ompt ./a.out
  ```
- Pthread: `% mpirun -np 64 tau_exec -T mpi,pthread -ebs ./a.out`
- Python+MPI+Sampling: `% mpirun -np 64 tau_python -ebs ./a.py`
- Python+MPI+OpenCL: `% mpirun -np 64 tau_python -opencl ./a.py`
- DPC++/SYCL (no MPI): `% tau_exec -T level_zero,serial -l0 ./a.out`
- CUDA+MPI `% mpirun -np 64 tau_exec -T cupti -ebs -cupti ./a.out`

Analysis: `% pprof -a -m | more;  % paraprof (GUI)`

Tracing:

- Vampir: MPI:
  ```
  % export TAU_TRACE=1; export TAU_TRACE_FORMAT=otf2
  % mpirun -np 64 tau_exec ./a.out; vampir traces.otf2 &
  ```
- Chrome:
  ```
  % export TAU_TRACE=1; mpirun -np 64 tau_exec ./a.out; tau_treemerge.pl;
  % tau_trace2json tau.trc tau.edf -chrome -ignoreatomic -o app.json
  ```

  Chrome browser: chrome://tracing (Load -> app.json)
- Jumpshot:
  ```
  % export TAU_TRACE=1; mpirun -np 64 tau_exec ./a.out; tau_treemerge.pl;
  % tau2slog2 tau.trc tau.edf -o app.slog2; jumpshot app.slog2 &
  ```

Challenges

- With growing hardware complexity, it is getting harder to accurately measure and optimize the performance of our HPC and AI/ML workloads.

- As our software gets more complex, it is getting harder to install tools and libraries correctly in an integrated and interoperable software stack.

Motivation: Improving Productivity

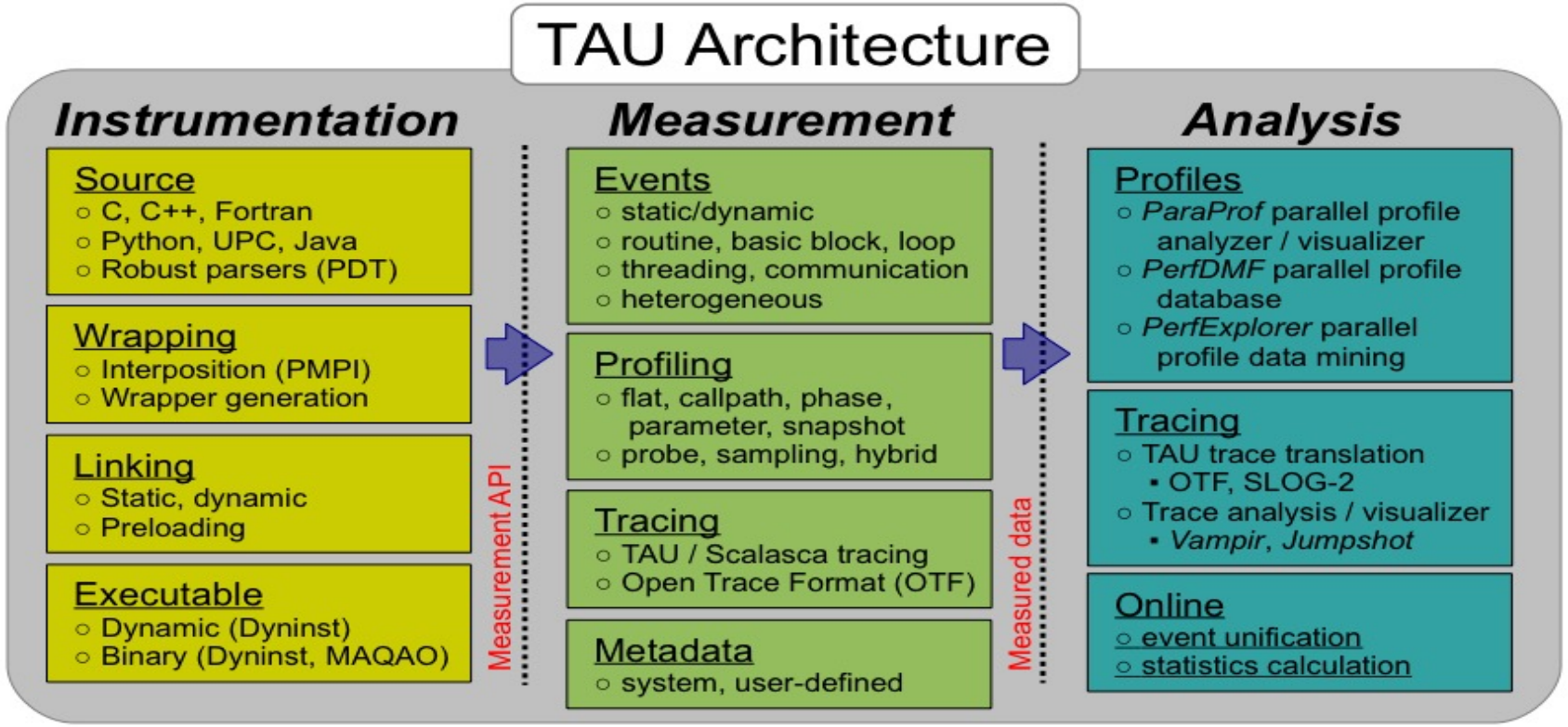
- TAU Performance System®:
  - Deliver a scalable, portable, performance evaluation toolkit for HPC and AI/ML workloads
- Extreme-scale Scientific Software Stack (E4S):
  - Delivering a modular, interoperable, and deployable software stack
  - Deliver expanded and vertically integrated software stacks to achieve full potential of extreme-scale computing
  - Lower barrier to using software technology (ST) products from ECP
  - Enable uniform APIs where possible

TAU Performance System®

Parallel performance framework and toolkit

Supports all HPC platforms, compilers, runtime system
Provides portable instrumentation, measurement, analysis

Tuning and Analysis Utilities



TAU Performance System

Instrumentation

- Fortran, C++, C, UPC, Java, Python, Chapel, Spark
- Automatic instrumentation

Measurement and analysis support

- MPI, OpenSHMEM, ARMCI, PGAS, DMAPP
- pthreads, OpenMP, OMPT interface, hybrid, other thread models
- GPU: Intel oneAPI DPC++/SYCL, AMD ROCm, CUDA, OpenCL, OpenACC, Kokkos
- Parallel profiling and tracing

Analysis

- Parallel profile analysis (ParaProf), data mining (PerfExplorer)
- Performance database technology (TAUdb)
- 3D profile browser

Application Performance Engineering using TAU

- How much time is spent in each application routine and outer *loops*? Within loops, what is the contribution of each *statement*? What is the time spent in OpenMP loops? In kernels on GPUs. How long did it take to transfer data between host and device (GPU)?
- How many instructions are executed in these code regions?
  Floating point, Level 1 and 2 *data cache misses*, hits, branches taken? What is the extent of vectorization for loops?
- What is the memory usage of the code? When and where is memory allocated/de-allocated? Are there any memory leaks? What is the memory footprint of the application? What is the memory high water mark?
- How much energy does the application use in Joules? What is the peak power usage?
- What are the I/O characteristics of the code? What is the peak read and write *bandwidth* of individual calls, total volume?
- How does the application *scale*? What is the efficiency, runtime breakdown of performance across different core counts?

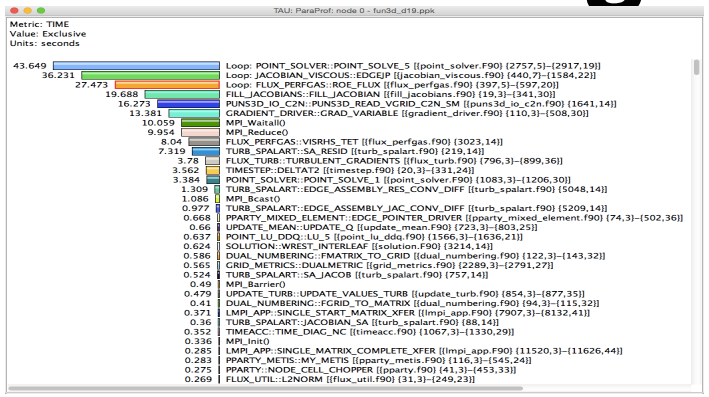
Instrumentation

Add hooks in the code to perform measurements

- **Source instrumentation using a preprocessor**
  - Add timer start/stop calls in a copy of the source code.
  - Use Program Database Toolkit (PDT) for parsing source code.
  - Requires recompiling the code using TAU shell scripts (tau_cc.sh, tau_f90.sh)
  - Selective instrumentation (filter file) can reduce runtime overhead and narrow instrumentation focus.
- **Compiler-based instrumentation**
  - Use system compiler to add a special flag to insert hooks at routine entry/exit.
  - Requires recompiling using TAU compiler scripts (tau_cc.sh, tau_f90.sh…)
- **Runtime preloading of TAU's Dynamic Shared Object (DSO)**
  - No need to recompile code! Use **aprun tau_exec ./app** with options.

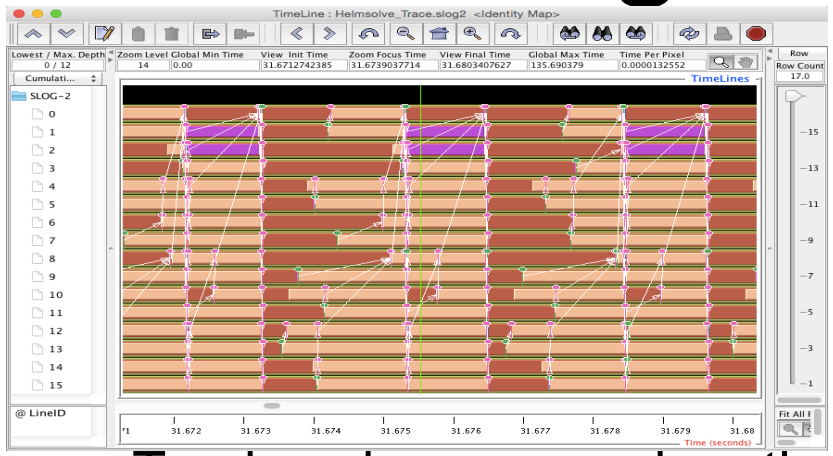
Profiling and Tracing

Profiling



- **Profiling** shows you **how much** (total) time was spent in each routine

Tracing



- Tracing shows you when the events take place on a timeline

- Profiling and tracing

  Profiling shows you **how much** (total) time was spent in each routine

  Tracing shows you **when** the events take place on a timeline

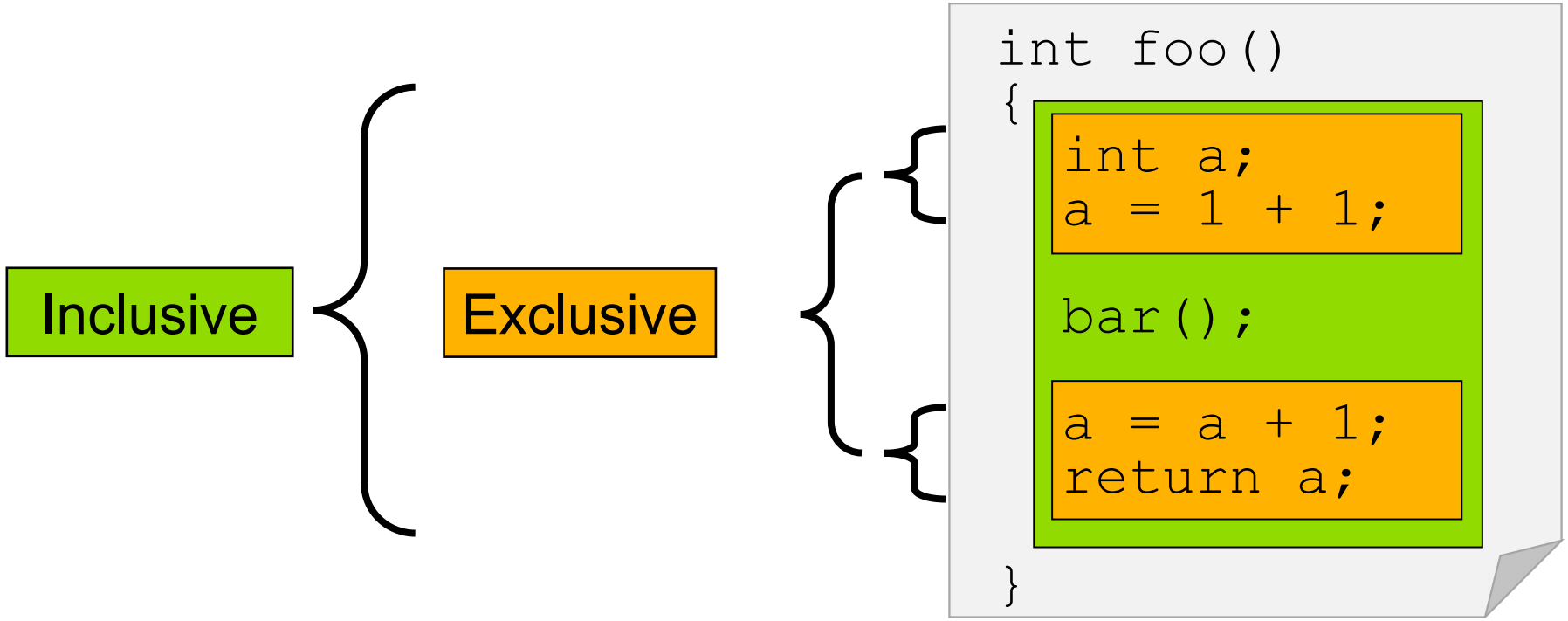
Instrumentation

- Direct and indirect performance observation
- Instrumentation invokes performance measurement
- Direct measurement with *probes*
- Indirect measurement with periodic sampling or hardware performance counter overflow interrupts
- Events measure performance data, metadata, context, etc.

- User-defined events
  - ***Interval*** (start/stop) events to measure exclusive & inclusive duration
  - ***Atomic events*** take measurements at a single point
    - Measures total, samples, min/max/mean/std. deviation statistics
  - ***Context events*** are atomic events with executing context
    - Measures above statistics for a given calling path

Inclusive vs. Exclusive values

- Inclusive
  - Information of all sub-elements aggregated into single value
- Exclusive
  - Information cannot be subdivided further



Inclusive Measurements

TAU: ParaProf: node 0 - fun3d_d19.ppk

Metric: TIME
Value: Inclusive
Units: seconds

221.305	.TAU application
221.304	NODET [{main.f90} {4,1}-{35,17}]
197.989	FLOW::ITERATE [{flow.F90} {1692,14}]
195.577	FLOW::STEP_SOLVER [{flow.F90} {1845,14}]
195.569	RELAX_STEADY::RELAX [{relax_steady.f90} {30,3}-{307,22}]
61.927	UPDATE_MEAN::UPDATE_LINEAR_SYSTEM_MEAN [{update_mean.F90} {195,3}-{275,42}]
61.28	UPDATE_MEAN::UPDATE_JACOBIAN_DRIVER_MEAN [{update_mean.F90} {460,3}-{505,44}]
61.275	UPDATE_MEAN::UPDATE_JACOBIAN [{update_mean.F90} {513,3}-{588,32}]
61.258	FILL_JACOBIANS::FILL_JACOBIAN [{fill_jacobians.f90} {19,3}-{341,30}]
59.068	GCR_SOLVE::GCR_SOLVER_QSET [{gcr_solve.f90} {47,3}-{415,32}]
57.635	GCR_SOLVE_UTIL::GCR_PRECONDITIONER_QSET [{gcr_solve_util.f90} {40,3}-{131,40}]
57.152	POINT_SOLVER::POINT_SOLVE [{point_solver.F90} {31,3}-{214,28}]
56.882	UPDATE_MEAN::UPDATE_RHS_MEAN [{update_mean.F90} {102,3}-{185,32}]
54.402	RELAX_MEAN::RELAX [{relax_mean.f90} {22,3}-{84,22}]
53.103	LINEARSOLVE_NODIVCHECK::NODIVCHECK_RELAX_Q [{linearsolve_nodivcheck.F90} {56,14}]
52.867	UPDATE_MEAN::RESIDUAL_S [{update_mean.F90} {42,3}-{94,27}]
52.866	FUN3D_RES_FLOW::RES_FLOW [{fun3d_res_flow.f90} {27,3}-{279,25}]
52.756	FLUX::RESIDUAL_COMPRESSIBLE [{flux.f90} {25,3}-{592,38}]
52.747	POINT_SOLVER::POINT_SOLVE_5 [{point_solver.F90} {2700,3}-{2921,30}]
52.744	Loop: POINT_SOLVER::POINT_SOLVE_5 [{point_solver.F90} {2757,5}-{2917,19}]
36.232	JACOBIAN_VISCOUS::VISCOUS_JACOBIAN [{jacobian_viscous.f90} {20,14}]
36.231	JACOBIAN_VISCOUS::EDGEJP [{jacobian_viscous.f90} {324,14}]
36.231	Loop: JACOBIAN_VISCOUS::EDGEJP [{jacobian_viscous.f90} {440,7}-{1584,22}]
27.474	FLUX_PERFGAS::INVISCID_FLUX_DRIVER [{flux_perfgas.f90} {37,14}]
27.474	FLUX_PERFGAS::ROE_FLUX [{flux_perfgas.f90} {236,14}]
27.473	Loop: FLUX_PERFGAS::ROE_FLUX [{flux_perfgas.f90} {397,5}-{597,20}]
22.707	FLOW::INITIALIZE_DATA [{flow.F90} {465,14}]
22.694	FLOW::INITIALIZE_DATA2 [{flow.F90} {663,14}]
20.916	PPARTY_PREPROCESSOR::PPARTY_PREPROCESS [{pparty_preprocessor.f90} {28,14}]
16.726	PPARTY_PREPROCESSOR::PPARTY_READ_GRID [{pparty_preprocessor.f90} {735,14}]
16.726	PUNS3D_IO_C2N::PUNS3D_READ_VGRID_C2N [{puns3d_io_c2n.f90} {1543,14}]
16.657	PUNS3D_IO_C2N::PUNS3D_READ_VGRID_C2N_SM [{puns3d_io_c2n.f90} {1641,14}]
14.159	GRADIENT_DRIVER::GRAD_VARIABLE [{gradient_driver.f90} {110,3}-{508,30}]
13.852	UPDATE_TURB::UPDATE_RHS_TURB [{update_turb.f90} {742,3}-{845,32}]

EXASCALE COMPUTING PROJECT

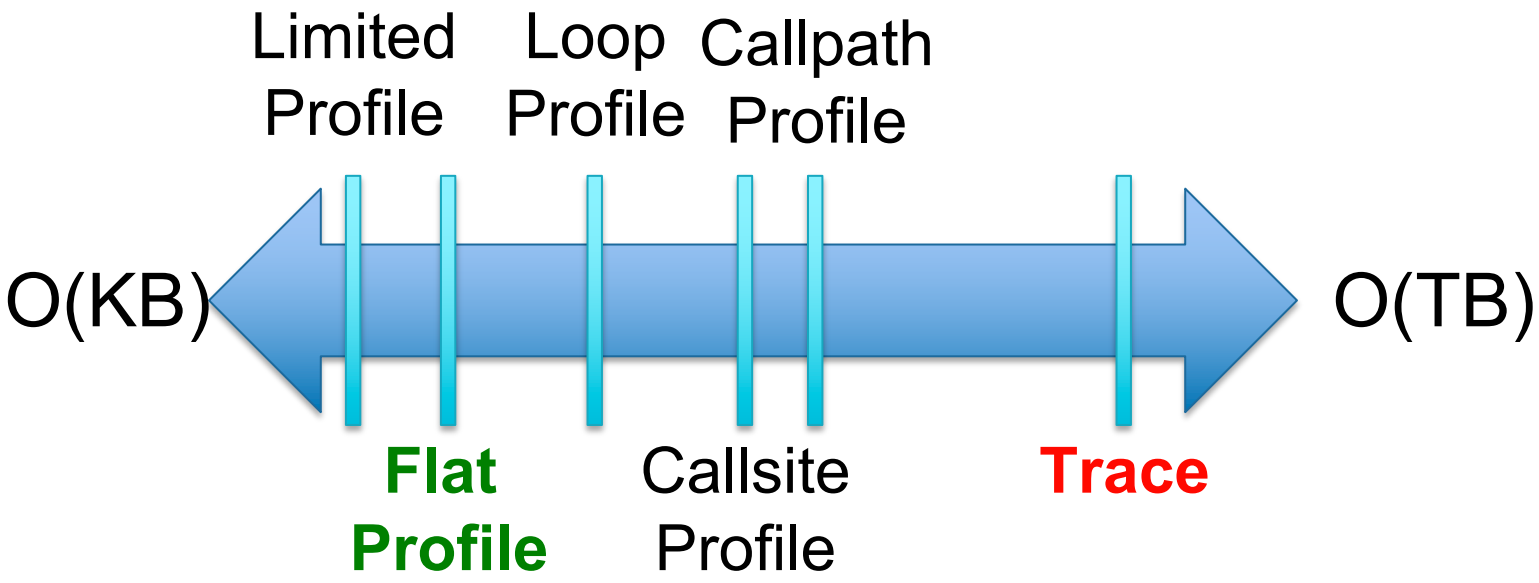
Exclusive Time

TAU: ParaProf: node 0 - fun3d_d19.ppk

Metric: TIME
Value: Exclusive
Units: seconds

43.649	Loop: POINT_SOLVER::POINT_SOLVE_5 [{point_solver.F90} {2757,5}-{2917,19}]
36.231	Loop: JACOBIAN_VISCOUS::EDGEJP [{jacobian_viscous.f90} {440,7}-{1584,22}]
27.473	Loop: FLUX_PERFGAS::ROE_FLUX [{flux_perfgas.f90} {397,5}-{597,20}]
19.688	FILL_JACOBIANS::FILL_JACOBIAN [{fill_jacobians.f90} {19,3}-{341,30}]
16.273	PUNS3D_IO_C2N::PUNS3D_READ_VGRID_C2N_SM [{puns3d_io_c2n.f90} {1641,14}]
13.381	GRADIENT_DRIVER::GRAD_VARIABLE [{gradient_driver.f90} {110,3}-{508,30}]
10.059	MPI_Waitall()
9.954	MPI_Reduce()
8.04	FLUX_PERFGAS::VISRHS_TET [{flux_perfgas.f90} {3023,14}]
7.319	TURB_SPALART::SA_RESID [{turb_spalart.f90} {219,14}]
3.78	FLUX_TURB::TURBULENT_GRADIENTS [{flux_turb.f90} {796,3}-{899,36}]
3.562	TIMESTEP::DELTAT2 [{timestep.f90} {20,3}-{331,24}]
3.384	POINT_SOLVER::POINT_SOLVE_1 [{point_solver.F90} {1083,3}-{1206,30}]
1.309	TURB_SPALART::EDGE_ASSEMBLY_RES_CONV_DIFF [{turb_spalart.f90} {5048,14}]
1.086	MPI_Bcast()
0.977	TURB_SPALART::EDGE_ASSEMBLY_JAC_CONV_DIFF [{turb_spalart.f90} {5209,14}]
0.668	PPARTY_MIXED_ELEMENT::EDGE_POINTER_DRIVER [{pparty_mixed_element.f90} {74,3}-{502,36}]
0.66	UPDATE_MEAN::UPDATE_Q [{update_mean.F90} {723,3}-{803,25}]
0.637	POINT_LU_DDQ::LU_5 [{point_lu_ddq.f90} {1566,3}-{1636,21}]
0.624	SOLUTION::WREST_INTERLEAF [{solution.F90} {3214,14}]
0.586	DUAL_NUMBERING::FMATRIX_TO_GRID [{dual_numbering.f90} {122,3}-{143,32}]
0.565	GRID_METRICS::DUALMETRIC [{grid_metrics.f90} {2289,3}-{2791,27}]
0.524	TURB_SPALART::SA_JACOB [{turb_spalart.f90} {757,14}]
0.49	MPI_Barrier()
0.479	UPDATE_TURB::UPDATE_VALUES_TURB [{update_turb.f90} {854,3}-{877,35}]
0.41	DUAL_NUMBERING::FGRID_TO_MATRIX [{dual_numbering.f90} {94,3}-{115,32}]
0.371	LMPI_APP::SINGLE_START_MATRIX_XFER [{lmpi_app.F90} {7907,3}-{8132,41}]
0.36	TURB_SPALART::JACOBIAN_SA [{turb_spalart.f90} {88,14}]
0.352	TIMEACC::TIME_DIAG_NC [{timeacc.f90} {1067,3}-{1330,29}]
0.336	MPI_Init()
0.285	LMPI_APP::SINGLE_MATRIX_COMPLETE_XFER [{lmpi_app.F90} {11520,3}-{11626,44}]
0.283	PPARTY_METIS::MY_METIS [{pparty_metis.F90} {116,3}-{545,24}]
0.275	PPARTY::NODE_CELL_CHOPPER [{pparty.f90} {41,3}-{453,33}]
0.269	FLUX_UTIL::L2NORM [{flux_util.f90} {31,3}-{249,23}]

How much data do you want?



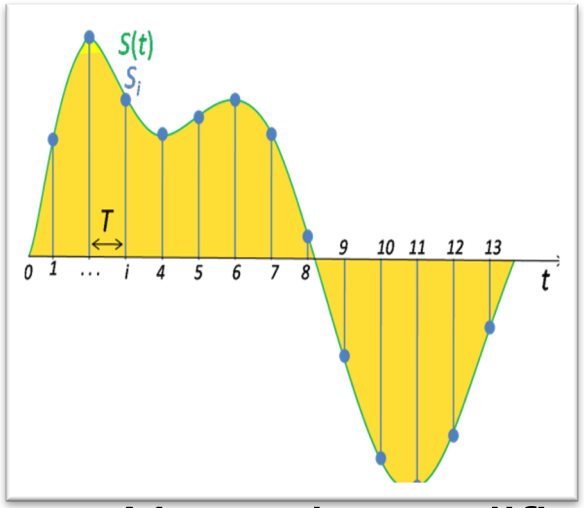
Performance Data Measurement

Direct via Probes

```
Call START('potential')
// code
Call STOP('potential')
```

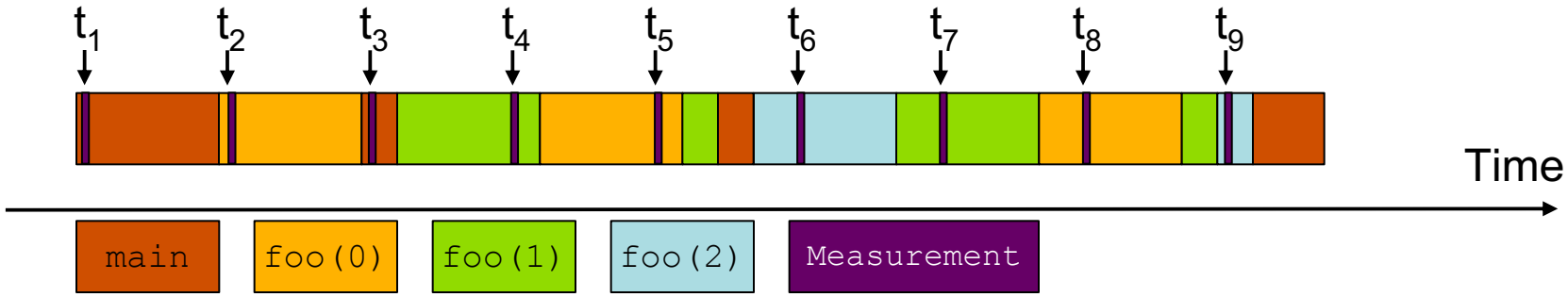
- Exact measurement
- Fine-grain control
- Calls inserted into code

Indirect via Sampling



- No code modification
- Minimal effort
- Relies on debug symbols (**-g**)

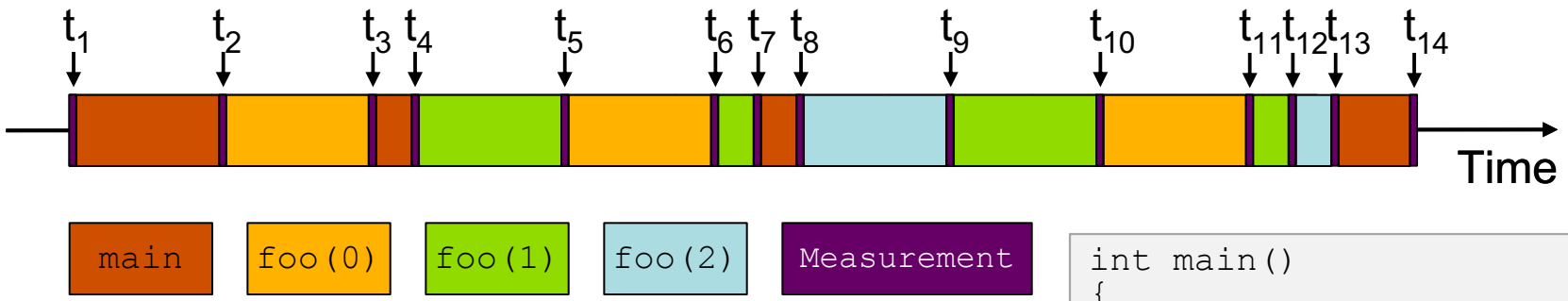
Sampling



- Running program is periodically interrupted to take measurement
  - Timer interrupt, OS signal, or HWC overflow
  - Service routine examines return-address stack
  - Addresses are mapped to routines using symbol table information
- Statistical inference of program behavior
  - Not very detailed information on highly volatile metrics
  - Requires long-running applications
- Works with unmodified executables

```
int main()
{
  int i;

  for (i=0; i < 3; i++)
    foo(i);

  return 0;
}

void foo(int i)
{

  if (i > 0)
    foo(i - 1);

}
```

Instrumentation



- Measurement code is inserted such that every event of interest is captured directly
  - Can be done in various ways
- Advantage:
  - Much more detailed information
- Disadvantage:
  - Processing of source-code / executable necessary
  - Large relative overheads for small functions

```
int main()
{
  int i;
  Start("main");
  for (i=0; i < 3; i++)
    foo(i);
  Stop("main");
  return 0;
}

void foo(int i)
{
  Start("foo");
  if (i > 0)
    foo(i - 1);
  Stop("foo");
}
```

Using TAU's Runtime Preloading Tool: tau_exec

Preload a wrapper that intercepts the runtime system call and substitutes with another

MPI

OpenMP

POSIX I/O

Memory allocation/deallocation routines

Wrapper library for an external package

No modification to the binary executable!

Enable other TAU options (communication matrix, OTF2, event-based sampling)

TAU Hands-On: Quickstart Guide

Setup:

- `% module load tau ; tar zxf /soft/perftools/tau/workshop.tgz (Theta/ACLF)`

Profiling with an un-instrumented application:

```
MPI: % aprun -n 64 tau_exec -T <tag> -ebs ./a.out
```

- MPI+OpenMP with Intel/Clang compilers: `% export TAU_OMPT_SUPPORT_LEVEL=full;`
  `% aprun -n 64 tau_exec -T ompt,v5 -ompt ./a.out`
- Pthread: `% aprun -n 64 tau_exec -T mpi,pthread -ebs ./a.out`
- Python+MPI+Sampling: `% aprun -n 64 tau_python -ebs ./a.py`
- Python+MPI+CUDA+Sampling: `% aprun -np 64 tau_python -cupti -ebs ./a.py`
- C+CUDA (no MPI): `% tau_exec -T cupti,serial -cupti ./a.out`

```
Analysis: % pprof -a -m | more;  % paraprof (GUI)
```

Tracing:

- Vampir: MPI: `% export TAU_TRACE=1; export TAU_TRACE_FORMAT=otf2`
  `% aprun -n 64 tau_exec ./a.out; vampir traces.otf2 &`
- Chrome: `% export TAU_TRACE=1; aprun -np 64 tau_exec ./a.out; tau_treemerge.pl;`
  `% tau_trace2json tau.trc tau.edf -chrome -ignoreatomic -o app.json`
  Chrome browser: chrome://tracing (Load -> app.json)
- Jumpshot: `% export TAU_TRACE=1; aprun -np 64 tau_exec ./a.out; tau_treemerge.pl;`
  `% tau2slog2 tau.trc tau.edf -o app.slog2; jumpshot app.slog2 &`

Simplifying TAU's usage (tau_exec)

Uninstrumented execution

```
% aprun -n  64  ./a.out
```

Track MPI performance

```
% aprun -n  64   tau_exec  ./a.out
```

Use event based sampling (compile with –g)

```
% aprun -n 64 tau_exec –ebs ./a.out
```

Also –ebs_source=<PAPI_COUNTER> -ebs_period=<overflow_count> -ebs_resolution=[file|function|line]
(line is default)

Track POSIX I/O and MPI performance (MPI enabled by default)

```
% aprun -n  64  tau_exec –T mpi,pdt,papi –io  ./a.out
```

Track OpenMP runtime routines

```
% aprun –n 64 tau_exec –T ompt,v5,pdt,mpi –ompt ./a.out
```

Track memory operations

```
% export TAU_TRACK_MEMORY_LEAKS=1
% aprun -n 64 tau_exec –memory_debug ./a.out (bounds check)
```

Load wrapper interposition library

```
% aprun –n 64 tau_exec –loadlib=<path/libwrapper.so> ./a.out
```

RUNTIME PRELOADING

- Injects TAU DSO in the executing application
- Requires dynamic executables
- We must compile with –dynamic –g
- Use tau_exec while launching the application

Copy the workshop tarball

Setup preferred program environment compilers

Default set Intel Compilers with Intel MPI. You must compile with **–dynamic -g**

```
% module load tau;
% tar zxf /soft/perftools/tau/workshop.tgz
% cd workshop/MZ-NPB3.3-MPI; cat README
% make clean
% make suite
% cd bin
In a second window:
% qsub -I -n 1 -A ATPESC_Day_8 -q ATPESC2020 -t 50
% cd bin; module load tau
% export OMP_NUM_THREADS=4
% aprun -n 16 ./bt-mz.B.16  (or ./r)
% export TAU_OMPT_SUPPORT_LEVEL=full
% aprun -n 16 tau_exec -T ompt,v5,mpi,pdt -ompt ./bt-mz.B.16
(OR ./rt)
% paraprof --pack ex1.ppk
In the first window or scp to laptop and launch locally:
% paraprof ex1.ppk &
```

ParaProf Profile Browser

```
% paraprof
```

ParaProf Profile Browser

TAU supports Python, MPI, and CUDA

Without any modification to the source code or DSOs or interpreter, it instruments and samples the application using Python, MPI, and CUDA instrumentation.

TAU: ParaProf: Statistics for: node 0, thread 2 - exafel1_230cores.ppk

Name	Exclusive ...	Inclusive T...	Calls	Child Calls
.TAU application	79.623	89.93	1	2,480
Memory copy Device to Host	8.216	8.216	425	0
Memory copy Host to Device	0.807	0.807	1,970	0
nanoBraggSpotsCUDAKernel(int, int, int, int, int,	1.284	1.284	85	0

Kernel on GPU

% aprun –np 230 tau_python –T cupti,mpi,pdt –ebs –cupti ./exafel.py
Instead of:
% aprun –np 230 python ./exafel.py

TAU Thread Statistics Table

TAU: ParaProf: Statistics for: node 0, thread 0 - exafel1_230cores.ppk

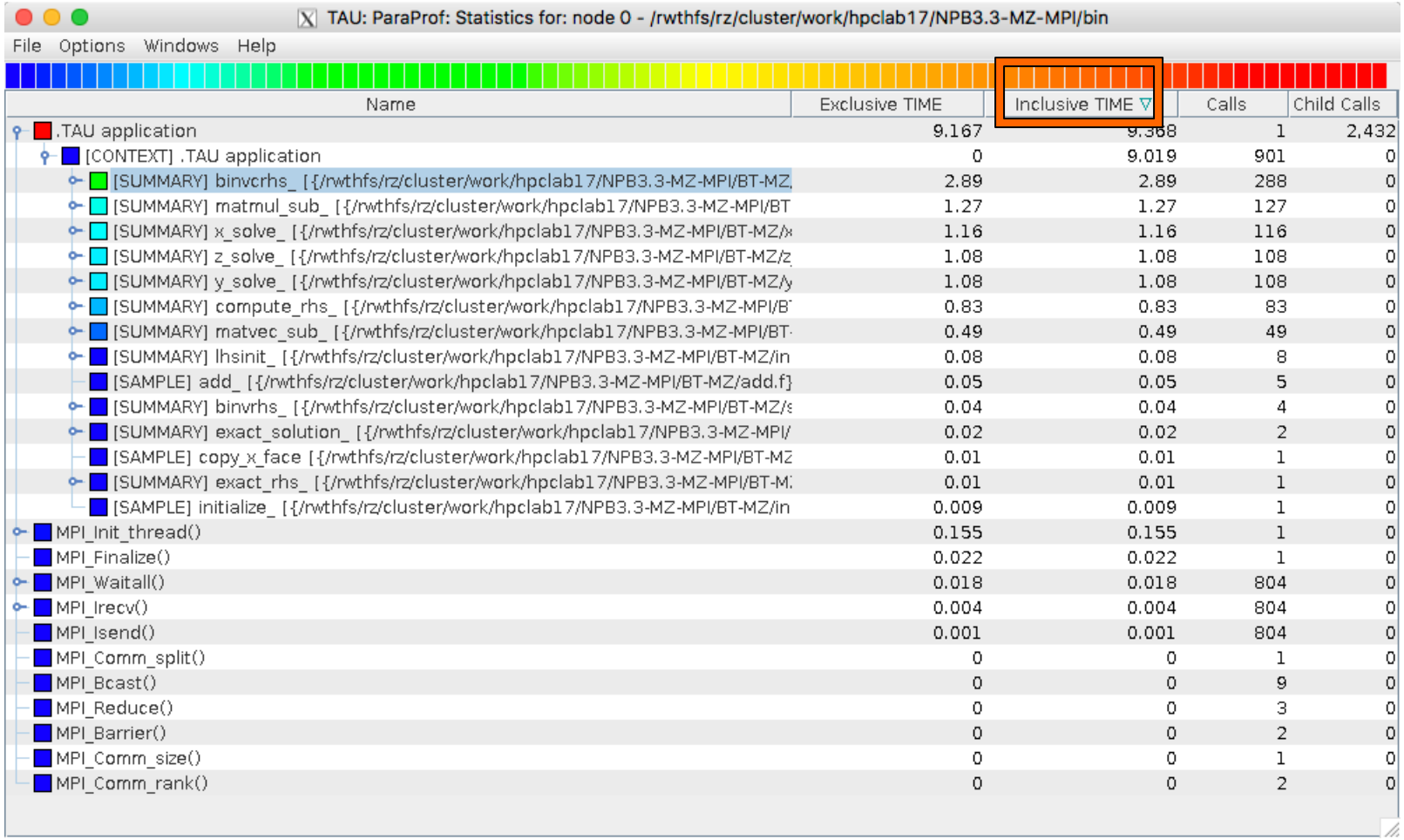
Name	Exclusive...	Inclusive ...	Calls	Child Calls
__init__ [{from_scatterers_fft.py}{13}]	20.036	20.362	303	10,914
run_sim2smv [{step5_pad.py}{138}]	16.78	134.9	1	1,066
__init__ [{__init__.py}{150}]	11.669	15.909	101	1,010
channel_pixels [{step5_pad.py}{79}]	11.029	107.657	100	13,358
[CONTEXT] channel_pixels [{step5_pad.py}{79}]	0	9.345	312	0
[SAMPLE] nanoBraggSpotsCUDA [{/autofs/nccs-svm1_home1/iris/adse13_161/psana-legion/simtbx/sun	4.755	4.755	159	0
[SAMPLE] simtbx::nanoBragg::nanoBragg::add_nanoBragg_spots_cuda() [{/autofs/nccs-svm1_home1/iris/	4.08	4.08	136	0
[SAMPLE] __memset_power8 [{} {0}]	0.3	0.3	10	0
[SAMPLE] UNRESOLVED /usr/lib64/libc-2.17.so	0.181	0.181	6	0
[SUMMARY] Tau_handle_driver_api_memcpy(void*, CUpti_CallbackDomain, unsigned int, CUpti_CallbackDa	0.03	0.03	1	0
cuMemcpyDtoH_v2	9.483	9.483	500	0
expand_to_p1_iselection [{__init__.py}{1376}]	7.349	7.35	101	606
load	7.004	7.009	2	2,251
reset_wavelength [{util_fmodel.py}{121}]	6.197	6.553	100	47,550
is_unique_set_under_symmetry [{__init__.py}{790}]	5.913	5.915	202	808
__import__	5.782	15.766	382	78
fp_fdp_at_wavelength [{fdp_plot.py}{44}]	5.616	5.723	800	1,600
MPI_Init_thread()	4.987	4.987	1	0
cuDevicePrimaryCtxRetain	4.735	4.735	2	0
<module> [{__init__.py}{1}]	4.255	23.888	85	756
MPI_Finalize()	3.829	3.829	1	1
match_bijvoet_mates [{__init__.py}{1032}]	3.146	3.684	101	707
bcast	3.073	3.448	1	9
__init__ [{__init__.py}{20}]	3.011	3.399	101	149,196
compute_f_mask [{__init__.py}{299}]	2.897	18.853	101	707

Python, MPI, CUDA, and samples from DSOs are all integrated in a single view

ParaProf

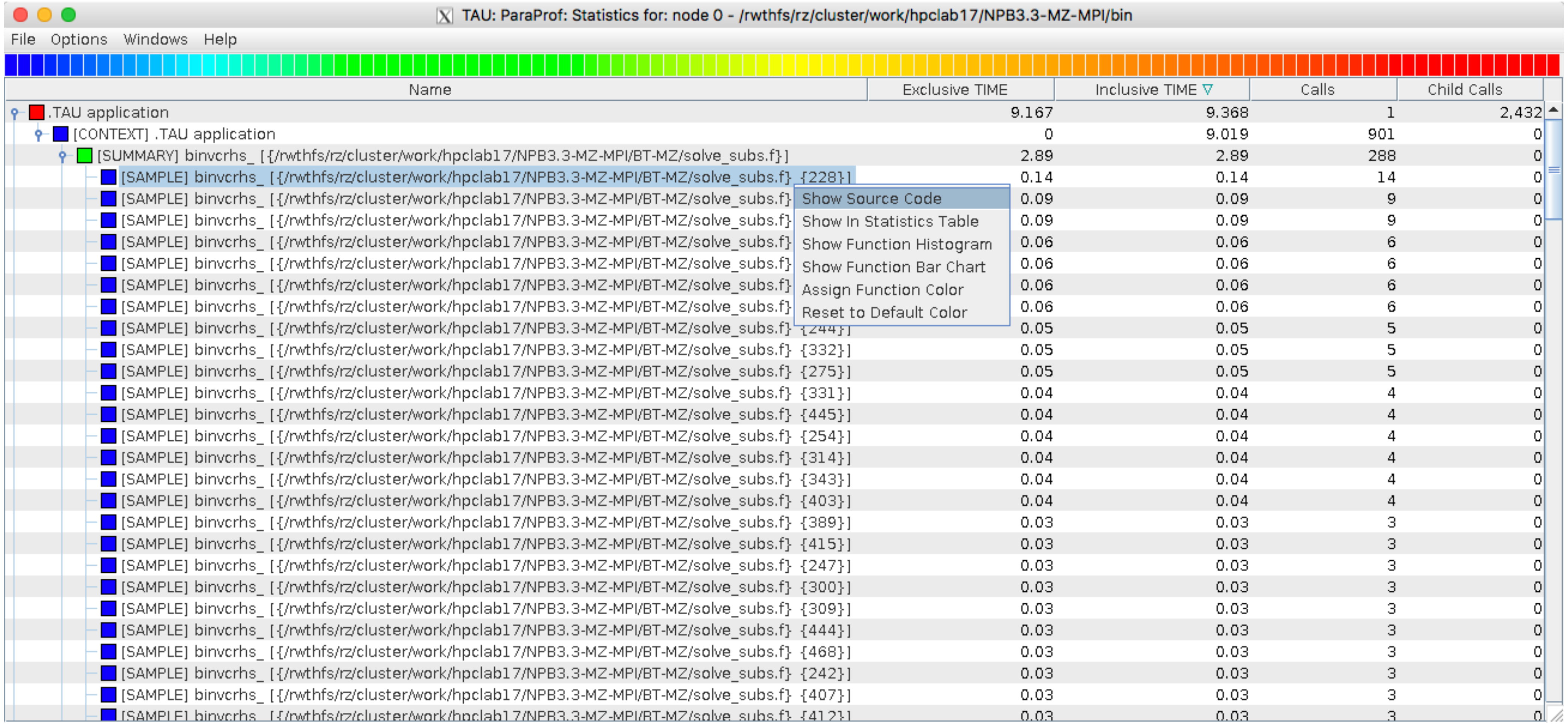
Click on Columns:
to sort by incl time

Open binvcrhs
Click on Sample



Name	Exclusive TIME	Inclusive TIME ▽	Calls	Child Calls
.TAU application	9.167	9.368	1	2,432
[CONTEXT] .TAU application	0	9.019	901	0
[SUMMARY] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ	2.89	2.89	288	0
[SUMMARY] matmul_sub_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT	1.27	1.27	127	0
[SUMMARY] x_solve_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/x	1.16	1.16	116	0
[SUMMARY] z_solve_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/z	1.08	1.08	108	0
[SUMMARY] y_solve_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/y	1.08	1.08	108	0
[SUMMARY] compute_rhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/B	0.83	0.83	83	0
[SUMMARY] matvec_sub_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT	0.49	0.49	49	0
[SUMMARY] lhsinit_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/in	0.08	0.08	8	0
[SAMPLE] add_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/add.f}	0.05	0.05	5	0
[SUMMARY] binvrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/s	0.04	0.04	4	0
[SUMMARY] exact_solution_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/	0.02	0.02	2	0
[SAMPLE] copy_x_face [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ	0.01	0.01	1	0
[SUMMARY] exact_rhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-M	0.01	0.01	1	0
[SAMPLE] initialize_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/in	0.009	0.009	1	0
MPI_Init_thread()	0.155	0.155	1	0
MPI_Finalize()	0.022	0.022	1	0
MPI_Waitall()	0.018	0.018	804	0
MPI_Irecv()	0.004	0.004	804	0
MPI_Isend()	0.001	0.001	804	0
MPI_Comm_split()	0	0	1	0
MPI_Bcast()	0	0	9	0
MPI_Reduce()	0	0	3	0
MPI_Barrier()	0	0	2	0
MPI_Comm_size()	0	0	1	0
MPI_Comm_rank()	0	0	2	0

ParaProf



Name	Exclusive TIME	Inclusive TIME ▽	Calls	Child Calls
🟥 .TAU application	9.167	9.368	1	2,432
🟦 [CONTEXT] .TAU application	0	9.019	901	0
🟩 [SUMMARY] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f}]	2.89	2.89	288	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {228}]	0.14	0.14	14	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f}	0.09	0.09	9	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f}	0.09	0.09	9	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f}	0.06	0.06	6	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f}	0.06	0.06	6	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f}	0.06	0.06	6	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f}	0.06	0.06	6	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {244}]	0.05	0.05	5	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {332}]	0.05	0.05	5	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {275}]	0.05	0.05	5	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {331}]	0.04	0.04	4	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {445}]	0.04	0.04	4	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {254}]	0.04	0.04	4	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {314}]	0.04	0.04	4	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {343}]	0.04	0.04	4	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {403}]	0.04	0.04	4	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {389}]	0.03	0.03	3	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {415}]	0.03	0.03	3	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {247}]	0.03	0.03	3	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {300}]	0.03	0.03	3	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {309}]	0.03	0.03	3	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {444}]	0.03	0.03	3	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {468}]	0.03	0.03	3	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {242}]	0.03	0.03	3	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {407}]	0.03	0.03	3	0
🟦 [SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {412}]	0.03	0.03	3	0

TAU Context Event Window

TAU: ParaProf: Context Events for: node 0, thread 0 - exafel1_230cores.ppk

Name	Total	NumSamples	MaxValue	MinValue	MeanValue	Std. Dev.
<module> [{step5_batch.py}{1}]						
tst_one [{step5_batch.py}{23}]						
run_sim2smv [{step5_pad.py}{138}]						
channel_pixels [{step5_pad.py}{79}]						
cudaMemcpy						
Bytes copied from Device to Host	15,300,000,000	500	36,000,000	9,000,000	30,600,000	10,800,000
Bytes copied from Host to Device	15,423,816,000	2,300	36,000,000	8	6,706,006.957	13,564,989.185
cuMemcpyHtoD_v2						
Bytes copied from Host to Device	15,423,816,000	2,300	36,000,000	8	6,706,006.957	13,564,989.185
cuMemcpyDtoH_v2						
Bytes copied from Device to Host	15,300,000,000	500	36,000,000	9,000,000	30,600,000	10,800,000
Bytes copied from Device to Host	30,600,000,000	1,000	36,000,000	9,000,000	30,600,000	10,800,000
Bytes copied from Host to Device	30,847,632,000	4,600	36,000,000	8	6,706,006.957	13,564,989.185
Message size for broadcast	827,971,798	2	827,971,794	4	413,985,899	413,985,895

TAU tracks the data transfers between the host and the GPU.

TAU's tracking of Python and MPI

TAU: ParaProf: Statistics for: node 1, thread 0 - exafel1_230cores.ppk

Name	Exclusive...	Inclusive ...	Calls	Child ...
__init__ [{from_scatterers_fft.py}{13}]	19.845	20.166	303	10,914
run_sim2smv [{step5_pad.py}{138}]	16.672	133.715	1	1,066
MPI_Bcast()	12.263	12.263	2	0
[CONTEXT] MPI_Bcast()	0	12.21	407	0
[SAMPLE] PAMI_Context_lock [{/autofs/nccs-svm1_sw/summit/.swci/1-compute/opt/spac	3.27	3.27	109	0
[SAMPLE] pthread_spin_lock [{/usr/lib64/libpthread-2.17.so}{0}]	2.34	2.34	78	0
[SAMPLE] start_libcoll_blocking_collective [{/autofs/nccs-svm1_sw/summit/.swci/1-compu	1.89	1.89	63	0
[SAMPLE] PAMI::Device::IBV::Device::advance() [{/autofs/nccs-svm1_sw/summit/.swci/1-cc	1.56	1.56	52	0
[SAMPLE] PAMI_Context_advancev [{/autofs/nccs-svm1_sw/summit/.swci/1-compute/opt	0.69	0.69	23	0
[SAMPLE] UNRESOLVED /usr/lib64/libmlx5.so.1.0.0	0.51	0.51	17	0
[SUMMARY] LIBCOLL_Advance_pami [{/__SMPI_build_dir_____/ibmsrc/r	0.42	0.42	14	0
[SAMPLE] LIBCOLL_Advance_pami [{/__SMPI_build_dir_____/ibmsrc/n	0.42	0.42	14	0
[SAMPLE] PAMI_Context_unlock [{/autofs/nccs-svm1_sw/summit/.swci/1-compute/opt/sp	0.39	0.39	13	0
[SAMPLE] pthread_spin_unlock [{/usr/lib64/libpthread-2.17.so}{0}]	0.36	0.36	12	0
[SAMPLE] __memcpy_power7 [{}{0}]	0.33	0.33	11	0
[SAMPLE] 0000003d.plt_call.PAMI_Context_lock [{}{0}]	0.15	0.15	5	0
[SAMPLE] verbs_get_exp_ctx [{pami.cc}{0}]	0.09	0.09	3	0
[SAMPLE] PAMI_Context_trylock_advancev [{/autofs/nccs-svm1_sw/summit/.swci/1-comp	0.06	0.06	2	0
[SAMPLE] 0000003d.plt_call.PAMI_Context_unlock [{}{0}]	0.06	0.06	2	0
[SAMPLE] opal_progress [{/autofs/nccs-svm1_sw/summit/.swci/1-compute/opt/spack/2C	0.03	0.03	1	0
[SAMPLE] 00000052.plt_call.PAMI_Context_advancev [{}{0}]	0.03	0.03	1	0
[SUMMARY] CCMI::Executor::ShmemBroadcastT<false, CCMI::Executor::ShmemAtomicBarrie	0.03	0.03	1	0
[SAMPLE] CCMI::Executor::ShmemBroadcastT<false, CCMI::Executor::ShmemAtomicBarrie	0.03	0.03	1	0
__init__ [{__init__.py}{150}]	11.518	15.698	101	1,010
channel_pixels [{step5_pad.py}{79}]	10.949	106.61	100	13,358
cuMemcpyDtoH_v2	9.433	9.433	500	0

TAU can observe events in closed-source vendor libraries (e.g., in MPI_Bcast)!

Callstack Sampling in TAU

TAU: ParaProf: Statistics for: n,c,t 2,0,0 - gamess_unw_call_ebs.ppk

Name	Inclusive TIME	Calls
.TAU application	79.592	1
MPI_Recv()	75.607	6,870
[CONTEXT] MPI_Recv()	74.848	1,497
[UNWIND] /gpfs/mira-home/sameer/gamess-theta-tau/object/unport.f.410 [@] MAIN__ [{/gpfs/mira-home/sameer/gamess-theta-t	26.196	524
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_fortran.c.67 [@] beging_ [{/gpfs/mira-home/sameer/ga	21.7	434
[UNWIND] /gpfs/mira-home/sameer/gamess-theta-tau/object/gamess.f.538 [@] main [{/gpfs/mira-home/sameer/gamess-theta-ta	11.85	237
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_init.c.113 [@] ddi_init_ [{/gpfs/mira-home/yuri/dist/Gi	8.701	174
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_server.c.99 [@] DDI_Init [{/gpfs/mira-home/yuri/dist/C	5.75	115
[UNWIND] /lib64/libc-2.22.so.0 [@] _start [{/home/abuild/rpmbuild/BUILD/glibc-2.22/csu/../sysdeps/x86_64/start.S} {118}]	0.2	4
[SAMPLE] GNII_DlaProgress [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0} {0}]	0.2	4
[UNWIND] [/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0.0] [@] UNRESOLVED UNKNOWN	0.15	3
[SAMPLE] GNI_CqGetEvent [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0} {0}]	0.051	1
[UNWIND] /opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1.0 [@] MPIDI_CH3I_Progress [{/opt/cray/pe/mpt/7	0.05	1
MPI_Finalize()	3.601	1
MPI_Send()	0.122	6,866
MPI_Init_thread()	0.112	1
[CONTEXT] .TAU application	0.05	1
MPI_Bcast()	0.014	6
MPI_Allgather()	0.004	3
MPI_Barrier()	0.003	7
MPI_Comm_create()	0.002	4
MPI_Gather()	0.002	1
MPI_Comm_split()	0.002	1
MPI_Group_intersection()	0.001	1
MPI_Comm_group()	0.001	1
MPI_Group_incl()	0	3
MPI_Comm_rank()	0	6
MPI_Comm_size()	0	2

% export TAU_SAMPLING=1; export TAU_EBS_UNWIND=1

UNWINDING CALLSTACKS

TAU: ParaProf: Statistics for: n,c,t 2,0,0 - gamess_unw_call_ebs.ppk

Name	Inclusive TIME	Calls
.TAU application	79.592	1
MPI_Recv()	75.607	6,870
[CONTEXT] MPI_Recv()	74.848	1,497
[UNWIND] /gpfs/mira-home/sameer/gamess-theta-tau/object/unport.f.410 [@] MAIN__ [{/gpfs/mira-home/sameer/gamess-theta-	26.196	524
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_fortran.c.67 [@] beging_ [{/gpfs/mira-home/sameer/g	21.7	434
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_init.c.113 [@] ddi_init_ [{/gpfs/mira-home/yuri/dist	21.7	434
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_server.c.99 [@] DDI_Init [{/gpfs/mira-home/yuri/	21.7	434
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_recv.c.65 [@] DDI_Server [{/gpfs/mira-home/y	21.7	434
[UNWIND] /lus/theta-fs0/software/perftools/tau/tau-2.26.3/src/Profile/TauMpi.c.2371 [@] DDI_Recv_request [{/gpfs/mira	21.7	434
[UNWIND] /opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1.0 [@] MPI_Recv [{/lus/theta-fs0/sof	21.7	434
[UNWIND] /opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1.0 [@] PMPI_Recv [{/opt/cray/pe/n	21.7	434
[UNWIND] /opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1.0 [@] MPIDI_CH3I_Progress [{/	21.45	429
[UNWIND] /opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0.0 [@] MPID_nem_gni_poll [{/	15.95	319
[SAMPLE] GNI_SmsgGetNextWTag [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0}	10.349	207
[SAMPLE] GNI_CqGetEvent [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0} {0}]	5.6	112
[UNWIND] gni_poll.c.0 [@] MPID_nem_gni_poll [{/opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_inte	5.25	105
[UNWIND] /opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1.0 [@] MPID_nem_gni_poll [{/	0.25	5
[UNWIND] UNRESOLVED [@] MPIDI_CH3I_Progress [{/opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_int	0.25	5
[UNWIND] /gpfs/mira-home/sameer/gamess-theta-tau/object/gamess.f.538 [@] main [{/gpfs/mira-home/sameer/gamess-theta-ta	11.85	237
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_init.c.113 [@] ddi_init_ [{/gpfs/mira-home/yuri/dist/G	8.701	174
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_server.c.99 [@] DDI_Init [{/gpfs/mira-home/yuri/dist/	5.75	115
[UNWIND] /lib64/libc-2.22.so.0 [@] _start [{/home/abuild/rpmbuild/BUILD/glibc-2.22/csu/../sysdeps/x86_64/start.S} {118}]	0.2	4
[SAMPLE] GNII_DlaProgress [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0} {0}]	0.2	4
[UNWIND] [/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0.0] [@] UNRESOLVED UNKNOWN	0.15	3
[SAMPLE] GNI_CqGetEvent [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0} {0}]	0.051	1
[UNWIND] /opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1.0 [@] MPIDI_CH3I_Progress [{/opt/cray/pe/mpt/	0.05	1
MPI_Finalize()	3.601	1
MPI_Send()	0.122	6,866
MPI_Init_thread()	0.112	1
[CONTEXT] .TAU application	0.05	1

% export TAU_SAMPLING=1; export TAU_EBS_UNWIND=1

EXASCALE COMPUTING PROJECT

Deep Learning: Tensorflow

TAU: ParaProf: Statistics for: node 0, thread 8 - nt3_baseline_keras2.ppk

Name	Inclusiv...	Calls
.TAU application	519.211	1
[CONTEXT] .TAU application	509.222	50,915
[SAMPLE] Eigen::internal::gebp_kernel<float, float, long, Eigen::internal::blas_data_mapper<float, long, 0, 0>,	240.632	24,089
[SAMPLE] __pthread_cond_wait [{} {0}]	86.384	8,634
[SAMPLE] Eigen::internal::gemm_pack_rhs<float, long, Eigen::internal::TensorContractionSubMapper<float, lor	51.345	5,135
[SAMPLE] Eigen::internal::gemm_pack_rhs<float, long, Eigen::internal::TensorContractionSubMapper<float, lor	24.375	2,416
[SAMPLE] void tensorflow::SpatialMaxPoolWithArgMaxHelper<Eigen::ThreadPoolDevice, float>(tensorflow::OpK	16.301	1,630
[SAMPLE] __memset_sse2 [{} {0}]	13.446	1,336
[SAMPLE] Eigen::TensorEvaluator<Eigen::TensorContractionOp<Eigen::array<Eigen::IndexPair<long>, 1ul> co	5.99	599
[SAMPLE] long Eigen::internal::operator/<long, false>(long const&, Eigen::internal::TensorIntDivisor<long, fals	5.843	585
[SAMPLE] std::_Function_handler<void (long, long), Eigen::internal::TensorExecutor<Eigen::TensorAssignOp<I	5.377	538
[SAMPLE] float __vector Eigen::TensorEvaluator<Eigen::TensorBroadcastingOp<Eigen::IndexList<int, Eigen::typ	4.862	487
[SAMPLE] Eigen::TensorEvaluator<Eigen::TensorContractionOp<Eigen::array<Eigen::IndexPair<long>, 1ul> co	4.775	478
[SAMPLE] Eigen::TensorEvaluator<Eigen::TensorAssignOp<Eigen::TensorMap<Eigen::Tensor<float, 1, 1, long>	4.037	404
[SAMPLE] Eigen::internal::gemm_pack_lhs<float, long, Eigen::internal::TensorContractionSubMapper<float, lon	3.679	367
[SAMPLE] Eigen::internal::EvalRange<Eigen::TensorEvaluator<Eigen::TensorAssignOp<Eigen::TensorMap<Eige	2.981	298
[SAMPLE] tensorflow::MaxPoolingOp<Eigen::ThreadPoolDevice, float>::SpatialMaxPool(tensorflow::OpKernelCo	2.915	295
[SAMPLE] std::_Function_handler<void (long, long), Eigen::internal::TensorExecutor<Eigen::TensorAssignOp<I	2.91	291
[SAMPLE] std::_Function_handler<void (long, long), Eigen::internal::TensorExecutor<Eigen::TensorAssignOp<I	2.772	277
[SAMPLE] Eigen::internal::gemm_pack_lhs<float, long, Eigen::internal::TensorContractionSubMapper<float, lon	2.481	248
[SAMPLE] std::_Function_handler<void (long, long), Eigen::internal::TensorExecutor<Eigen::TensorAssignOp<I	2.148	215
[SAMPLE] void Eigen::internal::call_dense_assignment_loop<Eigen::Map<Eigen::Matrix<float, -1, -1, 0, -1, -1>	2.008	197
[SAMPLE] Eigen::NonBlockingThreadPoolTempl<tensorflow::thread::EigenEnvironment>::WorkerLoop(int) [{/ho	1.999	200
[SAMPLE] Eigen::internal::ptranspose(Eigen::internal::PacketBlock<float __vector, 4>&) [{crtstuff.c} {0}]	1.919	192
[SAMPLE] Eigen::internal::gemm_pack_rhs<float, long, Eigen::internal::TensorContractionSubMapper<float, lor	1.607	160
[SAMPLE] Eigen::TensorEvaluator<Eigen::TensorContractionOp<Eigen::array<Eigen::IndexPair<long>, 1ul> co	1.518	152

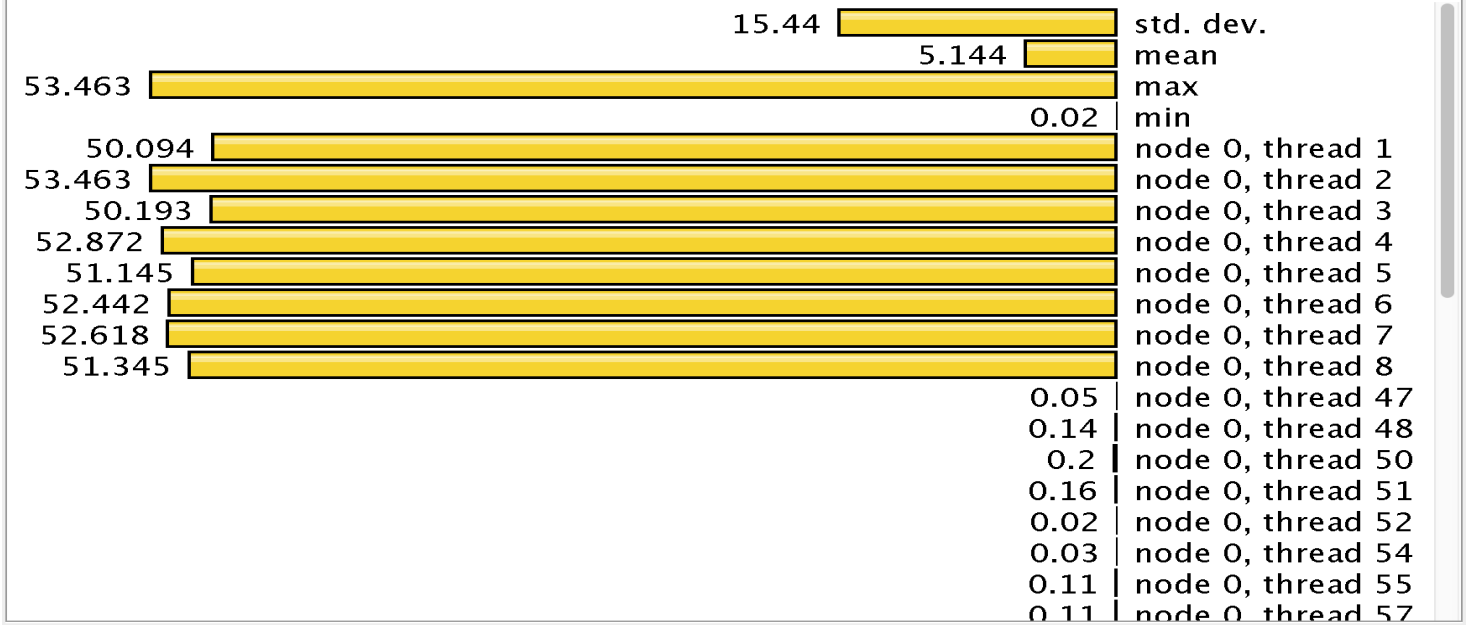
```
% tau_python -ebs nt3_baseline_keras2.py (CANDLE)
```

EXASCALE COMPUTING PROJECT

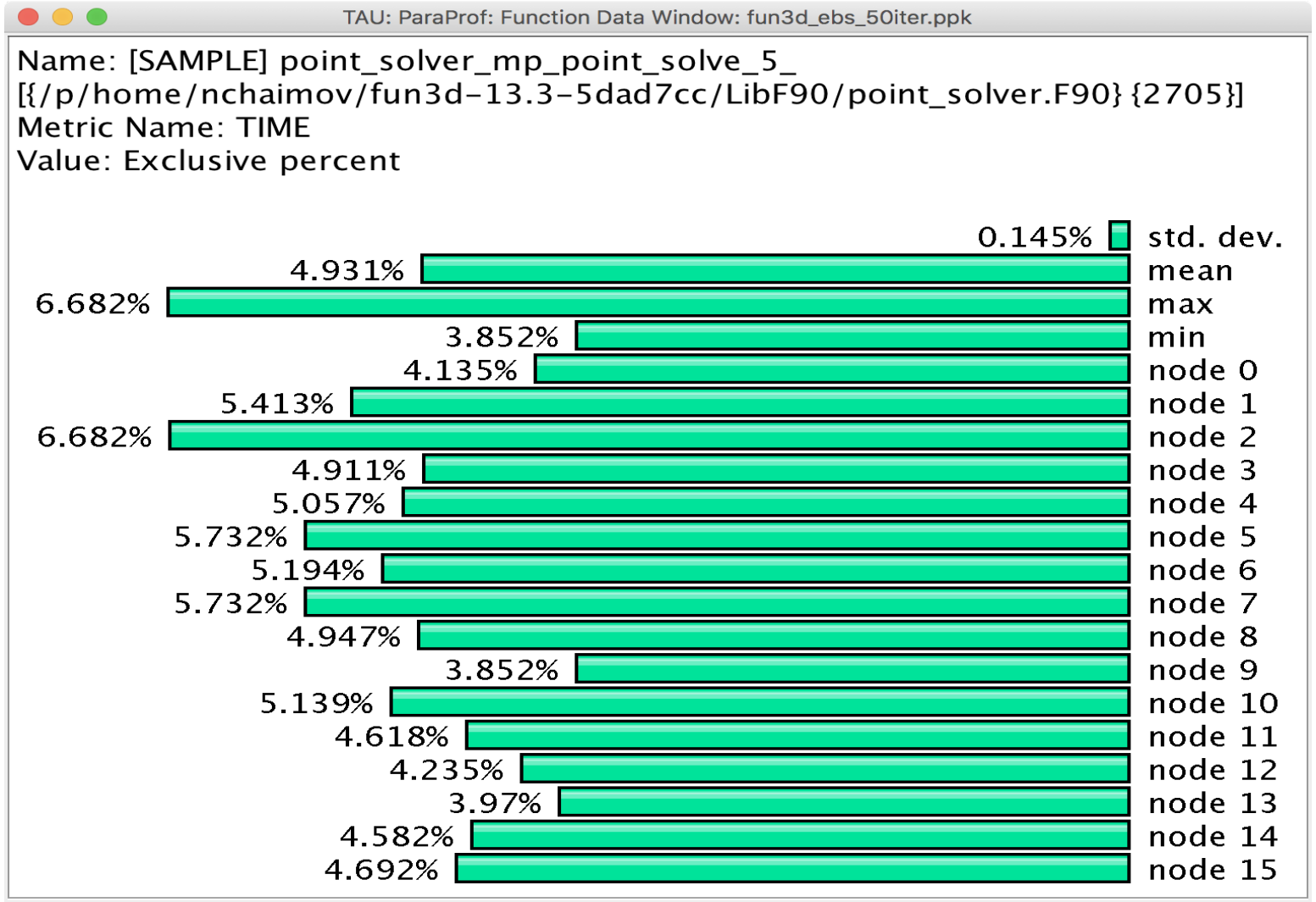
Sampling Tensorflow

TAU: ParaProf: Function Data Window: nt3_baseline_keras2.ppk

Name: .TAU application => [CONTEXT] .TAU application => [SAMPLE]
Eigen::internal::gemm_pack_rhs<float, long,
Eigen::internal::TensorContractionSubMapper<float, long, 0,
Eigen::TensorEvaluator<Eigen::TensorMap<Eigen::Tensor<float const, 2, 1, long>, 0,
Eigen::MakePointer> const, Eigen::ThreadPoolDevice>, Eigen::array<long, 1ul>,
Eigen::array<long, 1ul>, 8, false, false, 0, Eigen::MakePointer>, 4, 0, false,
false>::operator()(float*, Eigen::internal::TensorContractionSubMapper<float, long, 0,
Eigen::TensorEvaluator<Eigen::TensorMap<Eigen::Tensor<float const, 2, 1, long>, 0,
Eigen::MakePointer> const, Eigen::ThreadPoolDevice>, Eigen::array<long, 1ul>,
Eigen::array<long, 1ul>, 8, false, false, 0, Eigen::MakePointer> const&, long, long, long,
long) [{crtstuff.c} {0}]
Metric Name: TIME
Value: Exclusive
Units: seconds



Event Based Sampling (EBS)



Uninstrumented!

```
% aprun -n 16 tau_exec –ebs a.out
```

Callsite Profiling and Tracing

TAU: ParaProf: n,c,t 0,0,0 - lu_callsite.ppk

Metric: TIME
Value: Exclusive
Units: seconds

14.695	MPI_Recv()
12.627	[CALLSITE] MPI_Recv() [@] [exchange_1_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_1.f} {68}]
6.987	.TAU application
4.097	MPI_Send()
2.068	[CALLSITE] MPI_Recv() [@] [exchange_1_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_1.f} {86}]
2.053	[CALLSITE] MPI_Send() [@] [exchange_1_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_1.f} {113}]
1.926	[CALLSITE] MPI_Send() [@] [exchange_1_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_1.f} {130}]
0.365	MPI_Finalize()
0.365	[CALLSITE] MPI_Finalize() [@] [MAIN__] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/lu.f} {161}]
0.218	MPI_Init()
0.218	[CALLSITE] MPI_Init() [@] [init_comm_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/init_comm.f} {31}]
0.188	MPI_Wait()
0.104	[CALLSITE] MPI_Wait() [@] [exchange_3_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_3.f} {152}]
0.08	[CALLSITE] MPI_Wait() [@] [exchange_3_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_3.f} {288}]
0.063	[CALLSITE] MPI_Send() [@] [exchange_3_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_3.f} {209}]
0.057	MPI_Irecv()
0.055	[CALLSITE] MPI_Send() [@] [exchange_3_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_3.f} {73}]
0.03	[CALLSITE] MPI_Irecv() [@] [exchange_3_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_3.f} {108}]
0.026	[CALLSITE] MPI_Irecv() [@] [exchange_3_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_3.f} {244}]
0.012	MPI_Bcast()
0.009	[CALLSITE] MPI_Bcast() [@] [bcast_inputs_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/bcast_inputs.f} {28}]
0.008	MPI_Allreduce()
0.005	[CALLSITE] MPI_Allreduce() [@] [l2norm_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/l2norm.f} {55}]
0.002	[CALLSITE] MPI_Bcast() [@] [bcast_inputs_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/bcast_inputs.f} {33}]
0.001	[CALLSITE] MPI_Allreduce() [@] [ssor_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/ssor.f} {205}]
0.001	[CALLSITE] MPI_Wait() [@] [exchange_4_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_4.f} {59}]
0.001	[CALLSITE] MPI_Wait() [@] [exchange_6_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_6.f} {54}]
0.001	[CALLSITE] MPI_Wait() [@] [exchange_5_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_5.f} {54}]
7.6E-4	[CALLSITE] MPI_Wait() [@] [exchange_4_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_4.f} {104}]
4.9E-4	[CALLSITE] MPI_Irecv() [@] [exchange_4_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/exchange_4.f} {50}]
4.9E-4	MPI_Barrier()
4.9E-4	[CALLSITE] MPI_Barrier() [@] [ssor_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/ssor.f} {70}]
4.2E-4	[CALLSITE] MPI_Allreduce() [@] [error_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/error.f} {53}]
4.0E-4	MPI_Comm_size()
2.6E-4	[CALLSITE] MPI_Comm_size() [@] [read_input_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/read_input.f} {78}]
2.4E-4	MPI_Comm_rank()
2.4E-4	[CALLSITE] MPI_Allreduce() [@] [pintgr_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/pintgr.f} {272}]
2.4E-4	[CALLSITE] MPI_Comm_rank() [@] [init_comm_] [{/lus/theta-fs0/projects/Tools/tau/workshop/NPB3.1/LU/init_comm.f} {36}]

% export TAU_CALLSITE=1

TAU – Context Events

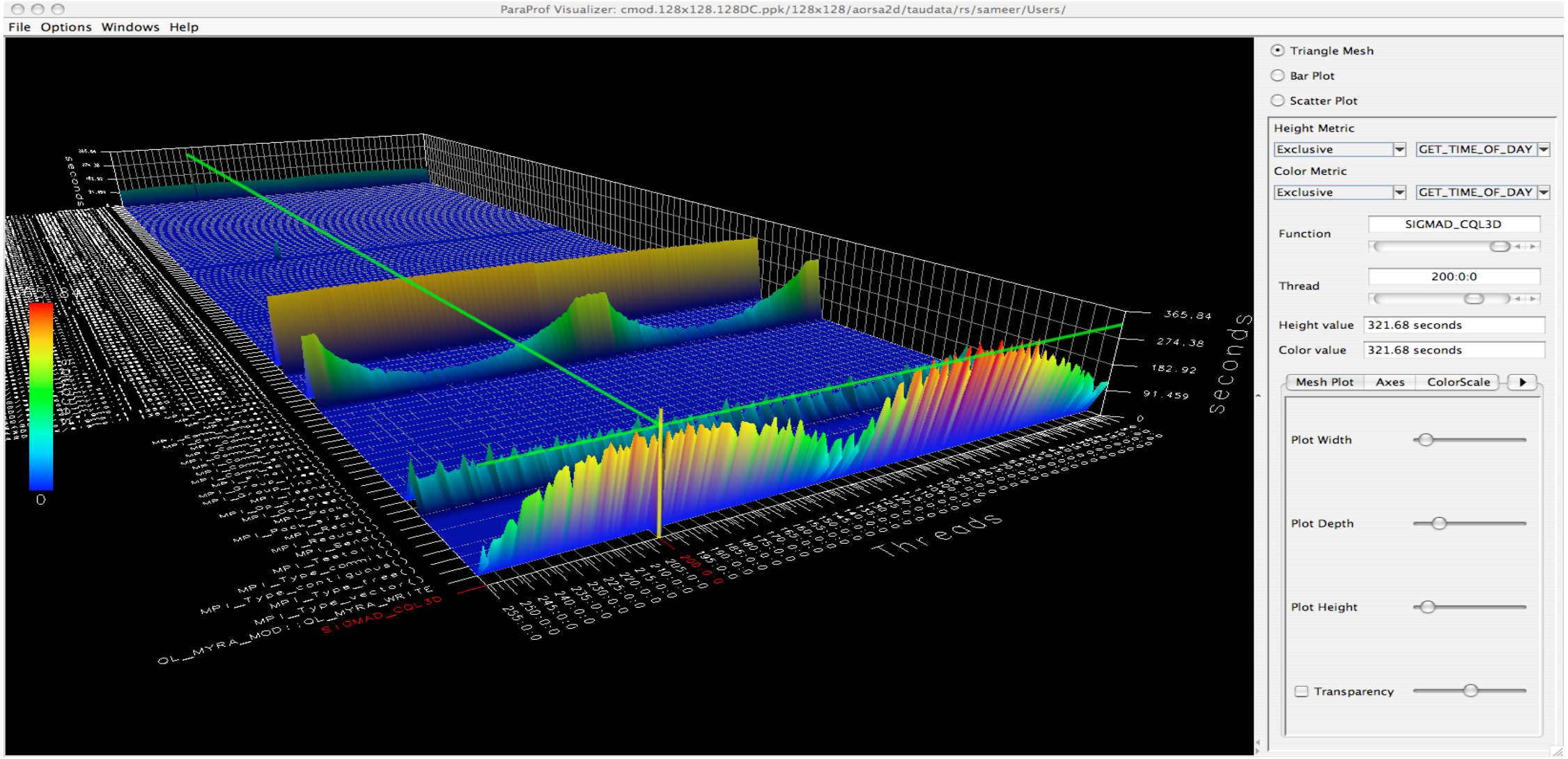
TAU: ParaProf: Context Events for thread: n,c,t, 1,0,0 – samarc_obe_4p_iomem_cp.ppk

Name	Total	MeanValue	NumSamples	MinValue	MaxValue	Std. Dev.
.TAU application						
read()						
fopen64()						
fclose()						
OurMain()						
malloc size	25,235	1,097.174	23	11	12,032	2,851.143
free size	22,707	1,746.692	13	11	12,032	3,660.642
OurMain [{wrapper.py}{3}]						
read()						
malloc size	3,877	323.083	12	32	981	252.72
free size	1,536	219.429	7	32	464	148.122
fopen64()						
fclose()						
<module> [{obe.py}{8}]						
writeRestartData [{samarcInterface.py}{145}]						
samarcWriteRestartData						
write()						
WRITE Bandwidth (MB/s) <file="samarc/restore.00002/nodes.00004/proc.00001">		74.565	117	0	2,156.889	246.386
WRITE Bandwidth (MB/s) <file="samarc/restore.00001/nodes.00004/proc.00001">		77.594	117	0	1,941.2	228.366
WRITE Bandwidth (MB/s)		76.08	234	0	2,156.889	237.551
Bytes Written <file="samarc/restore.00002/nodes.00004/proc.00001">	2,097,552	17,927.795	117	1	1,048,576	133,362.946
Bytes Written <file="samarc/restore.00001/nodes.00004/proc.00001">	2,097,552	17,927.795	117	1	1,048,576	133,362.946
Bytes Written	4,195,104	17,927.795	234	1	1,048,576	133,362.946
open64()						

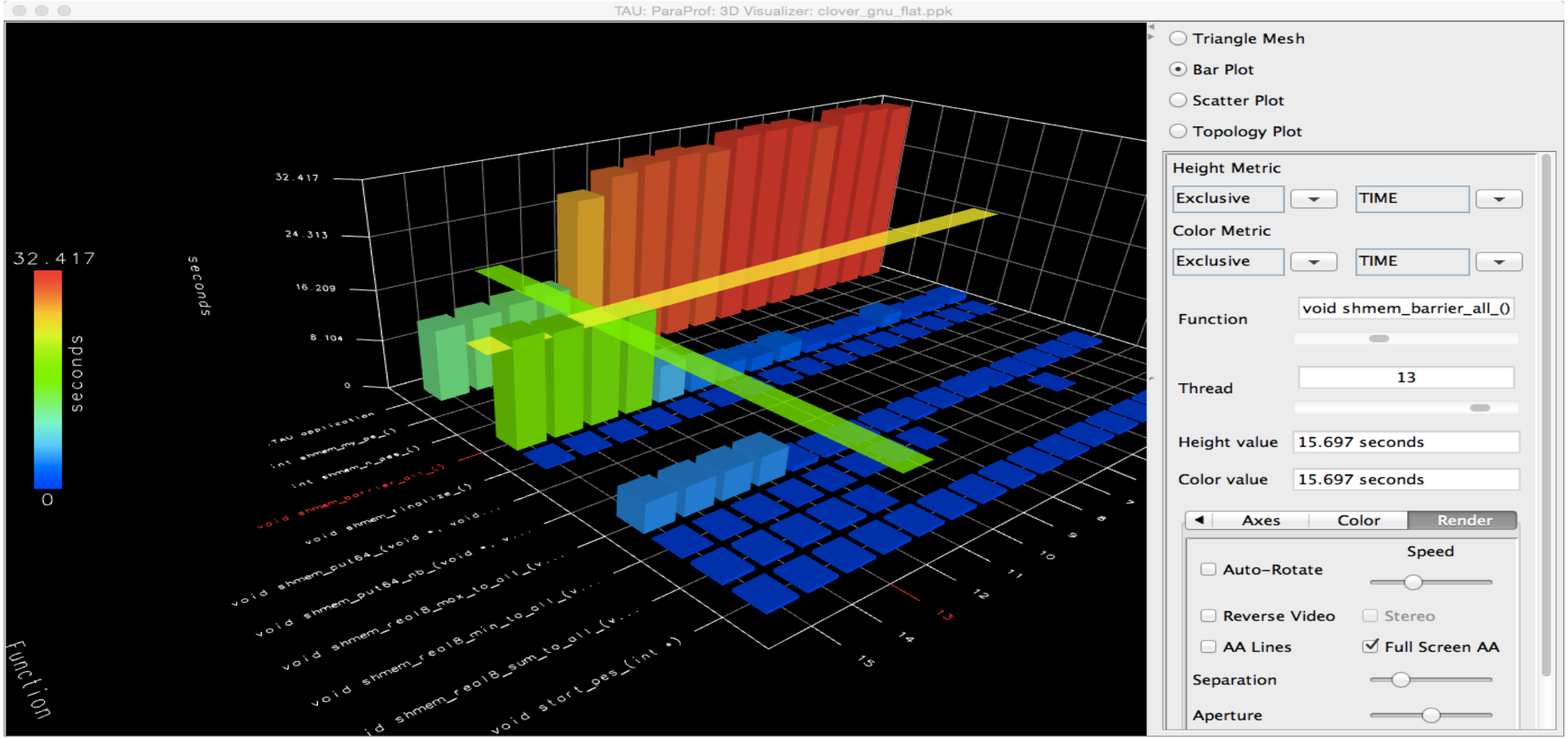
Write bandwidth per file

Bytes written to each file

ParaProf 3D Profile Browser

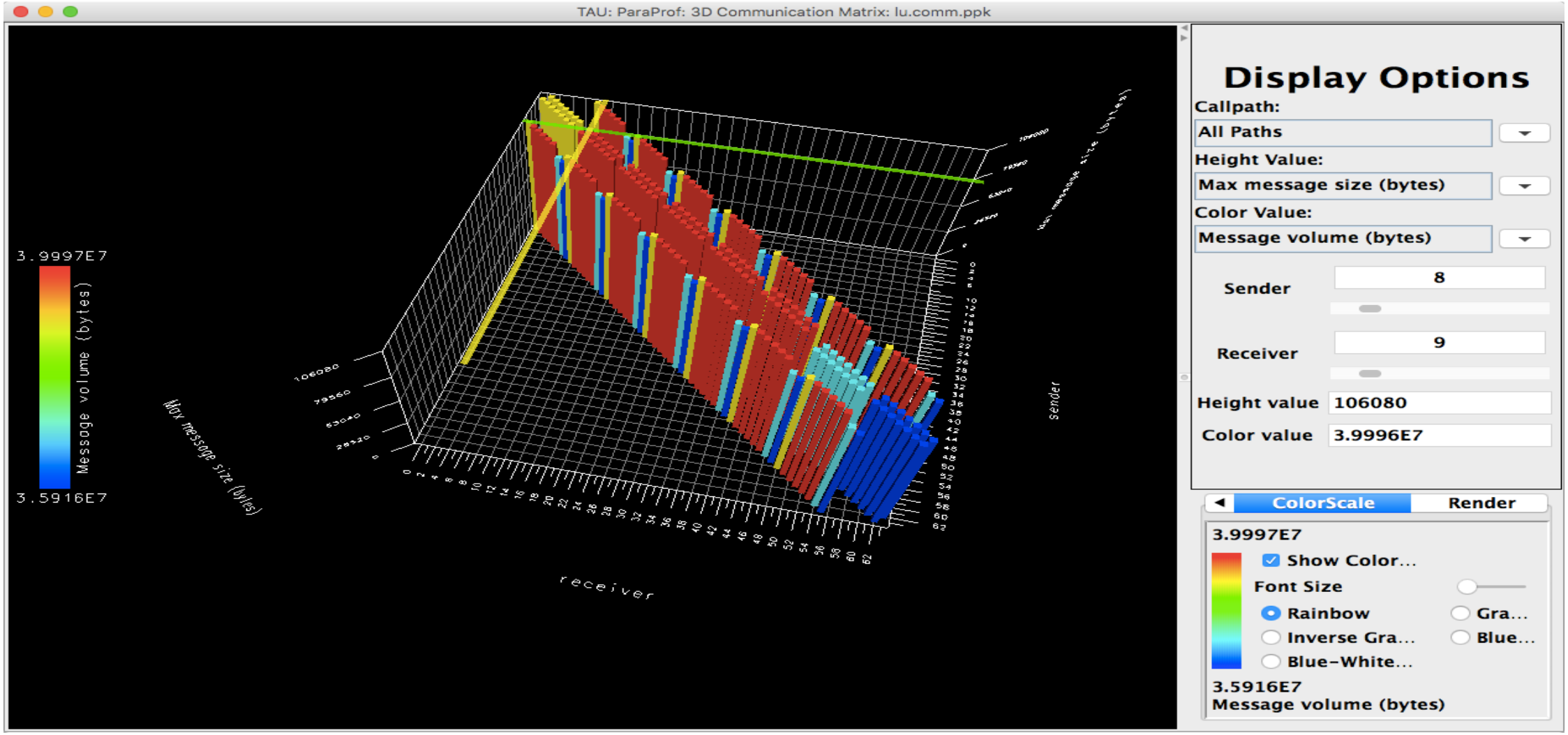


TAU – ParaProf 3D Visualization



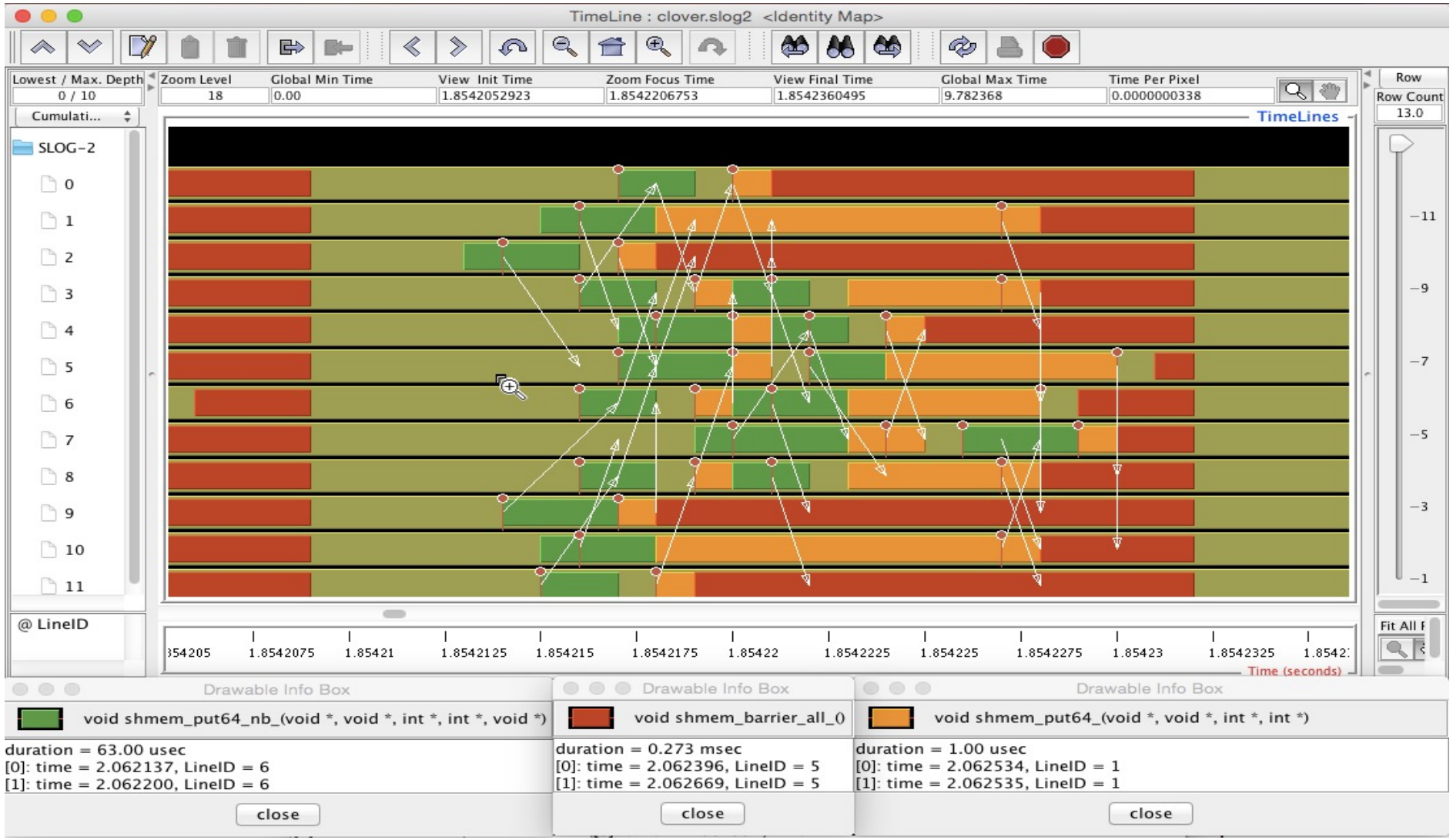
% paraprof app.ppk
Windows -> 3D Visualization -> Bar Plot (right pane)

TAU – 3D Communication Window



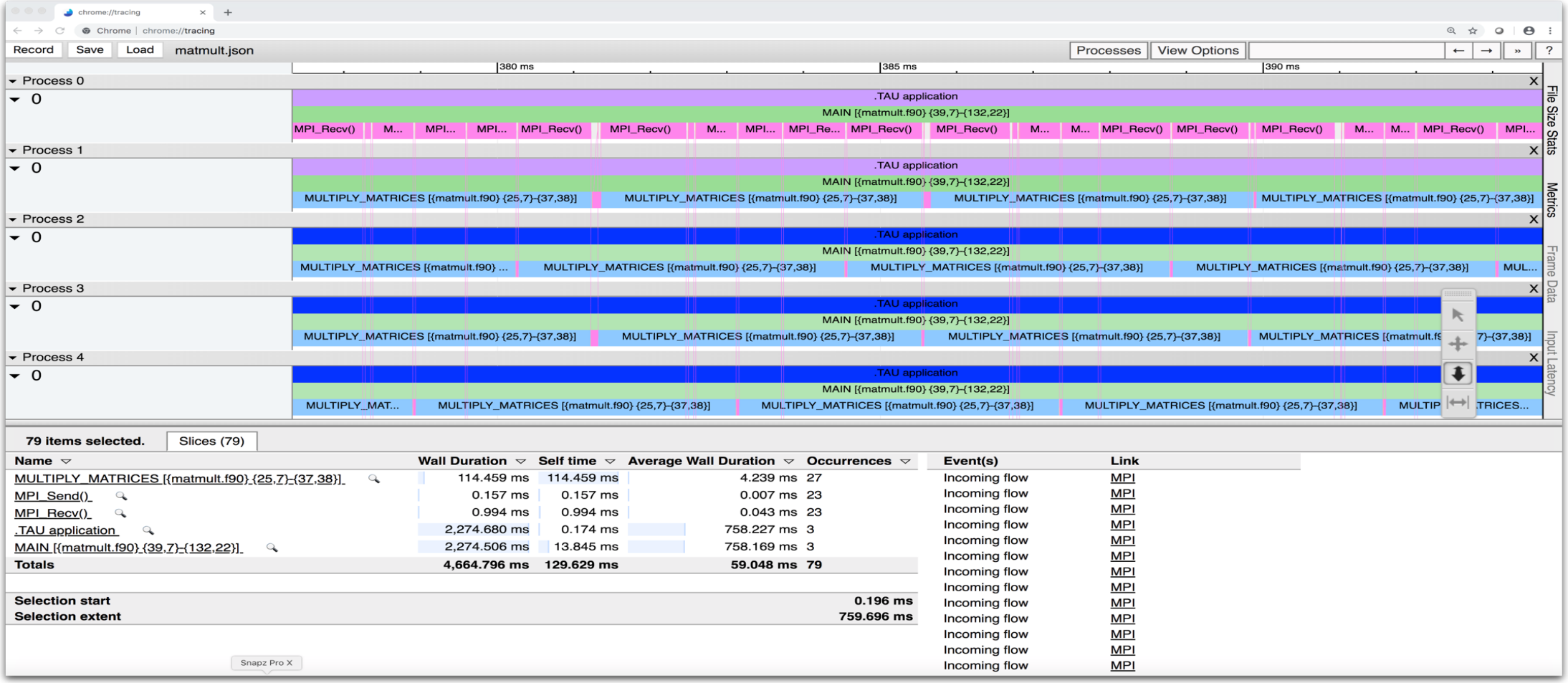
% export TAU_COMM_MATRIX=1; aprun … tau_exec ./a.out
% paraprof ; Windows -> 3D Communication Matrix

Tracing: Jumpshot (ships with TAU)



EXASCALE COMPUTING PROJECT

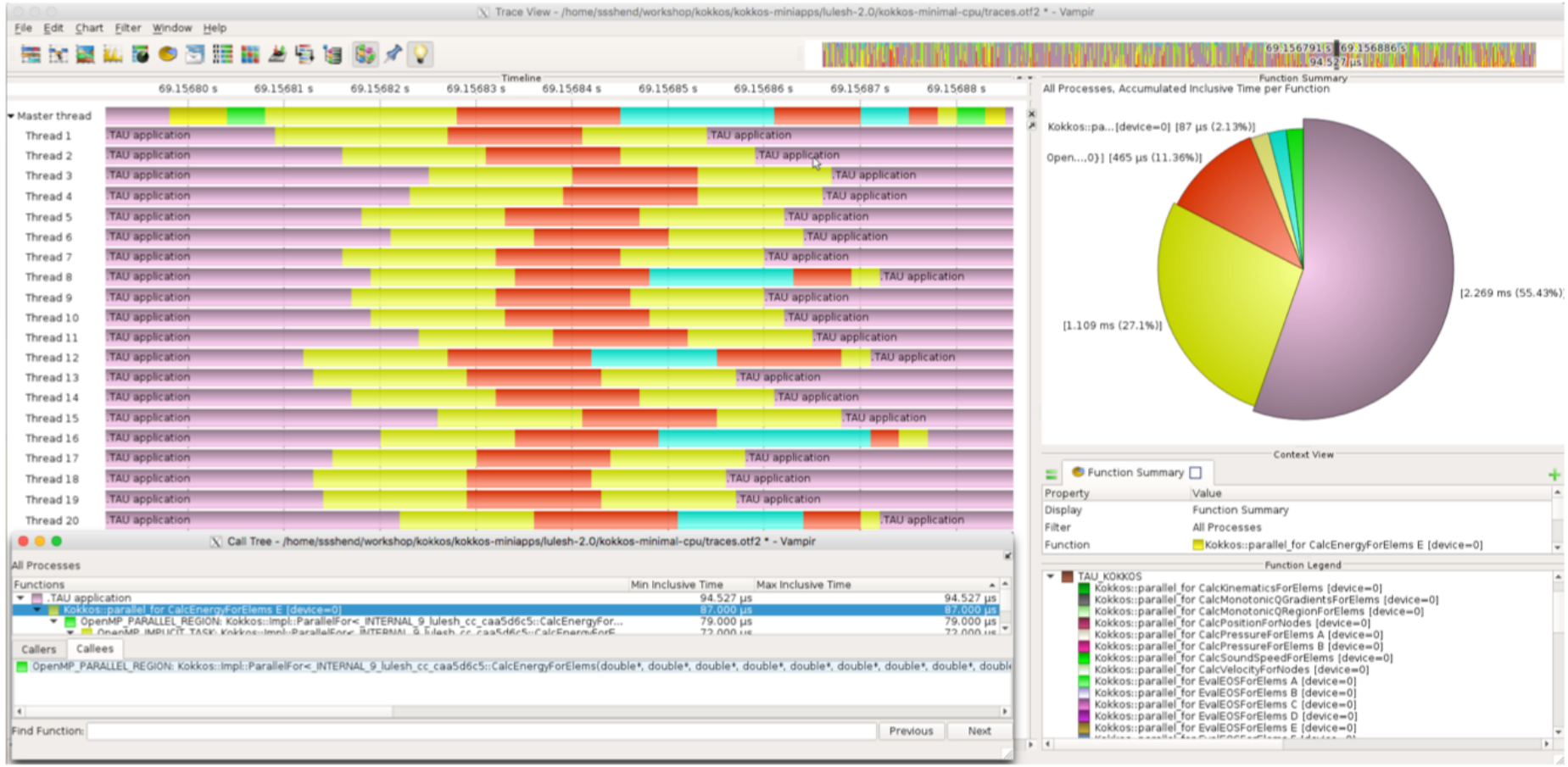
Tracing: Chrome Browser



% export TAU_TRACE=1
% aprun –np 256 tau_exec ./a.out
% tau_treemerge.pl; tau_trace2json tau.trc tau.edf –chrome –ignoreatomic –o app.json

Chrome browser: chrome://tracing (Load -> app.json)

Vampir [TU Dresden] Timeline: Kokkos




```
% export TAU_TRACE=1; export TAU_TRACE_FORMAT=otf2
% tau_exec –ompt  ./a.out
% vampir traces.otf2 &
```

Kokkos

- Provides abstractions for node level parallelism (X in MPI+X)
- Productive, portable, and performant shared-memory programming model
- Helps you create single source performance portable codes
- Provides data abstractions
- C++ API for expressing parallelism in your program
- Aggressive compiler transformations using C++ templates
- Low level code targets backends such as OpenMP, Pthread, CUDA
- Creates a problem for performance evaluation tools
- Gap: performance data and higher-level abstractions
- Solution: Kokkos profiling API for mapping performance data

Kokkos API use in ExaMiniMD

20. sameer@pegasus:~/pkgs/ORNL/DEMO/BUILD/ExaMiniMD-pthread/ExaMiniMD/src/comm_types (ssh)

```
void CommMPI::update_halo() {

  Kokkos::Profiling::pushRegion("Comm::update_halo");

  N_ghost = 0;
  s=*system;

  pack_buffer_update = t_buffer_update((T_X_FLOAT*)pack_buffer.data(),pack_indicies_all.extent(1));
  unpack_buffer_update = t_buffer_update((T_X_FLOAT*)unpack_buffer.data(),pack_indicies_all.extent(1));

  for(phase = 0; phase<6; phase++) {
    pack_indicies = Kokkos::subview(pack_indicies_all,phase,Kokkos::ALL());
    if(proc_grid[phase/2]>1) {

      Kokkos::parallel_for("CommMPI::halo_update_pack",
         Kokkos::RangePolicy<TagHaloUpdatePack, Kokkos::IndexType<T_INT> >(0,proc_num_send[phase]),
         *this);
      MPI_Request request;
      MPI_Status status;
      MPI_Irecv(unpack_buffer.data(),proc_num_recv[phase]*sizeof(T_X_FLOAT)*3/sizeof(int),MPI_INT, proc_neighbors_recv[phase],100002,MPI_COMM_WORLD,&request);
      MPI_Send (pack_buffer.data(),proc_num_send[phase]*sizeof(T_X_FLOAT)*3/sizeof(int),MPI_INT, proc_neighbors_send[phase],100002,MPI_COMM_WORLD);
      s = *system;
      MPI_Wait(&request,&status);
      const int count = proc_num_recv[phase];
      if(unpack_buffer_update.extent(0)<count) {
        unpack_buffer_update = t_buffer_update((T_X_FLOAT*)unpack_buffer.data(),count);
      }
      Kokkos::parallel_for("CommMPI::halo_update_unpack",
                Kokkos::RangePolicy<TagHaloUpdateUnpack, Kokkos::IndexType<T_INT> >(0,proc_num_recv[phase]),
                *this);

    } else {
      //printf("HaloUpdateCopy: %i %i %i\n",phase,proc_num_send[phase],pack_indicies.extent(0));
      Kokkos::parallel_for("CommMPI::halo_update_self",
        Kokkos::RangePolicy<TagHaloUpdateSelf, Kokkos::IndexType<T_INT> >(0,proc_num_send[phase]),
        *this);
    }
    N_ghost += proc_num_recv[phase];
  }

  Kokkos::Profiling::popRegion();
};
```

pushRegion("Comm::update_halo")

Kokkos::parallel_for

popRegion

ExaMiniMD: TAU Phase

TAU: ParaProf: Statistics for: node 0, thread 0 - examinimd_ompt_phase.ppk

Name	Exclusive TIME	Inclusive TIME	Calls	Child Calls
.TAU application	0.143	96.743	1	832
Comm::exchange	0.001	0.967	6	142
Comm::exchange_halo	0.001	4.702	6	184
Comm::update_halo	0.004	31.347	95	1,330
Kokkos::parallel_for CommMPI::halo_update_pack [device=0]	0.002	0.506	190	190
Kokkos::parallel_for CommMPI::halo_update_self [device=0]	0.003	0.597	380	380
Kokkos::parallel_for CommMPI::halo_update_unpack [device=0]	0.002	0.97	190	190
MPI_Irecv()	0.001	0.001	190	0
MPI_Send()	29.268	29.268	190	0
MPI_Wait()	0.001	0.001	190	0
OpenMP_Implicit_Task	0.041	1.985	760	760
OpenMP_Parallel_Region parallel_for<Kokkos::RangePolicy<CommMPI::Ta	0	0.504	190	190
OpenMP_Parallel_Region parallel_for<Kokkos::RangePolicy<CommMPI::Ta	0.08	0.968	190	190
OpenMP_Parallel_Region void Kokkos::parallel_for<Kokkos::RangePolicy<(	0.001	0.594	380	380
OpenMP_Sync_Region_Barrier parallel_for<Kokkos::RangePolicy<CommMI	0.489	0.489	190	0
OpenMP_Sync_Region_Barrier parallel_for<Kokkos::RangePolicy<CommMI	0.875	0.875	190	0
OpenMP_Sync_Region_Barrier void Kokkos::parallel_for<Kokkos::RangePol	0.58	0.58	380	0

Comm::update_halo phase in TAU ParaProf's Thread Statistics Table

ExaMiniMD: ParaProf Node Window

TAU: ParaProf: node 0, thread 0 - examinimd_ompt_phase.ppk Phase: Comm::update_halo

Phase: Comm::update_halo
Metric: TIME
Value: Exclusive
Units: seconds

29.268	MPI_Send()
0.875	OpenMP_Sync_Region_Barrier parallel_for<Kokkos::RangePolicy<CommMPI::TagHaloUpdateUnpack, Kokkos::IndexType<int> >, CommMPI> [{/home/u
0.58	OpenMP_Sync_Region_Barrier void Kokkos::parallel_for<Kokkos::RangePolicy<CommMPI::TagHaloUpdateSelf, Kokkos::IndexType<int> >, CommMPI>(I
0.489	OpenMP_Sync_Region_Barrier parallel_for<Kokkos::RangePolicy<CommMPI::TagHaloUpdatePack, Kokkos::IndexType<int> >, CommMPI> [{/home/user
0.08	OpenMP_Parallel_Region parallel_for<Kokkos::RangePolicy<CommMPI::TagHaloUpdateUnpack, Kokkos::IndexType<int> >, CommMPI> [{/home/users/
0.041	OpenMP_Implicit_Task
0.004	Comm::update_halo
0.003	Kokkos::parallel_for CommMPI::halo_update_self [device=0]
0.002	Kokkos::parallel_for CommMPI::halo_update_unpack [device=0]
0.002	Kokkos::parallel_for CommMPI::halo_update_pack [device=0]
7.8E-4	MPI_Wait()
7.2E-4	MPI_Irecv()
6.9E-4	OpenMP_Parallel_Region void Kokkos::parallel_for<Kokkos::RangePolicy<CommMPI::TagHaloUpdateSelf, Kokkos::IndexType<int> >, CommMPI>(Kokk
4.4E-4	OpenMP_Parallel_Region parallel_for<Kokkos::RangePolicy<CommMPI::TagHaloUpdatePack, Kokkos::IndexType<int> >, CommMPI> [{/home/users/sa

Event-based Sampling (EBS): CabanaMD on an IBM AC922 with NVIDIA V100 GPUs

TAU: ParaProf: Statistics for: node 0, thread 0 - cabana.ppk

Name	Exclusive...	Inclusive...	Calls	Child Calls
.TAU application	0.655	5.132	1	2,424
Comm::update_halo	0.129	1.634	95	21,755
[CONTEXT] Comm::update_halo	0	0.12	3	0
[SAMPLE] __strlen_power8 [{} {0}]	0.09	0.09	2	0
[SAMPLE] Kokkos::Impl::SharedAllocationRecord<void, void>::increment(Kokkos::Impl::SharedAllocationRecord<void, void>*) [{/g/g20/reeve5/bin/CabanaMD}	0.03	0.03	1	0
cudaDeviceSynchronize	0.991	0.991	3,043	0
[CONTEXT] .TAU application	0	0.54	18	0
[SUMMARY] LAMMPS_RandomVelocityGeom::reset(int, double*) [{/g/g20/reeve5/pr/CabanaMD/src/input.h}]	0.27	0.27	9	0
[SAMPLE] LAMMPS_RandomVelocityGeom::reset(int, double*) [{/g/g20/reeve5/pr/CabanaMD/src/input.h} {128}]	0.09	0.09	3	0
[SAMPLE] LAMMPS_RandomVelocityGeom::reset(int, double*) [{/g/g20/reeve5/pr/CabanaMD/src/input.h} {129}]	0.09	0.09	3	0
[SAMPLE] LAMMPS_RandomVelocityGeom::reset(int, double*) [{/g/g20/reeve5/pr/CabanaMD/src/input.h} {130}]	0.06	0.06	2	0
[SAMPLE] LAMMPS_RandomVelocityGeom::reset(int, double*) [{/g/g20/reeve5/pr/CabanaMD/src/input.h} {140}]	0.03	0.03	1	0
[SUMMARY] Input::create_lattice(Comm*) [{/g/g20/reeve5/pr/CabanaMD/src/input.cpp}]	0.15	0.15	5	0
[SAMPLE] Input::create_lattice(Comm*) [{/g/g20/reeve5/pr/CabanaMD/src/input.cpp} {745}]	0.03	0.03	1	0
[SAMPLE] Input::create_lattice(Comm*) [{/g/g20/reeve5/pr/CabanaMD/src/input.cpp} {665}]	0.03	0.03	1	0
[SAMPLE] Input::create_lattice(Comm*) [{/g/g20/reeve5/pr/CabanaMD/src/input.cpp} {721}]	0.03	0.03	1	0
[SAMPLE] Input::create_lattice(Comm*) [{/g/g20/reeve5/pr/CabanaMD/src/input.cpp} {713}]	0.03	0.03	1	0
[SAMPLE] Input::create_lattice(Comm*) [{/g/g20/reeve5/pr/CabanaMD/src/input.cpp} {714}]	0.03	0.03	1	0
[SAMPLE] reference<unsigned int, unsigned int, unsigned int> [{/g/g20/reeve5/build_v100/install/kokkos/include/impl/Kokkos_ViewMapping.hpp} {2740}]	0.06	0.06	2	0
[SAMPLE] unsigned long Kokkos::Impl::ViewOffset<Kokkos::Impl::ViewDimension<0ul, 16ul, 3ul>, Kokkos::LayoutCabanaSlice<176, 16, 3, 0, 0, 0, 0, 0>, void>::	0.03	0.03	1	0
[SUMMARY] LAMMPS_RandomVelocityGeom::uniform() [{/g/g20/reeve5/pr/CabanaMD/src/input.h}]	0.03	0.03	1	0
[SAMPLE] LAMMPS_RandomVelocityGeom::uniform() [{/g/g20/reeve5/pr/CabanaMD/src/input.h} {93}]	0.03	0.03	1	0
Comm::exchange	0.024	0.392	6	3,371
MPI_Finalize()	0.367	0.369	1	68
Comm::exchange_halo	0.026	0.351	6	4,772
MPI_Init()	0.323	0.323	1	0
Cabana::Verlet	0.004	0.256	6	438
Kokkos::parallel_for ForceLJCabanaNeigh::compute [device=0]	0.002	0.164	101	606
MPI_Allreduce()	0.082	0.082	39	0
[CONTEXT] MPI_Allreduce()	0	0.09	3	0
[SAMPLE] __GI___sched_yield [{} {0}]	0.03	0.03	1	0
[SAMPLE] pthread_spin_unlock [{/usr/lib64/libpthread-2.17.so} {0}]	0.03	0.03	1	0
[SAMPLE] pthread_spin_lock [{/usr/lib64/libpthread-2.17.so} {0}]	0.03	0.03	1	0
Kokkos::parallel_for Kokkos::View::initialization [device=0]	0.001	0.072	35	170
Kokkos::parallel_for Kokkos::ViewFill-3D [device=0]	0.001	0.047	101	303
Kokkos::parallel_reduce ForceLJCabanaNeigh::compute_energy [device=0]	0	0.042	11	77
cudaLaunchKernel	0.015	0.028	527	1,581

Kokkos sample within Comm::update_halo

Kokkos sample within top-level application code

Instrumented Kokkos::parallel_for

Instrumented Kokkos::parallel_reduce

Event-based sampling (EBS) with Kokkos API

CabanaMD: CUDA Events

TAU: ParaProf: Function Data Window: cabana.ppk

Phase: .TAU application
Name: void Kokkos::Impl::cuda_parallel_launch_constant_memory<Kokkos::Impl::ParallelFor<ForceLJ<Cabana::VerletList<Kokkos::Device<Kokkos::Cuda, Kokkos::CudaUVMSpace>, Cabana::FullNeighborTag, Cabana::VerletLayout2D> >, Kokkos::RangePolicy<ForceLJ<Cabana::VerletList<Kokkos::Device<Kokkos::Cuda, Kokkos::CudaUVMSpace>, Cabana::FullNeighborTag, Cabana::VerletLayout2D> >::TagFullNeigh, Kokkos::IndexType<int> >, Kokkos::Cuda> >()
Metric Name: TAUGPU_TIME
Value: Exclusive
Units: microseconds

152387	max
151120	min
449.383	std. dev.
151787.562	mean
151120	node 0, thread 1
151807	node 1, thread 1
152387	node 2, thread 1
151836	node 3, thread 1

TAU's Support for Runtime Systems

MPI

- PMPI profiling interface
- MPI_T tools interface using performance and control variables

Pthread

- Captures time spent in routines per thread of execution

OpenMP

- OMPT tools interface to track salient OpenMP runtime events
- Opari source rewriter
- Preloading wrapper OpenMP runtime library when OMPT is not supported

OpenACC

- OpenACC instrumentation API
- Track data transfers between host and device (per-variable)
- Track time spent in kernels

TAU's Support for Runtime Systems (contd.)

OpenCL

- OpenCL profiling interface
- Track timings of kernels

CUDA

- Cuda Profiling Tools Interface (CUPTI)
- Track data transfers between host and GPU
- Track access to uniform shared memory between host and GPU

ROCm

- Rocprofiler and Roctracer instrumentation interfaces
- Track data transfers and kernel execution between host and GPU

Kokkos

- Kokkos profiling API
- Push/pop interface for region, kernel execution interface

Python

- Python interpreter instrumentation API
- Tracks Python routine transitions as well as Python to C transitions

Examples of Multi-Level Instrumentation

MPI + OpenMP

MPI_T + PMPI + OMPT may be used to track MPI and OpenMP

MPI + CUDA

PMPI + CUPTI interfaces

OpenCL + ROCm

Rocprofiler + OpenCL instrumentation interfaces

Kokkos + OpenMP

Kokkos profiling API + OMPT to transparently track events

Kokkos + pthread + MPI

Kokkos + pthread wrapper interposition library + PMPI layer

Python + CUDA + MPI

Python + CUPTI + pthread profiling interfaces (e.g., Tensorflow, PyTorch) + MPI

MPI + OpenCL

PMPI + OpenCL profiling interfaces

TAU Execution Command (tau_exec)

Uninstrumented execution

```
% aprun -n 256  ./a.out
```

Track GPU operations

```
% aprun –np 256  tau_exec –rocm ./a.out
% aprun –np 256  tau_exec –cupti ./a.out
% aprun –np 256 tau_exec –opencl ./a.out
% aprun  -np 256 tau_exec –l0 ./a.out
% aprun –np 256 tau_exec –openacc ./a.out
```

Track MPI performance

```
% aprun -n 256   tau_exec ./a.out
```

Track I/O, and MPI performance (MPI enabled by default)

```
% aprun -n 256  tau_exec -io  ./a.out
```

Track OpenMP and MPI execution (using OMPT for Intel v19+ or Clang 8+)

```
% export TAU_OMPT_SUPPORT_LEVEL=full;
% aprun –np 256  tau_exec –T ompt,v5,mpi  -ompt  ./a.out
```

Track memory operations

```
% export TAU_TRACK_MEMORY_LEAKS=1
% aprun –np 256 tau_exec –memory_debug ./a.out (bounds check)
```

Use event based sampling (compile with –g)

```
% aprun –np 256 tau_exec –ebs ./a.out
```

Also -ebs_source=<PAPI_COUNTER> -ebs_period=<overflow_count> -ebs_resolution=<file | function | line>

tau_exec

```
$ tau_exec

Usage: tau_exec [options] [--] <exe> <exe options>

Options:
        -v             Verbose mode
        -s             Show what will be done but don't actually do anything (dryrun)
        -qsub          Use qsub mode (BG/P only, see below)
        -io            Track I/O
        -memory        Track memory allocation/deallocation
        -memory_debug Enable memory debugger
        -cuda          Track GPU events via CUDA
        -cupti         Track GPU events via CUPTI (Also see env. variable TAU_CUPTI_API)
        -opencl        Track GPU events via OpenCL
        -openacc       Track GPU events via OpenACC (currently PGI only)
        -ompt          Track OpenMP events via OMPT interface
        -armci         Track ARMCI events via PARMCI
        -ebs           Enable event-based sampling
        -ebs_period=<count> Sampling period (default 1000)
        -ebs_source=<counter> Counter (default itimer)
        -um           Enable Unified Memory events via CUPTI
        -T <DISABLE,GNU,ICPC,MPI,OMPT,OPENMP,PAPI,PDT,PROFILE,PTHREAD,
           SCOREP,SERIAL>
           : Specify TAU tags
        -loadlib=<file.so>   : Specify additional load library
        -XrunTAUsh-<options> : Specify TAU library directly
        -gdb           Run program in the gdb debugger

Notes:
           Defaults if unspecified: -T MPI
           MPI is assumed unless SERIAL is specified
```

tau_exec
- preloads the TAU wrapper libraries and performs measurements

No need to recompile the application!

tau_exec Example (continued)

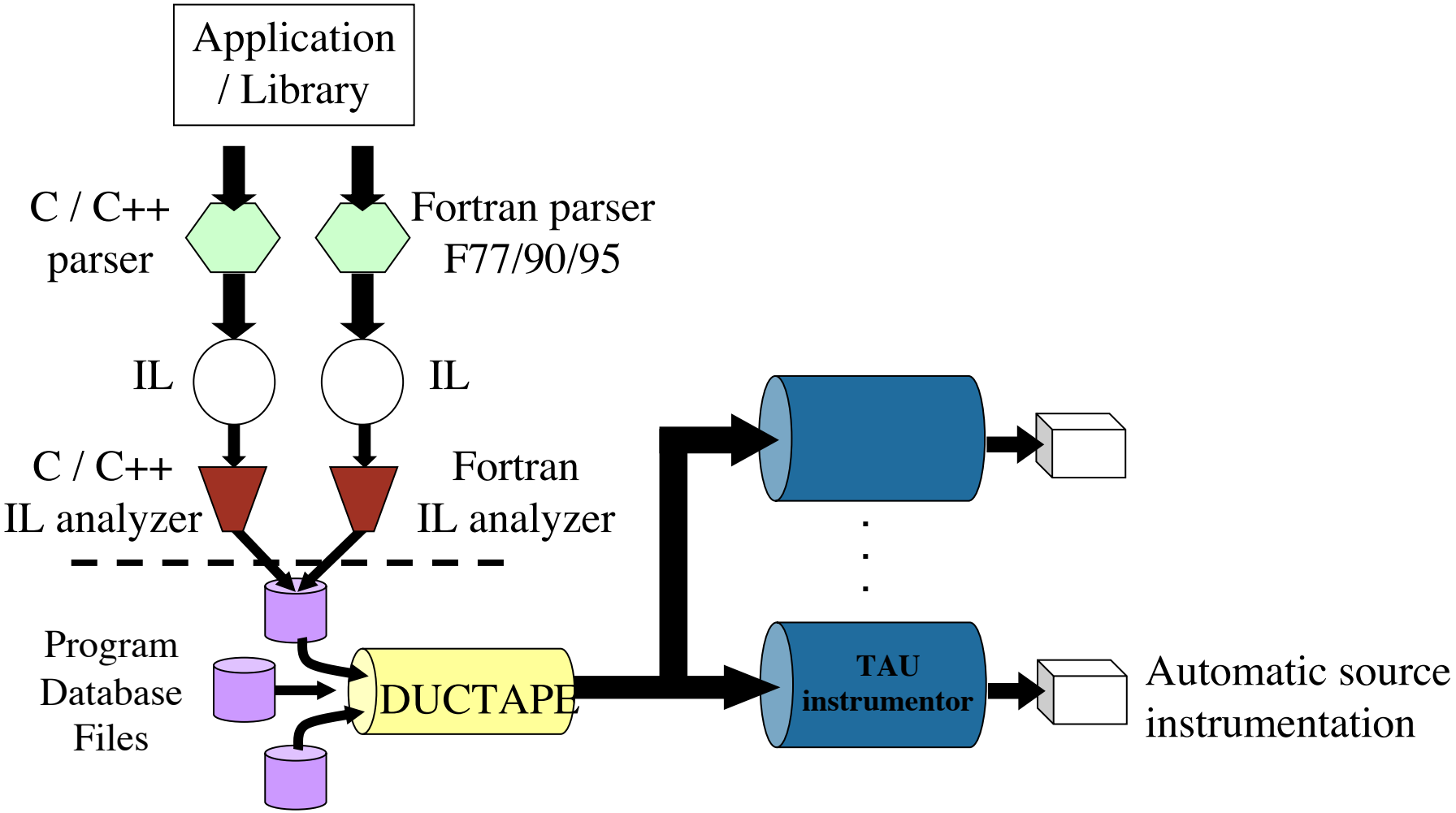
```
Example:
    aprun -np 2 tau_exec -T icpc,ompt,mpi  -ompt ./a.out
    aprun -n  2 tau_exec -io ./a.out
Example - event-based sampling with samples taken every 1,000,000 FP instructions
    aprun -n  8 tau_exec -ebs -ebs_period=1000000 -ebs_source=PAPI_FP_INS ./ring
Examples - GPU:
    tau_exec -T serial,cupti -cupti ./matmult (Preferred for CUDA 4.1 or later)
    tau_exec -openacc ./a.out
    tau_exec -T serial -opencl ./a.out (OPENCL)
    aprun -np 2 tau_exec -T mpi,cupti,papi -cupti -um ./a.out (Unified Virtual Memory in CUDA 6.0+)

qsub mode (IBM BG/Q only):
    Original:
      qsub -n 1 --mode smp -t 10 ./a.out
    With TAU:
      tau_exec -qsub -io -memory -- qsub -n 1 … -t 10 ./a.out

Memory Debugging:
    -memory option:
      Tracks heap allocation/deallocation and memory leaks.
    -memory_debug option:
      Detects memory leaks, checks for invalid alignment, and checks for
      array overflow.  This is exactly like setting TAU_TRACK_MEMORY_LEAKS=1
      and TAU_MEMDBG_PROTECT_ABOVE=1 and running with -memory
```

tau_exec can enable event based sampling while launching the executable using environment var TAU_SAMPLING=1 or tau_exec -ebs

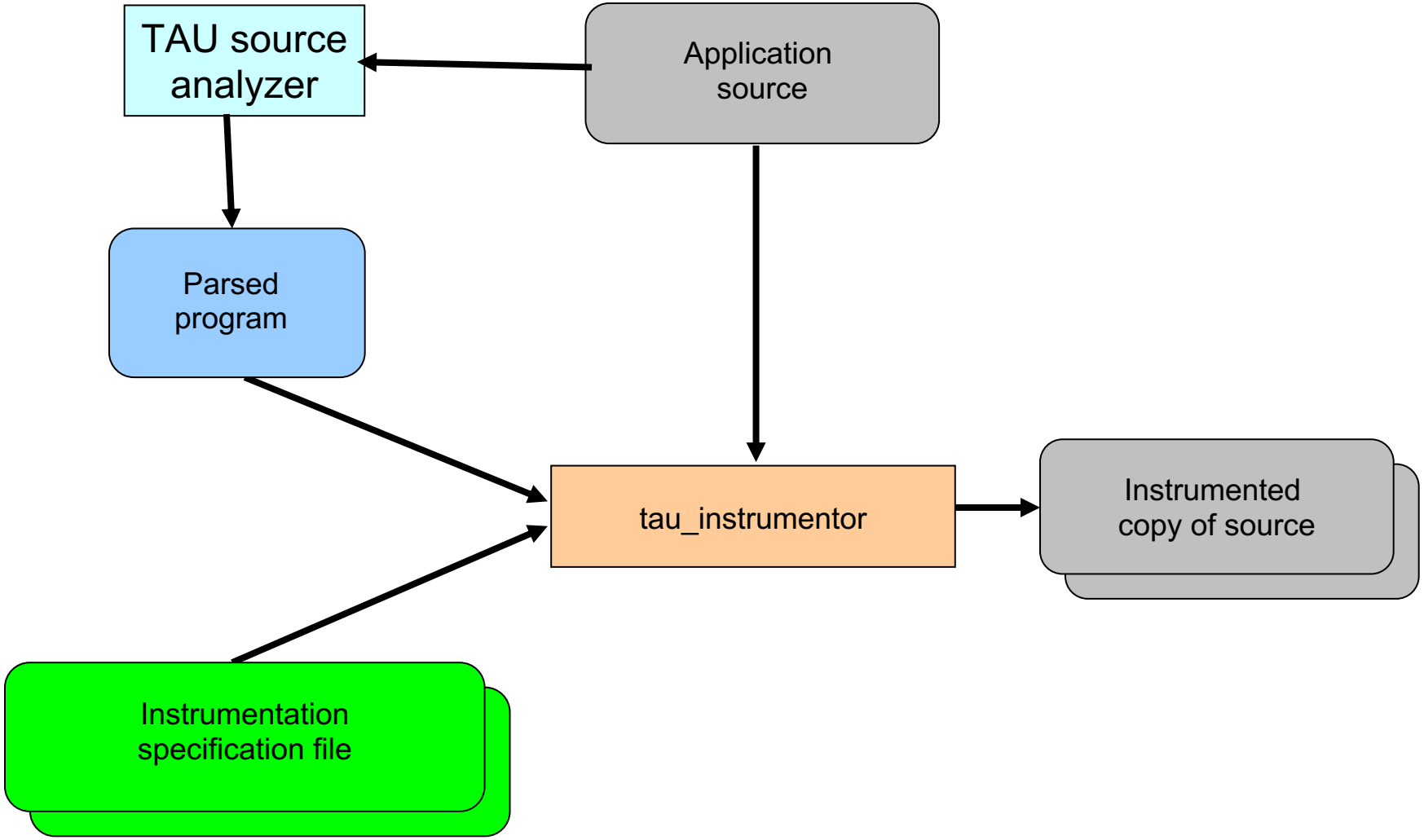
Automatic Source Instrumentation in TAU using PDT

EXASCALE COMPUTING PROJECT

TAU's Static Analysis System: Program Database Toolkit (PDT)



PDT: automatic source instrumentation



Installing TAU

- Installing PDT:
  - wget http://tau.uoregon.edu/pdt_lite.tgz
  - ./configure –prefix=<dir>; make ; make install
- Installing TAU:
  - wget http://tau.uoregon.edu/tau.tgz
  - ./configure -mpi –pdt=<dir> -bfd=download –unwind=download –iowrapper …
  - make install
- Using TAU:
  - export TAU_MAKEFILE=<taudir>/ibm64linux/lib/Makefile.tau-<TAGS>
  - make CC=tau_cc.sh CXX=tau_cxx.sh F90=tau_f90.sh

Installing TAU on Laptops

- Installing TAU under Mac OS X:
  - wget http://tau.uoregon.edu/tau.dmg
  - Install tau.dmg
- Installing TAU under Linux
  - http://tau.uoregon.edu/tau.exe
- Installing TAU under Linux
  - http://tau.uoregon.edu/tau.tgz
- ./configure; make install
- export PATH=<taudir>/x86_64/bin:$PATH

Source Instrumentation in TAU

- TAU supports several compilers, measurement, and thread options
  - Intel, GNU, Clang, PGI compilers, profiling with hardware counters using PAPI, MPI library, OpenMP…
  - Each measurement configuration of orresponds to a unique stub makefile (configuration file) and library that is generated when you configure it
- To instrument source code automatically using PDT
  - Choose an appropriate TAU stub makefile in <arch>/lib:
    - **% module load tau**
    - **% export TAU_MAKEFILE=<tau_root>/**craycnl/lib/Makefile.tau-<options>
    - **% export TAU_OPTIONS= '-optVerbose …' (see tau_compiler.sh)**
  - Use tau_f90.sh, tau_cxx.sh, tau_upc.sh, tau_caf.sh, or tau_cc.sh as F90, C++, UPC, CAF, or C compilers respectively:
    - **% ftn foo.f90 changes to**
    - **% tau_f90.sh foo.f90**
  - Set runtime environment variables, execute application and analyze performance data:
    - **% pprof (for text based profile display)**
    - **% paraprof (for GUI)**

Different Makefiles for TAU Compiler on Summit at ORNL

```
% module load tau
% ls $TAU_DIR/lib/Makefile*
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-5-papi-cupti
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-5-papi-cupti-openmp-opari
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-5-papi-mpi
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-5-papi-mpi-cupti
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-5-papi-mpi-cupti-openmp-opari
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-5-papi-mpi-openmp-opari
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-6-papi-cupti
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-6-papi-cupti-openmp-opari
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-6-papi-mpi
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-6-papi-mpi-cupti
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-6-papi-mpi-cupti-openmp-opari
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-xl_16.1.1-6-papi-mpi-openmp-opari
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-gcc_8.1.1-papi-gnu-cupti
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-gcc_8.1.1-papi-gnu-cupti-pdt
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-gcc_8.1.1-papi-gnu-mpi
/sw/summit/tau/2.29.1/ibm64linux/lib/Makefile.tau-gcc_8.1.1-papi-gnu-mpi-cupti
…
```

Different Makefiles for TAU Compiler on Theta at ALCF

```
% module load tau
% ls $TAU_DIR/lib/Makefile*
/soft/perftools/tau/tau-2.30.1/craycnl/lib/Makefile.tau-intel-papi-mpi-pdt
/soft/perftools/tau/tau-2.30.1/craycnl/lib/Makefile.tau-intel-papi-mpi-pthread-pdt
/soft/perftools/tau/tau-2.30.1/craycnl/lib/Makefile.tau-intel-papi-ompt-v5-mpi-pdt-openmp
/soft/perftools/tau/tau-2.30.1/craycnl/lib/Makefile.tau-intel-papi-ompt-v5-pdt-openmp
/soft/perftools/tau/tau-2.30.1/craycnl/lib/Makefile.tau-intel-papi-pthread-pdt
…
```

Configuration tags for tau_exec

```
% ./configure -pdt=<dir> -mpi -papi=<dir>; make install
```

Creates in <taudir>/<arch>/lib:

```
Makefile.tau-papi-mpi-pdt
shared-papi-mpi-pdt/libTAU.so
```

```
% ./configure -pdt=<dir> -mpi; make install
```
creates

```
Makefile.tau-mpi-pdt
shared-mpi-pdt/libTAU.so
```

To explicitly choose preloading of shared-<options>/libTAU.so change:

```
% aprun -np 8 ./a.out     to
% aprun -np 8 tau_exec -T <comma_separated_options> ./a.out

% aprun -np 8 tau_exec -T papi,mpi,pdt ./a.out
```

Preloads `<taudir>/<arch>/shared-papi-mpi-pdt/libTAU.so`

```
% aprun -np 8 tau_exec -T papi ./a.out
```

Preloads `<taudir>/<arch>/shared-papi-mpi-pdt/libTAU.so by matching.`

```
% aprun -np 8 tau_exec -T papi,mpi,pdt -s ./a.out
```

Does not execute the program. Just displays the library that it will preload if executed without the –s option.
NOTE: -mpi configuration is selected by default. Use –T serial for
Sequential programs.

Compile-Time Options

Optional parameters for the TAU_OPTIONS environment variable:

% tau_compiler.sh

-optVerbose	Turn on verbose debugging messages
-optCompInst	Use compiler based instrumentation
-optNoCompInst	Do not revert to compiler instrumentation if source instrumentation fails.
-optTrackIO	Wrap POSIX I/O call and calculates vol/bw of I/O operations (configure TAU with *–iowrapper*)
-optTrackGOMP	Enable tracking GNU OpenMP runtime layer (used without –opari)
-optMemDbg	Enable runtime bounds checking (see TAU_MEMDBG_* env vars)
-optKeepFiles	Does not remove intermediate .pdb and .inst.* files
-optPreProcess	Preprocess sources (OpenMP, Fortran) before instrumentation
-optTauSelectFile=”<file>"	Specify selective instrumentation file for *tau_instrumentor*
-optTauWrapFile=”<file>"	Specify path to *link_options.tau* generated by *tau_gen_wrapper*
-optHeaderInst	Enable Instrumentation of headers
-optTrackUPCR	Track UPC runtime layer routines (used with tau_upc.sh)
-optLinking=""	Options passed to the linker. Typically $(TAU_MPI_FLIBS) $(TAU_LIBS) $(TAU_CXXLIBS)
-optCompile=""	Options passed to the compiler. Typically $(TAU_MPI_INCLUDE) $(TAU_INCLUDE) $(TAU_DEFS)
-optPdtF95Opts=""	Add options for Fortran parser in PDT (f95parse/gfparse) …

Compile-Time Options (contd.)

Optional parameters for the TAU_OPTIONS environment variable:

% tau_compiler.sh

-optShared	Use TAU's shared library (libTAU.so) instead of static library (default)
-optPdtCxxOpts=""	Options for C++ parser in PDT (cxxparse).
-optPdtF90Parser=""	Specify a different Fortran parser
-optPdtCleanscapeParser	Specify the Cleanscape Fortran parser instead of GNU gfparser
-optTau=""	Specify options to the tau_instrumentor
-optTrackDMAPP	Enable instrumentation of low-level DMAPP API calls on Cray
-optTrackPthread	Enable instrumentation of pthread calls

See tau_compiler.sh for a full list of TAU_OPTIONS.

…

Using TAU_OPTIONS

To use the compiler based instrumentation instead of PDT (source-based):

```
% export TAU_OPTIONS= '-optCompInst -optVerbose'
```

If your Fortran code uses C preprocessor directives (#include, #ifdef, #endif):

```
% export TAU_OPTIONS= '-optPreProcess -optVerbose -optDetectMemoryLeaks'
```

To use an instrumentation specification file:

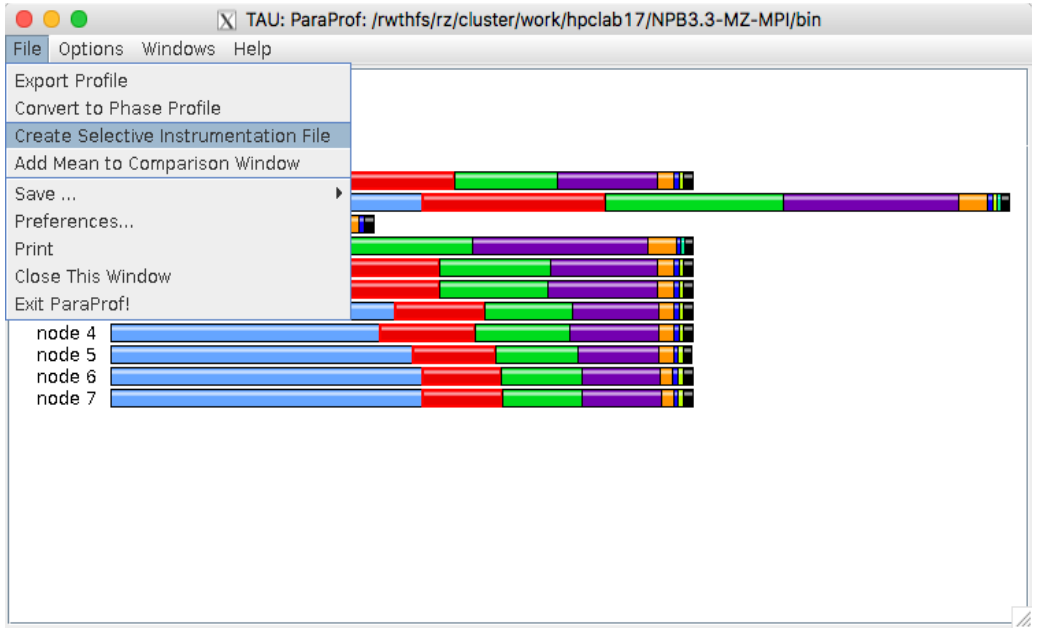
```
% export TAU_OPTIONS= '-optTauSelectFile=select.tau -optVerbose -optPreProcess'
% cat select.tau
BEGIN_INSTRUMENT_SECTION
loops  routine="#"
# this statement instruments all outer loops in all routines. # is wildcard as well as comment in first column.
END_INSTRUMENT_SECTION
```

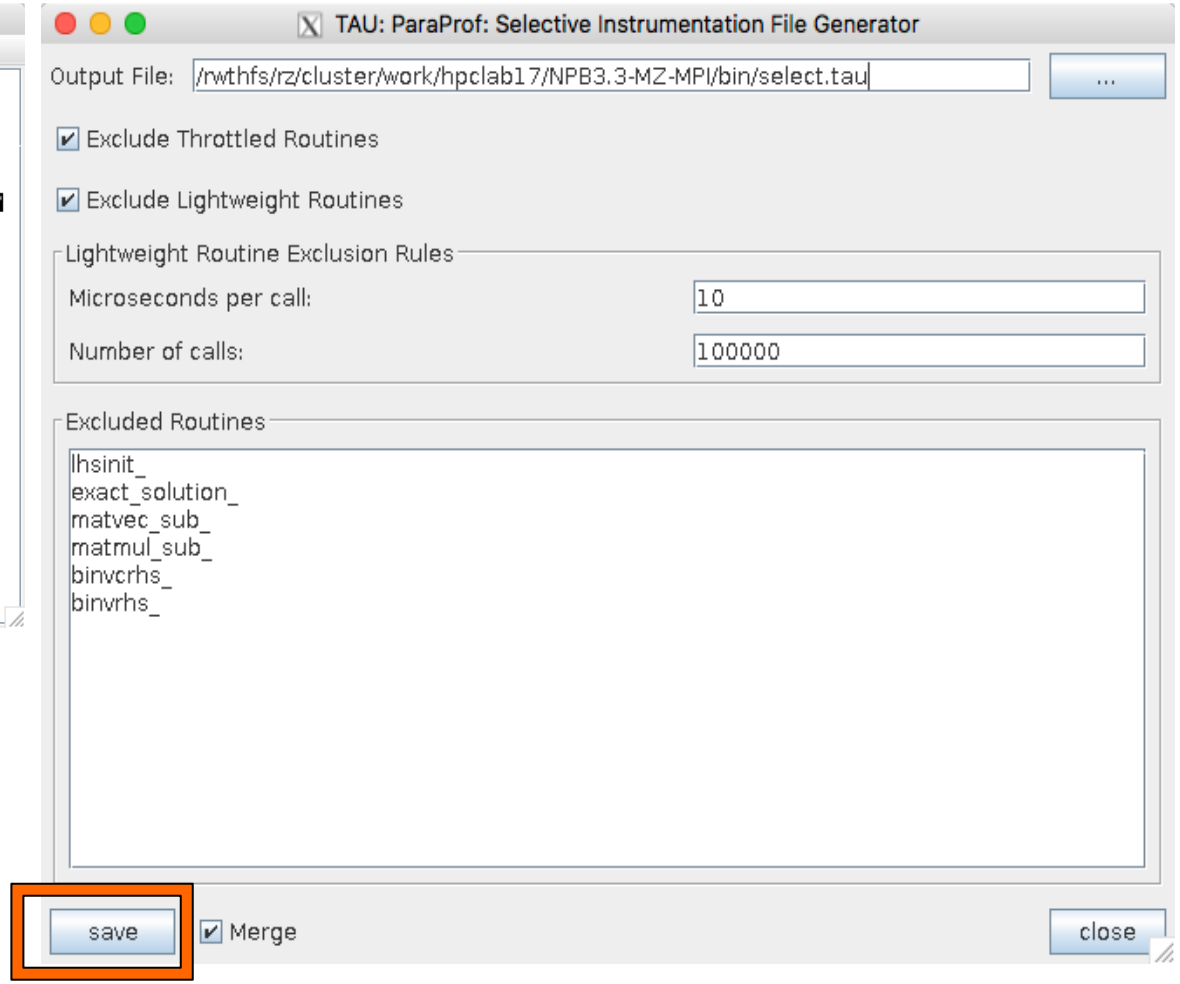
Selective Instrumentation File With Program Database Toolkit (PDT)

To use an instrumentation specification file for source instrumentation:

```
% export TAU_OPTIONS= '-optTauSelectFile=/path/to/select.tau –optVerbose '
% cat select.tau
  BEGIN_EXCLUDE_LIST
  BINVCRHS
  MATMUL_SUB
  MATVEC_SUB
  EXACT_SOLUTION
  BINVRHS
  LHS#INIT
  TIMER_#
  END_EXCLUDE_LIST
NOTE: paraprof can create this file from an earlier execution for you.
File -> Create Selective Instrumentation File -> save
Selective instrumentation at runtime:
% export TAU_SELECT_FILE=select.tau
```

Create a Selective Instrumentation File, Re-instrument, Re-run





TAU's Runtime Environment Variables

Environment Variable	Default	Description
TAU_TRACE	0	Setting to 1 turns on tracing
TAU_CALLPATH	0	Setting to 1 turns on callpath profiling
TAU_TRACK_MEMORY_FOOTPRINT	0	Setting to 1 turns on tracking memory usage by sampling periodically the resident set size and high water mark of memory usage
TAU_TRACK_POWER	0	Tracks power usage by sampling periodically.
TAU_CALLPATH_DEPTH	2	Specifies depth of callpath. Setting to 0 generates no callpath or routine information, setting to 1 generates flat profile and context events have just parent information (e.g., Heap Entry: foo)
TAU_SAMPLING	1	Setting to 1 enables event-based sampling.
TAU_TRACK_SIGNALS	0	Setting to 1 generate debugging callstack info when a program crashes
TAU_COMM_MATRIX	0	Setting to 1 generates communication matrix display using context events
TAU_THROTTLE	1	Setting to 0 turns off throttling. Throttles instrumentation in lightweight routines that are called frequently
TAU_THROTTLE_NUMCALLS	100000	Specifies the number of calls before testing for throttling
TAU_THROTTLE_PERCALL	10	Specifies value in microseconds. Throttle a routine if it is called over 100000 times and takes less than 10 usec of inclusive time per call
TAU_CALLSITE	0	Setting to 1 enables callsite profiling that shows where an instrumented function was called. Also compatible with tracing.
TAU_PROFILE_FORMAT	Profile	Setting to "merged" generates a single file. "snapshot" generates xml format
TAU_METRICS	TIME	Setting to a comma separated list generates other metrics. (e.g., ENERGY,TIME,P_VIRTUAL_TIME,PAPI_FP_INS,PAPI_NATIVE_<event>:<subevent>)

Runtime Environment Variables

Environment Variable	Default	Description
TAU_TRACE	0	Setting to 1 turns on tracing
TAU_TRACE_FORMAT	Default	Setting to “otf2” turns on TAU’s native OTF2 trace generation (configure with –otf=download)
TAU_EBS_UNWIND	0	Setting to 1 turns on unwinding the callstack during sampling (use with tau_exec –ebs or TAU_SAMPLING=1)
TAU_EBS_RESOLUTION	line	Setting to “function” or “file” changes the sampling resolution to function or file level respectively.
TAU_TRACK_LOAD	0	Setting to 1 tracks system load on the node
TAU_SELECT_FILE	Default	Setting to a file name, enables selective instrumentation based on exclude/include lists specified in the file.
TAU_OMPT_SUPPORT_LEVEL	basic	Setting to “full” improves resolution of OMPT TR6 regions on threads 1.. N-1. Also, “lowoverhead” option is available.
TAU_OMPT_RESOLVE_ADDRESS_EAGERLY	1	Setting to 1 is necessary for event based sampling to resolve addresses with OMPT. Setting to 0 allows the user to do offline address translation.

Runtime Environment Variables

Environment Variable	Default	Description
TAU_TRACK_MEMORY_LEAKS	0	Tracks allocates that were not de-allocated (needs –optMemDbg or tau_exec –memory)
TAU_EBS_SOURCE	TIME	Allows using PAPI hardware counters for periodic interrupts for EBS (e.g., TAU_EBS_SOURCE=PAPI_TOT_INS when TAU_SAMPLING=1)
TAU_EBS_PERIOD	100000	Specifies the overflow count for interrupts
TAU_MEMDBG_ALLOC_MIN/MAX	0	Byte size minimum and maximum subject to bounds checking (used with TAU_MEMDBG_PROTECT_*)
TAU_MEMDBG_OVERHEAD	0	Specifies the number of bytes for TAU's memory overhead for memory debugging.
TAU_MEMDBG_PROTECT_BELOW/ABOVE	0	Setting to 1 enables tracking runtime bounds checking below or above the array bounds (requires –optMemDbg while building or tau_exec –memory)
TAU_MEMDBG_ZERO_MALLOC	0	Setting to 1 enables tracking zero byte allocations as invalid memory allocations.
TAU_MEMDBG_PROTECT_FREE	0	Setting to 1 detects invalid accesses to deallocated memory that should not be referenced until it is reallocated (requires –optMemDbg or tau_exec –memory)
TAU_MEMDBG_ATTEMPT_CONTINUE	0	Setting to 1 allows TAU to record and continue execution when a memory error occurs at runtime.
TAU_MEMDBG_FILL_GAP	Undefined	Initial value for gap bytes
TAU_MEMDBG_ALINGMENT	Sizeof(int)	Byte alignment for memory allocations
TAU_EVENT_THRESHOLD	0.5	Define a threshold value (e.g., .25 is 25%) to trigger marker events for min/max

Extreme-scale Scientific Software Stack (E4S)

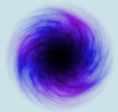
https://e4s.io

EXASCALE COMPUTING PROJECT

E4S: Better Quality, Documentation, Test, Integration, Delivery, Build & Use

Delivering HPC software to facilities, vendors, agencies, industry, international partners in a brand-new way

Community Policies
Commitment to software quality



DocPortal
Single portal to all E4S product info

Portfolio testing
Especially leadership platforms

Curated collection
The end of dependency hell

Quarterly releases
Release 1.2 – November

Build caches
10X build time improvement

Turnkey stack
A new user experience

https://e4s.io

E4S Strategy Group
US agencies, industry, international

E4S: Extreme-scale Scientific Software Stack

- Curated, Spack based software distribution
- Spack binary build caches for bare-metal installs
  - x86_64, ppc64le (IBM Power 9), and aarch64 (ARM64)
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products
- Base images and full featured containers (with GPU support)
- GitHub recipes for creating custom images from base images
- GitLab integration for building E4S images
- E4S validation test suite on GitHub
- E4S-cl container launcher tool for MPI substitution in applications using MPICH ABI
- E4S VirtualBox image with support for container runtimes
  - Docker
  - Singularity
  - Shifter
  - Charliecloud
- AWS and GCP images to deploy E4S

https://e4s.io

Spack is a flexible package manager for HPC

- How to install Spack (works out of the box):

```
$ git clone https://github.com/spack/spack
$ . spack/share/spack/setup-env.sh
```

- How to install a package:

```
$ spack install tau
```

- TAU and its dependencies are installed within the Spack directory.
- Unlike typical package managers, Spack can also install many variants of the same build.
  - Different compilers
  - Different MPI implementations
  - Different build options

Visit spack.io

github.com/spack/spack

@spackpm

Spack provides the *spec* syntax to describe custom configurations

```
$ git clone https://github.com/spack/spack
$ . spack/share/spack/setup-env.sh
$ spack compiler find                                    # set up compilers
$ spack external find                                    # set up external packages
```

```
$ spack install tau                                      unconstrained
$ spack install tau@2.30.1                               @ custom version
$ spack install tau@2.30.1 %gcc@7.3.0                    % custom compiler
$ spack install tau@2.30.1 %gcc@7.3.0 +level_zero        +/- build option
$ spack install tau@2.30.1 %gcc@7.3.0 +mpi ^mvapich2@2.3~wrapperrpath ^ dependency information
```

- Each expression is a ***spec*** for a particular configuration
  - Each clause adds a constraint to the spec
  - Constraints are optional – specify only what you need.
  - Customize install on the command line!
- Spec syntax is recursive
  - Full control over the combinatorial build space

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```
1: adios2       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/adios2-2.6.0-nkp24j7enorn3dt7626chuqm3pbkrvfe
2: aml  /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/aml-0.1.0-3mwyb6cf6ervfnruqb5u33v46buyuqth
3: arborx       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/arborx-0.9-beta-qjzxlkcgplto6pnpjwejoh5xpoik3adr
4: argobots     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/argobots-1.0-yoafg2slps7kp4dkmb6pzu5z2a37sgs4
5: ascent       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ascent-develop-ciwqg6lh6unww3hjsnu47wr7cpqptqgy
6: axom         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/axom-0.3.3-tzyejxpy3p3ekaev35k2bhpkr74cnuhh
7: bolt         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/bolt-1.0-uxku5w5qdfnpa4atgzcbraq7wop7lunc
8: caliper      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/caliper-2.4.0-lfdx3gc6qodg2abbpovib3thdsmsamnn
9: darshan-runtime      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/darshan-runtime-3.2.1-jqugqxx2uunyaduoe3owhd2snves6mlr
10: dyninst     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/dyninst-10.2.1-xad3v6rvosm6qfai5fc7d4nn33svtzzf
11: faodel      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/faodel-1.1906.1-ijilel2vjionmj56mscqkw2hpecfsuym
12: flecsi      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/flecsi-1-c7sevlnc2ak4pf2jgq6wh3mwictch5l2
13: flit        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/flit-2.1.0-yvvog7kmax22ei2yyrwfxj3heinmz5am
14: gasnet      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/gasnet-2020.3.0-ufrq5hym67eq3jsg4jtttjjqgo4i6hnq
15: ginkgo      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ginkgo-1.2.0-r6lorgchpr5qrcwyqqxtewqdhtpi4rmt
16: globalarrays        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/globalarrays-5.7-bow6d32j63j6gusotzjuityznwqvv64b
17: gotcha      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/gotcha-1.0.3-7n7bjnzsnf5w5tnihiok3otbaewdhjmu
18: hdf5        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hdf5-1.10.6-k74avubedd5knvlc73dr3ib5oyw6bcwn
19: hpctoolkit  /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hpctoolkit-2020.08.03-wck4g3h3jhfvzvxorelxqunbe3xsesry
20: hpx         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hpx-1.5.0-pynmocntkmuwkowyo5jxtycvg34w6kue
21: hypre       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/hypre-2.19.0-vqo72wn6ei7ruitpg7drkje2rdbdfguo
22: kokkos      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/kokkos-3.2.00-pqv3uugd6cv3qftyur3rx6dm2gao2tg3
23: kokkos-kernels      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/kokkos-kernels-3.1.00-y4veufypftworlbehxusg4yzh6n7anhp
24: legion      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/legion-20.03.0-zkbz7h2wuze4dgbwcbo4w5fvqltugmog
25: libnrm      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/libnrm-0.1.0-kp5jb7o4kow25rnggiditwtmdbeebojs
26: libquo      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/libquo-1.3.1-w45wcw6dqbiajeeauj3ryaeskqu7bzx6
27: magma       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/magma-2.5.3-yksxthffslhjrhzwgcx7smz2tca6ojfn
28: mercury     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mercury-1.0.1-ppledsr3drk2upciytfsuawfxrtjp73q
29: mfem        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mfem-4.1.0-kivaike2qintplgufwp5yf2mj3n36ay3
30: mpich       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mpich-3.2.1-kgwtpelzobpkrvg24ct6padfbhw7nene
31: mpifileutils        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/mpifileutils-develop-djje5g7ts55g3yic3bms426c2zi7gqsj
32: ninja       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/ninja-1.10.1-7zbbtuslw25nmqo4ur6abyyf3tchnqvv
33: omega-h     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/omega-h-9.29.0-eln73w7ytpvgqtkmkqyjm4gsabsu2w4p
```

- 67 ECP ST products
- Ubuntu v18.04 x86_64
- AI/ML package support
  - TensorFlow 2.3.5
  - PyTorch 1.8
  - Horovod
- Support for GPUs
  - Intel oneAPI 2021.1

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```
34: openpmd-api         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/openpmd-api-0.12.0-4myph6pbjnupgupxdlvbxvqqeqx6atyp
35: openmpi     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/openmpi-3.1.6-6yqtoym56as6xso2pdgkmn4bcsoyufku
36: papi        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/papi-6.0.0.1-gorrfrvrik575lldzgq46qmmu63kxl7x
37: papyrus     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/papyrus-develop-iu3dgpmwwyykgv5mpw2dwcrol4wbwbai
38: parallel-netcdf     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/parallel-netcdf-1.12.1-tmmkzibn43xr7su76msxxusyzrphdtn5
39: pdt         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/pdt-3.25.1-kvi5wuu5y72fypijti3nxqvdn7zpj6ni
40: petsc       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/petsc-3.13.4-llg3u4rrt5axrqlim75tt73epewxu4fb
41: plasma      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/plasma-19.8.1-tji7bojb5ne5hqj2mwn5bqq2tfkm23ke
42: precice     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/precice-2.1.0-ozdmbat2hlivccha3nklbeahikgynewu
43: pumi        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/pumi-2.2.2-52czzdbxeg7pmjkd55nub5jgxzodcprh
44: py-jupyterhub       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-jupyterhub-1.0.0-tr3wcolaij3kbzb6xm4mbbvakcstwsw3
45: py-libensemble      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-libensemble-0.7.0-mxvqxhiiblqnmhlfepbxboyiskqyvbej
46: qthreads    /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/qthreads-1.14-neshsclplh7ttkebm34grztaijqohnxt
47: raja        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/raja-0.11.0-w25bj2dys6cjqn7isgcjfyvte3tuulev
48: rempi       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/rempi-1.1.0-sideqdbiik2yseshs3loh4sictbis3t6
49: scr         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/scr-2.0.0-yh3chyq5gayuk6r4juejjiye6zg3rh3u
50: slate       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/slate-develop-jnysy2rh5vxhwua5ubtvq4bsfd3py7d5
51: slepc       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/slepc-3.13.4-q3lalpbqoshiyvjjgrnhb2iqiisvnfrp
52: strumpack   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/strumpack-4.0.0-rlbti5eqc5rjhfisxv2uxevj6m3fn5gg
53: sundials    /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/sundials-5.3.0-3g52gh4a6h4ohucqart5i4m6pi66woj6
54: superlu-dist        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/superlu-dist-6.3.1-o2hkund66coxn2rrbtlalda2vq35uu7j
55: stc         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/stc-0.8.3-oxfik7nsmgufoqyy7xilzsrct7it63ej
56: swig        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/swig-4.0.1-htxmzjd5sed5yfibw6j7jn5cx6p7g72x
57: sz  /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/sz-2.1.9-tcatyiuzh6quctrgd2g3dcli7xa7gvtj
58: tasmanian   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tasmanian-7.1-quo3grs5kb2xrvjufpi7vn66cpjfnadv
59: tau         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tau-2.29-ijw2nbphmlfkt42ubwz7g5a5yru22ikn
60: trilinos    /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/trilinos-13.0.0-6xfnp44g5xm7gpn2en6gkwzfceykfd3x
61: turbine     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/turbine-1.2.3-q4qjvgxjl3cbuyquo6zrurb4mwfn6wkp
62: umap        /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/umap-2.0.0-5tob3exzrmwoitudu5pstbb2dms3xnto
63: umpire      /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/umpire-3.0.0-6woo2uuvazcucxikc6xad6g3zksu2ygi
64: unifyfs     /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/unifyfs-0.9.0-be7mqbng7kdeewdlgvlhdm4jkxnquiil
65: upcxx       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/upcxx-2020.3.0-pshe62qyvmnrvesqa4pkj6bdq3fxxucf
66: veloc       /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/veloc-1.4-gk3iwfjhmgkwlawp7rmxf2eh37rqpqm2
67: zfp         /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/zfp-0.5.5-6r6yaco7gga5w4gbuvid3zt2iohrnepj
```

`spack find` shows what is installed

```
Singularity> spack find
==> 319 installed packages
-- linux-ubuntu18.04-power9le / gcc@7.3.0 ------------------------
autoconf@2.69     diffutils@3.7     libiconv@1.16       m4@1.4.18      ncurses@6.2              openssl@1.1.1g       texinfo@6.5
automake@1.16.2   findutils@4.6.0   libpciaccess@0.16   matio@1.5.17   netcdf-c@4.7.4           parmetis@4.0.3       trilinos@13.0.0
boost@1.74.0      glm@0.9.7.1       libsigsegv@2.12     metis@5.1.0    netlib-scalapack@2.1.0   perl@5.26.1          util-macros@1.19.1
bzip2@1.0.8       hdf5@1.10.7       libtool@2.4.6       mpich@3.2.1    omega-h@9.29.0           pkgconf@1.7.3        xz@5.2.5
cmake@3.18.4      hypre@2.20.0      libxml2@2.9.10      mumps@5.3.3    openblas@0.3.10          suite-sparse@5.7.2   zlib@1.2.11

-- linux-ubuntu18.04-ppc64le / gcc@7.3.0 -------------------------
adiak@0.1.1              flit@2.1.0               libpfm4@4.11.0           papyrus@develop                py-more-itertools@7.2.0     qthreads@1.14
adios@1.13.1             gasnet@2020.3.0          libpng@1.6.37            parallel-netcdf@1.12.1         py-mpi4py@3.0.3             raja@0.12.1
adios2@2.6.0             gasnet@2020.3.0          libpthread-stubs@0.4     parmetis@4.0.3                 py-nbclient@0.5.0           rankstr@0.0.2
adlbx@0.9.2              gdbm@1.18.1              libquo@1.3.1             pcre@8.44                      py-nbconvert@6.0.1          readline@8.0
aml@0.1.0                gettext@0.20.2           libsigsegv@2.12          pcre2@10.35                    py-nbformat@5.0.7           redset@0.0.3
amrex@20.10              gettext@0.21             libsodium@1.0.18         pdsh@2.31                      py-nest-asyncio@1.4.0       rempi@1.1.0
arborx@0.9-beta          ginkgo@1.3.0             libtool@2.4.6            pdt@3.25.1                     py-notebook@6.1.4           scr@2.0.0
argobots@1.0             git@2.28.0               libunistring@0.9.10      perl@5.26.1                    py-numpy@1.19.2             shuffile@0.0.3
arpack-ng@3.7.0          git@2.28.0               libunwind@1.4.0          petsc@3.13.6                   py-oauthlib@3.1.0           slate@develop
ascent@develop           glm@0.9.7.1              libunwind@1.4.0          petsc@3.14.0                   py-pamela@1.0.0             slepc@3.14.0
autoconf@2.69            globalarrays@5.7         libuuid@1.0.3            pkgconf@1.7.3                  py-pandocfilters@1.4.2      snappy@1.1.8
automake@1.16.2          gmake@4.2.1              libxml2@2.9.10           plasma@20.9.20                 py-parso@0.6.1              sqlite@3.31.1
axl@0.3.0                gmp@6.1.2                libyogrt@1.24            precice@2.1.1                  py-petsc4py@3.13.0          strumpack@5.0.0
axom@0.3.3               googletest@1.10.0        libzmq@4.3.2             pumi@2.2.2                     py-pexpect@4.7.0            suite-sparse@5.7.2
bash@5.0                 gotcha@0.0.2             lmod@8.3                 py-alembic@1.0.7               py-pickleshare@0.7.5        sundials@5.4.0
binutils@2.33.1          gotcha@1.0.3             lua@5.3.5                py-argon2-cffi@20.1.0          py-prometheus-client@0.7.1  superlu@5.2.1
bmi@develop              gperftools@2.7           lua-luafilesystem@1_7_0_2 py-asn1crypto@0.24.0          py-prompt-toolkit@2.0.9     superlu-dist@6.3.0
bolt@1.0                 hdf5@1.8.21              lua-luaposix@33.4.0      py-async-generator@1.10        py-psutil@5.7.2             superlu-dist@6.3.1
boost@1.73.0             hdf5@1.8.21              lwgrp@1.0.3              py-attrs@19.3.0                py-ptyprocess@0.6.0         swig@4.0.2
boost@1.73.0             hdf5@1.10.6              lz4@1.9.2                py-babel@2.7.0                 py-py@1.8.0                 sz@1.4.12.3
boost@1.73.0             hdf5@1.10.6              lzo@2.10                 py-backcall@0.1.0              py-pycparser@2.20           sz@2.0.2.0
boost@1.73.0             hpctoolkit@2020.08.03    m4@1.4.18                py-bleach@3.1.0                py-pyelftools@0.26          sz@2.1.10
butterflypack@1.2.0      hpx@1.5.1                magma@2.5.4              py-blinker@1.4                 py-pygments@2.6.1           tar@1.32
bzip2@1.0.8              hwloc@1.11.11            margo@0.4.3              py-certifi@2020.6.20           py-pyjwt@1.7.1              tasmanian@7.3
c-blosc@1.17.0           hwloc@2.2.0              matio@1.5.17             py-certipy@0.1.3               py-pyopenssl@19.0.0         tau@2.29
caliper@2.4.0            hypre@2.18.2             mbedtls@2.16.7           py-cffi@1.14.3                 py-pyrsistent@0.15.7        tcl@8.6.10
cinch@master             hypre@2.20.0             mercury@1.0.1            py-chardet@3.0.4               py-pytest-runner@5.1        texinfo@6.5
cmake@3.17.3             intel-tbb@2020.3         mercury@1.0.1            py-cryptography@2.7            py-python-dateutil@2.8.0    turbine@1.2.3
conduit@master           kokkos@3.2.00            metis@5.1.0              py-cython@0.29.21              py-python-editor@1.0.4      umap@2.1.0
conduit@master           kokkos-kernels@3.2.00    mfem@4.1.0               py-decorator@4.4.2             py-python-oauth2@1.1.1      umpire@4.0.1
cuda@10.2.89             kvtree@1.0.2             mpark-variant@1.4.0      py-defusedxml@0.6.0            py-pytz@2020.1              umpire@4.0.1
curl@7.72.0              legion@20.03.0           mpich@3.2.1              py-entrypoints@0.3             py-pyzmq@18.1.0             unifyfs@0.9.0
darshan-runtime@3.2.1    leveldb@1.22             mpifileutils@develop     py-idna@2.8                    py-requests@2.24.0          unzip@6.0
da[illegible]3.2.1       libarchive@3.4.1         mumps@5.3.3              py-importlib-metadata@2.0.0    py-send2trash@1.5.0         upcxx@2.020.3.0
di[illegible]            libbsd@0.10.0            ncurses@6.2              py-ipykernel@5.3.4             py-setuptools@50.1.0        util-macros@1.19.1
```

Snapz Pro X

All the versions coexist!

- Multiple versions of same package are ok.

Packages are installed to automatically find correct dependencies.

Binaries work *regardless of user's environment*.

Spack also generates module files.

- Don't *have* to use them.

E4S Spack environment spack.yaml

https://github.com/UO-OACISS/e4s/blob/master/docker-recipes/ubuntu18.04-e4s-x86_64/spack

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eugeneswalker remove old recipes Latest commit 096d2ec on Mar 23, 2020 History

1 contributor

201 lines (201 sloc) 3.04 KB Raw Blame

```yaml
spack:
  concretization: separately
  definitions:
  - e4s:
    - openpmd-api
    - slate
    - magma
    - stc
    - py-libensemble^python@3.7.3
    - flecsi+cinch
    - hypre
    - mfem
    - trilinos@12.14.1+dtk+intrepid2+shards
    - sundials
    - petsc
    - strumpack
    - superlu-dist
    - superlu
    - tasmanian
    - openblas threads=openmp
    - faodel
    - mercury
    - hdf5
    - adios2
    - adios
    - darshan-runtime
    - darshan-util
    - veloc
    - scr
```

- Bare-metal install
  % cat spack.yaml
  % spack -e . install
- Docker build:

Executable File | 2 lines (2 sloc) | 78 Bytes

```bash
#!/bin/bash -x
docker build --no-cache -t ecpe4s/ubuntu18.04-e4s-x86_64:1.2 .
```

E4S Validation Test Suite

- Provides automated build and run tests
- Validate container environments and products
- New LLVM validation test suite for DOE LLVM

https://github.com/E4S-Project/testsuite/tree/master/validation_tests/magma

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eugeneswalker use bash -xe in compile/run.sh Latest commit a1dfb32 9 hours ago

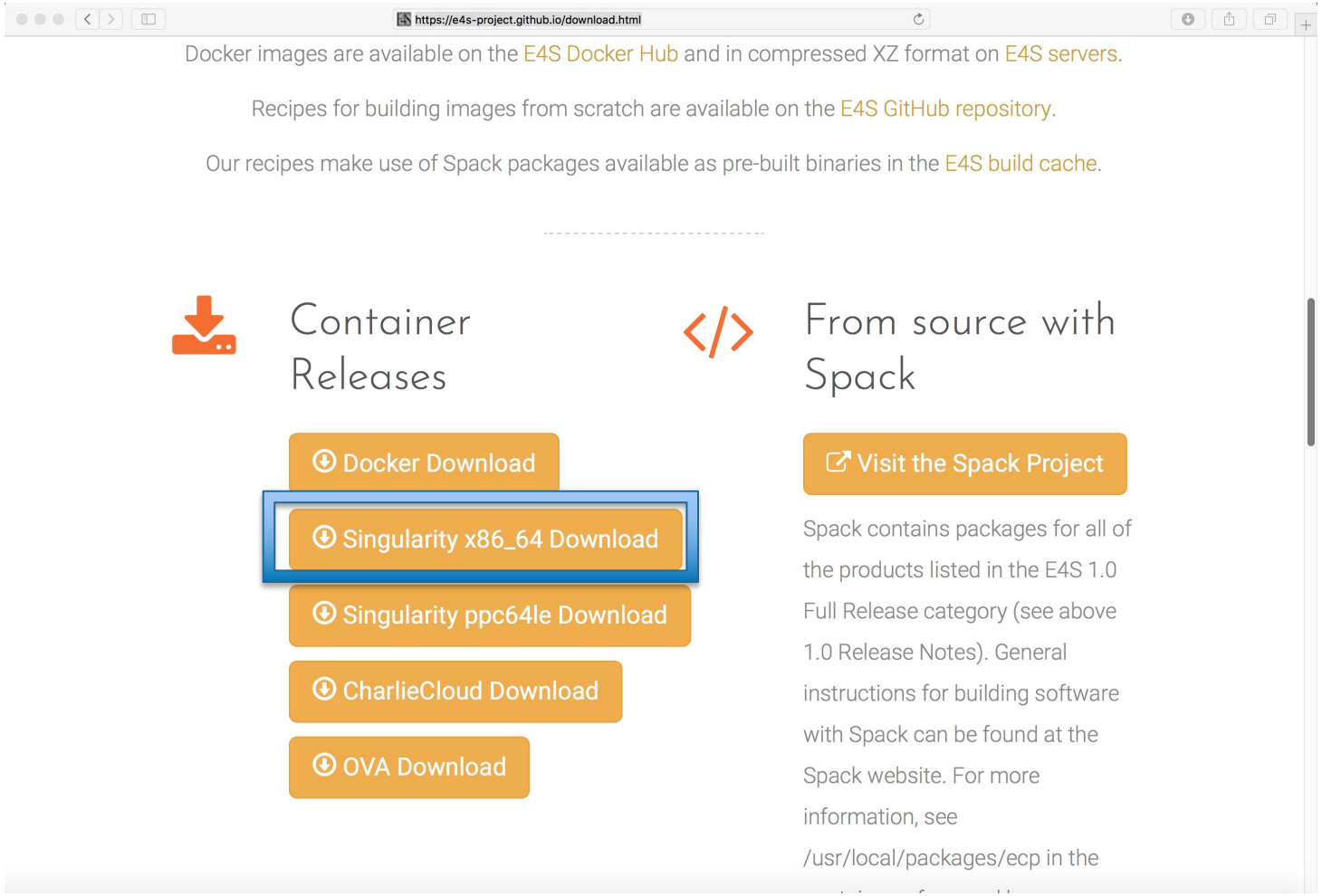
..		
Makefile	use env variables set by `spack load`	4 months ago
README.txt	Added basic magma test.	11 months ago
clean.sh	Added basic magma test.	11 months ago
compile.sh	use bash -xe in compile/run.sh	9 hours ago
example_f.F90	Added basic magma test.	11 months ago
example_sparse.c	Added basic magma test.	11 months ago
example_sparse_operator.c	Added basic magma test.	11 months ago
example_v1.c	Added basic magma test.	11 months ago
example_v2.c	Added basic magma test.	11 months ago
run.sh	use bash -xe in compile/run.sh	9 hours ago
setup.sh	Remove some .o files. Don't load special openblas. Don't specify spec...	3 months ago

README.txt

```
Getting started with MAGMA.

This is a simple, standalone example to show how to use MAGMA, once it is
compiled. More involved examples for individual routines are in the testing
directory. The testing code includes some extra utilities that we use for
testing, such as testings.h and libtest.a, which are not required to use MAGMA,
though you may use them if desired.

----------------------------------------
C example

See example_v2.c for sample code.

Include the MAGMA header:

    #include "magma_v2.h"

(For the legacy MAGMA v1 interface, see example_v1.c. It includes magma.h
instead. By default, magma.h includes the legacy cuBLAS v1 interface (cublas.h).
You can include cublas_v2.h before magma.h if desired.)
```

- git clone https://github.com/E4S-Project/testsuite.git

E4S Supports Singularity and Docker container runtimes



https://e4s.io

- wget http://tau.uoregon.edu/ecp.simg
- singularity run ecp.simg; module load intel
- Supports Intel OneAPI
- which dpcpp

e4s-cl: A tool to simplify the launch of MPI jobs in E4S containers

- E4S containers support replacement of MPI libraries using MPICH ABI compatibility layer.
- Applications binaries built using E4S can be launched with Singularity using MPI library substitution for efficient inter-node communications.
- e4s-cl is a new tool that simplifies the launch and MPI replacement.
- Usage:

```
. /opt/intel/oneapi/setvars.sh
e4s-cl init --backend singularity --image /home/tutorial/ecp.simg --source /home/tutorial/source.sh
e4s-cl mpirun -np 4 ./a.out
```

https://github.com/E4S-Project/e4s-cl

Download TAU from U. Oregon

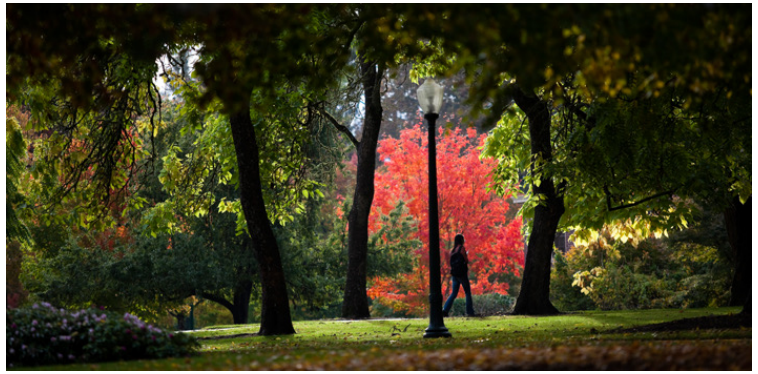
Tuning and Analysis Utilities

http://tau.uoregon.edu

for more information

Free download, open source, BSD license

Performance Research Laboratory, University of Oregon, Eugene



www.uoregon.edu

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