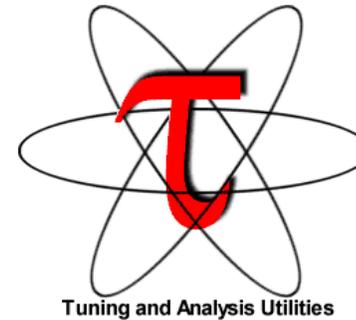


TAU

August 10, 2022, 4:50pm – 5:30pm CT
ATPESC workshop Tools Track
Q Center, St. Charles, IL

Sameer Shende
Performance Research Laboratory, OACISS, University of Oregon and ParaTools, Inc.
http://tau.uoregon.edu/tau_atpesc22.pdf



TAU: Quickstart Guide

Setup:

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

Profiling with an un-instrumented application:

- **MPI:** `% srun -n 64 tau_exec -ebs ./a.out`
- **MPI+OpenMP with Intel 19+:**
`% export TAU_OMPT_SUPPORT_LEVEL=full;`
`% srun -n 64 tau_exec -T ompt,mpi -ompt ./a.out`
- **Pthread:** `% srun -n 64 tau_exec -T mpi,pthread -ebs ./a.out`
- **Python+MPI+Sampling:** `% srun -n 64 tau_python -ebs ./a.py`
- **Python+MPI+OpenCL:** `% srun -n 64 tau_python -opencl ./a.py`
- **DPC++/SYCL (no MPI):** `% tau_exec -T level_zero,serial -l0 ./a.out`
- **CUDA+MPI** `% srun -n 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`
`% srun -n 64 tau_exec ./a.out; vampir traces.otf2 &`
- **Chrome:** `% export TAU_TRACE=1; srun -n 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) or Perfetto.dev
- **Jumpshot:** `% export TAU_TRACE=1; srun -n 64 tau_exec ./a.out; tau_treemerge.pl;`
`% tau2slog2 tau.trc tau.edf -o app.slog2; jumpshot app.slog2 &`

Setup: Installing TAU on Laptops

Prerequisites: Java in your path

- Microsoft Windows
 - Install Java from Oracle.com
 - <http://tau.uoregon.edu/tau.exe>
 - Install, click on a ppk file to launch paraprof
- macOS (x86_64)
 - Install Java 11.0.3:
 - Download and install <http://tau.uoregon.edu/java.dmg>
 - If you have multiple Java installations, add to your `~/.zshrc` (or `~/.bashrc` as appropriate):
 - `export PATH=/Library/Java/JavaVirtualMachines/jdk-11.0.3.jdk/Contents/Home/bin:$PATH`
 - `java -version`
 - Download and install TAU (copy to /Applications from dmg):
 - <http://tau.uoregon.edu/tau.dmg>
 - `export PATH=/Applications/TAU/tau/apple/bin:$PATH`
 - `paraprof app.ppk &`
 - macOS (arm64, M1)
 - http://tau.uoregon.edu/java_arm64.dmg
 - http://tau.uoregon.edu/tau_arm64.dmg
 - Linux (<http://tau.uoregon.edu/tau.tgz>)
 - `./configure; make install; export PATH=<taudir>/x86_64/bin:$PATH; paraprof app.ppk &`

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

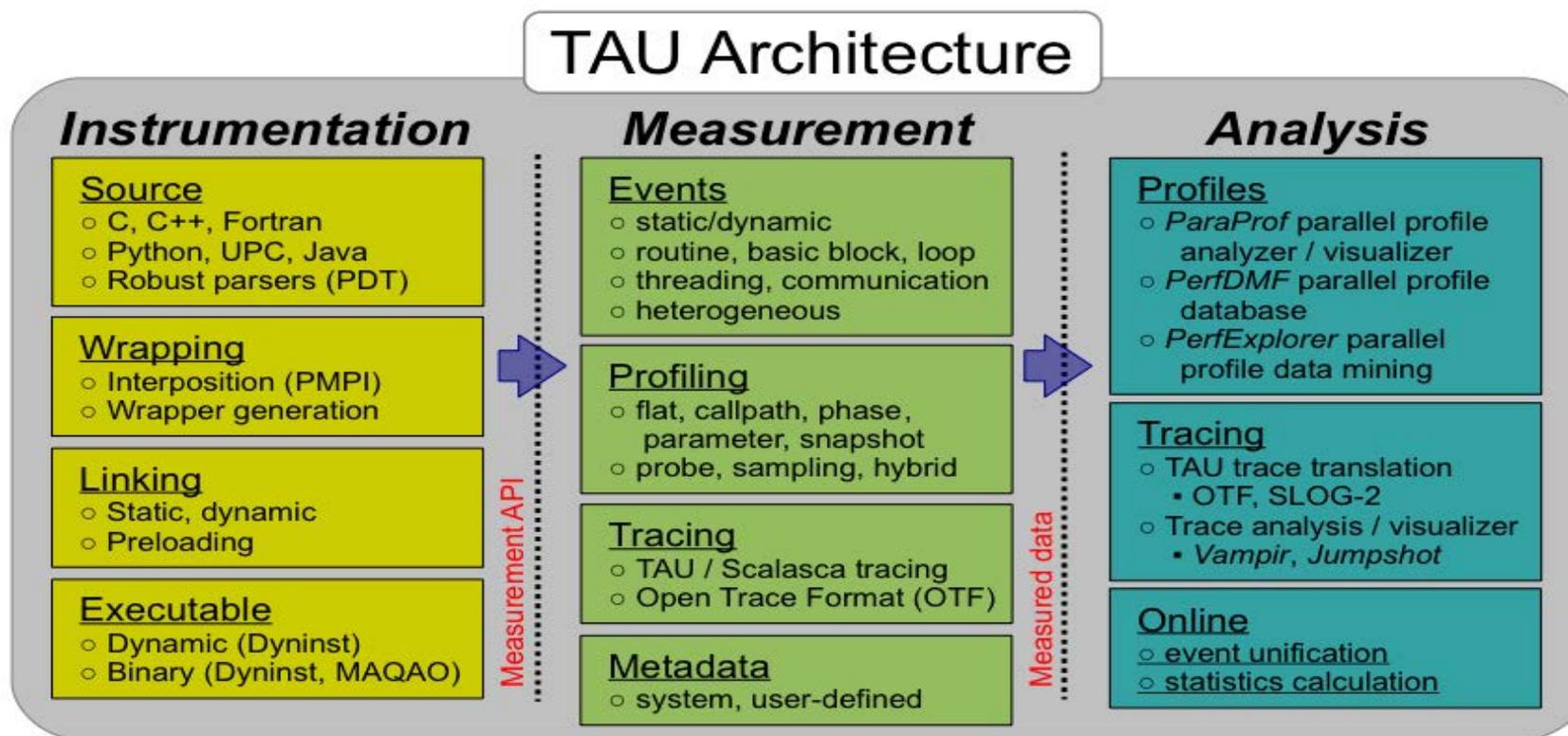
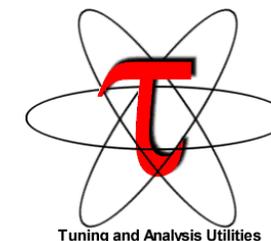
- TAU Performance System[®]:
 - Deliver a scalable, portable, performance evaluation toolkit for HPC and AI/ML workloads
- Extreme-scale Scientific Software Stack (E4S):
 - Delivering a modular, interoperable, and deployable software stack
 - Deliver expanded and vertically integrated software stacks 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



TAU Performance System

Instrumentation

- Fortran, C++, C, UPC, Java, Python, Chapel, Spark
- Automatic instrumentation
- Map manual instrumentation APIs from other tools to TAU
 - NVTX, ROCTx
 - CAMTimers, PerfStubs, PETSc, Caliper, Kokkos API

Measurement and analysis support

- MPI, OpenSHMEM, ARMCI, PGAS, DMAPP
- pthreads, OpenMP, OMPT interface, hybrid, other thread models
- GPU: Intel oneAPI DPC++/SYCL, AMD ROCm (RocProfiler and RocTracer), 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?
- How much time did my application spend waiting at a barrier in MPI collective operations?
- How can I use my app multi-node GPU systems? With unmodified binary on all 3 vendor GPUs?
- 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?

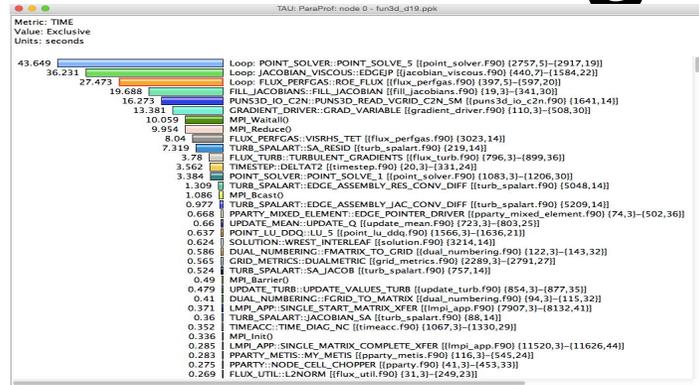
Instrumentation

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

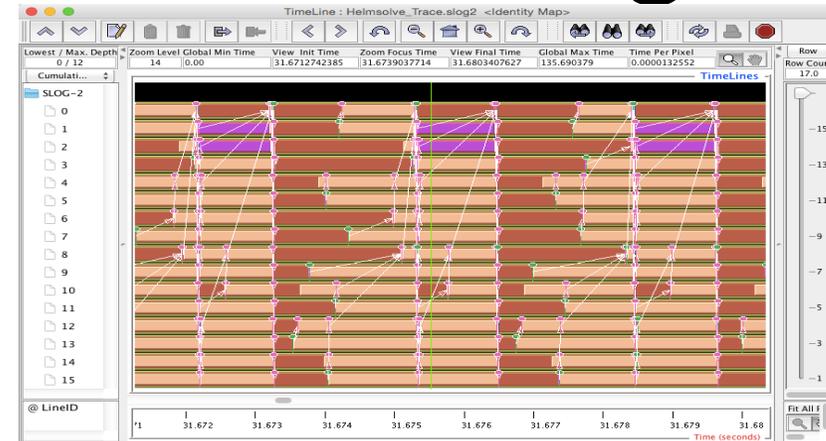


- **Profiling** shows you **how much** (total) time was spent in each routine
- Profiling and tracing

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

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

Tracing



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

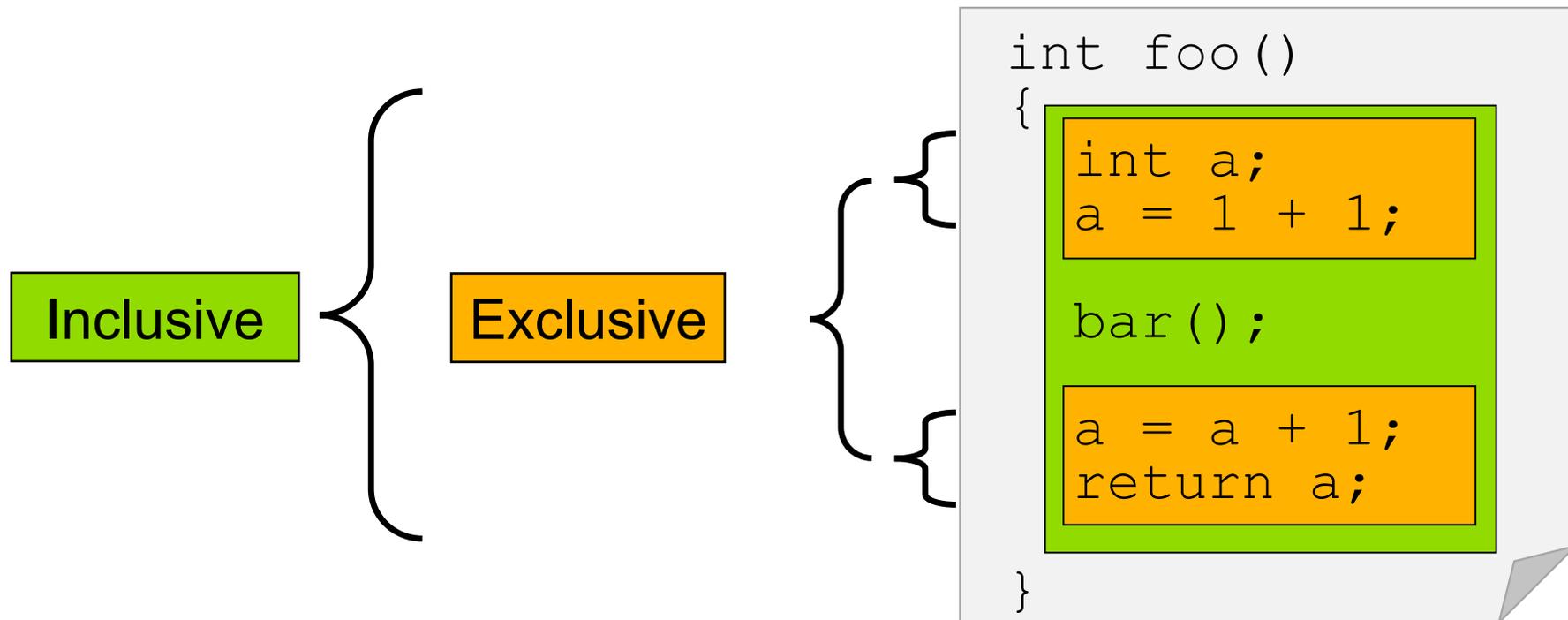
Instrumentation

- 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.

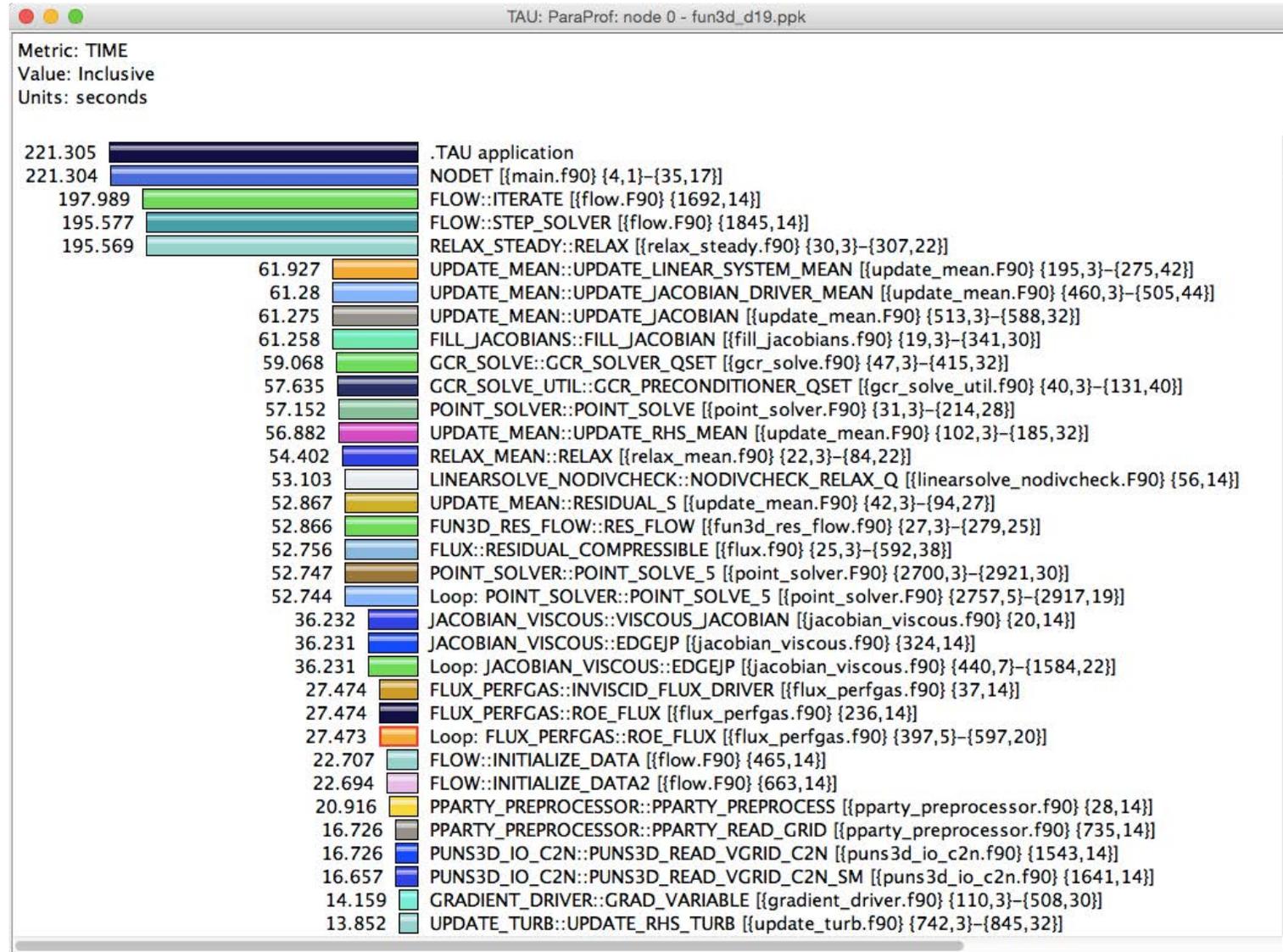
- User-defined events
 - **Interval** (start/stop) events to measure exclusive & inclusive duration
 - **Atomic events** take measurements at a single point
 - Measures total, samples, min/max/mean/std. deviation statistics
 - **Context events** are atomic events with executing context
 - Measures above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

Inclusive vs. Exclusive values

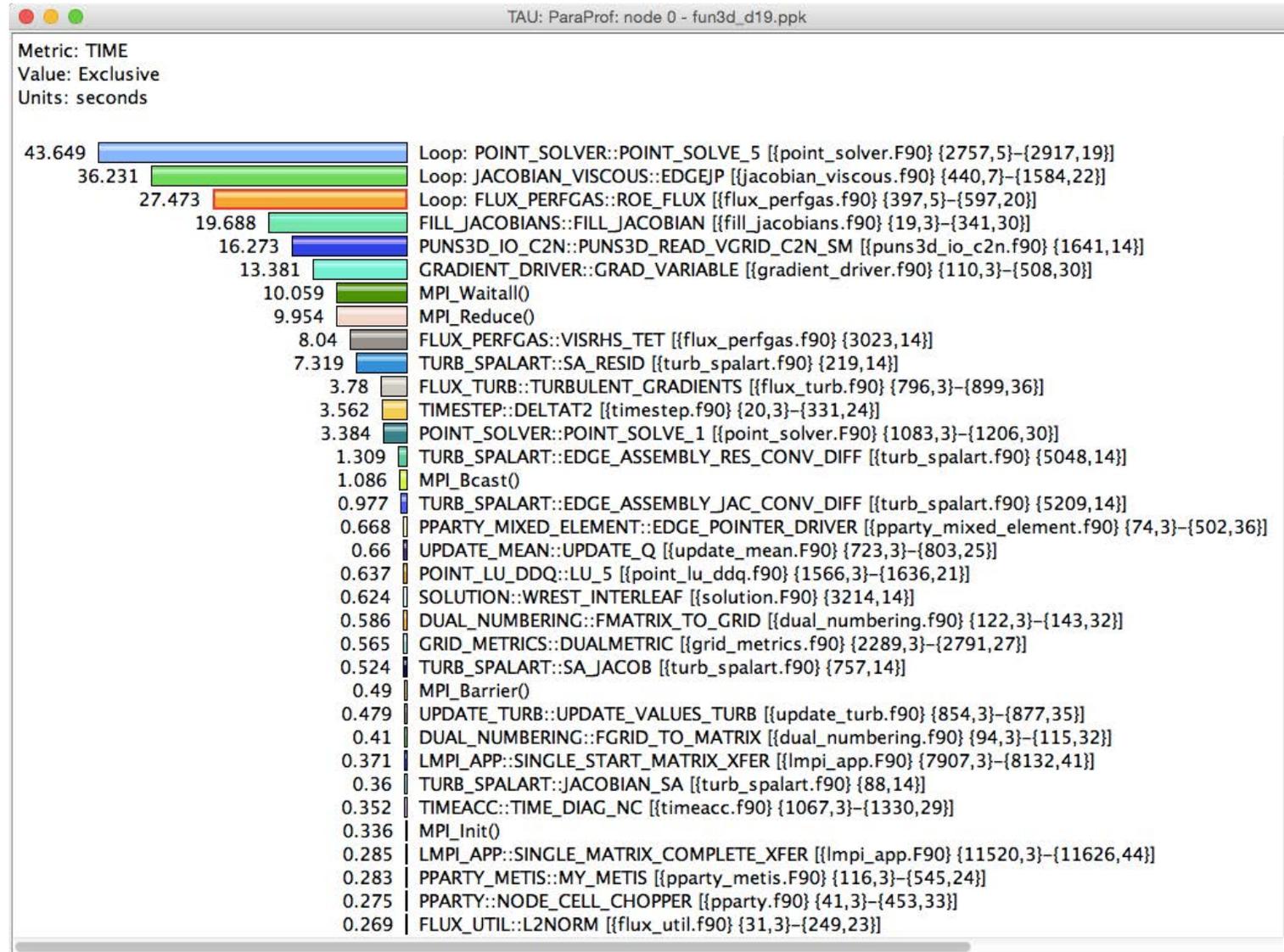
- Inclusive
 - Information of all sub-elements aggregated into single value
- Exclusive
 - Information cannot be subdivided further



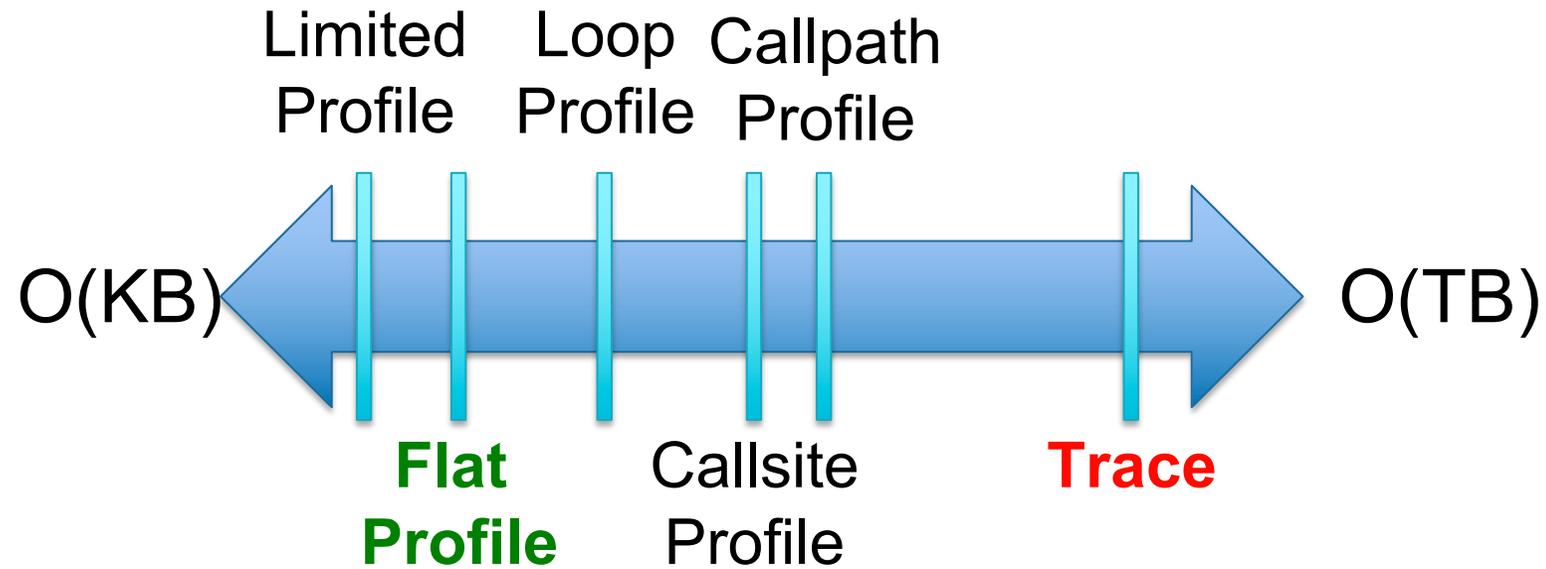
Inclusive Measurements



Exclusive Time



How much data do you want?



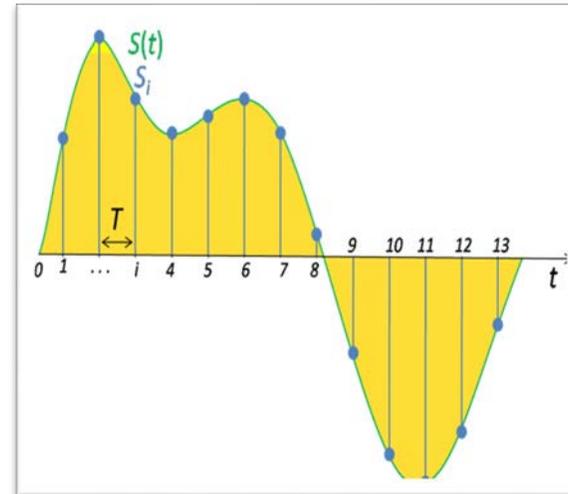
Performance Data Measurement

Direct via Probes

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

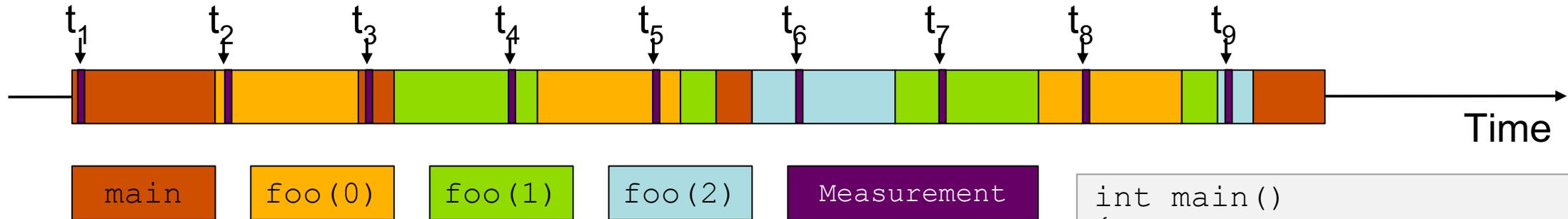
- Exact measurement
- Fine-grain control
- Calls inserted into code

Indirect via Sampling



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

Event-Based Sampling (EBS)



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 (tau_exec -ebs)

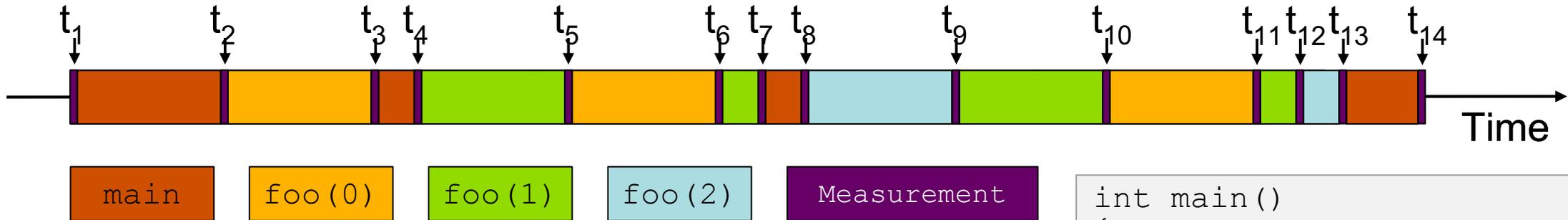
```
int main()
{
    int i;

    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;
    TAU_START("main");
    for (i=0; i < 3; i++)
        foo(i);
    TAU_STOP("main");
    return 0;
}

void foo(int i)
{
    TAU_START("foo");
    if (i > 0)
        foo(i - 1);
    TAU_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 Execution Command (tau_exec)

Uninstrumented execution

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

Track GPU operations

```
% srun -n 256 tau_exec -T rocprofiler -rocm ./a.out
```

```
% srun -n 256 tau_exec -l0 ./a.out
```

```
% srun -n 256 tau_exec -cupti -um ./a.out (CUDA with Uniform memory)
```

```
% srun -n 256 tau_exec -opencl ./a.out
```

```
% srun -n 256 tau_exec -openacc ./a.out
```

Track MPI performance

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

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

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

Track OpenMP and MPI execution (using OMPT)

```
% export TAU_OMPT_SUPPORT_LEVEL=full;
```

```
% srun -n 256 tau_exec -T ompt,intel,mpi -ompt ./a.out
```

Track memory operations

```
% export TAU_TRACK_MEMORY_LEAKS=1
```

```
% srun -n 256 tau_exec -memory_debug ./a.out (bounds check)
```

Use event based sampling (compile with -g)

```
% srun -n 256 tau_exec -ebs ./a.out
```

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

Configuring TAU and choosing a configuration in tau_exec

```
% cd /soft/perftools/tau/tau-2.31.1; cat .all_configs
./configure -ompt -mpi -bfd=download -unwind=download -iowrapper -dwarf=download
        -papi=<dir> -pdt=<dir> -pdt_c++=g++ -otf=download
% make install
% module load tau/2.31.1
% ls $TAU/Makefile*
/soft/perftools/tau/tau-2.31.1/craycn1/lib/Makefile.tau-intel-papi-mpi-pdt
/soft/perftools/tau/tau-2.31.1/craycn1/lib/Makefile.tau-intel-papi-mpi-pthread-pdt
/soft/perftools/tau/tau-2.31.1/craycn1/lib/Makefile.tau-intel-papi-ompt-mpi-pdt-openmp
/soft/perftools/tau/tau-2.31.1/craycn1/lib/Makefile.tau-intel-papi-pthread-pdt

% aprun -n 4 tau_exec -T ompt,papi -ebs ./a.out
Will preload libTAU.so from
/soft/perftools/tau/tau-2.31.1/craycn1/lib/shared-intel-papi-ompt-mpi-pdt-openmp/

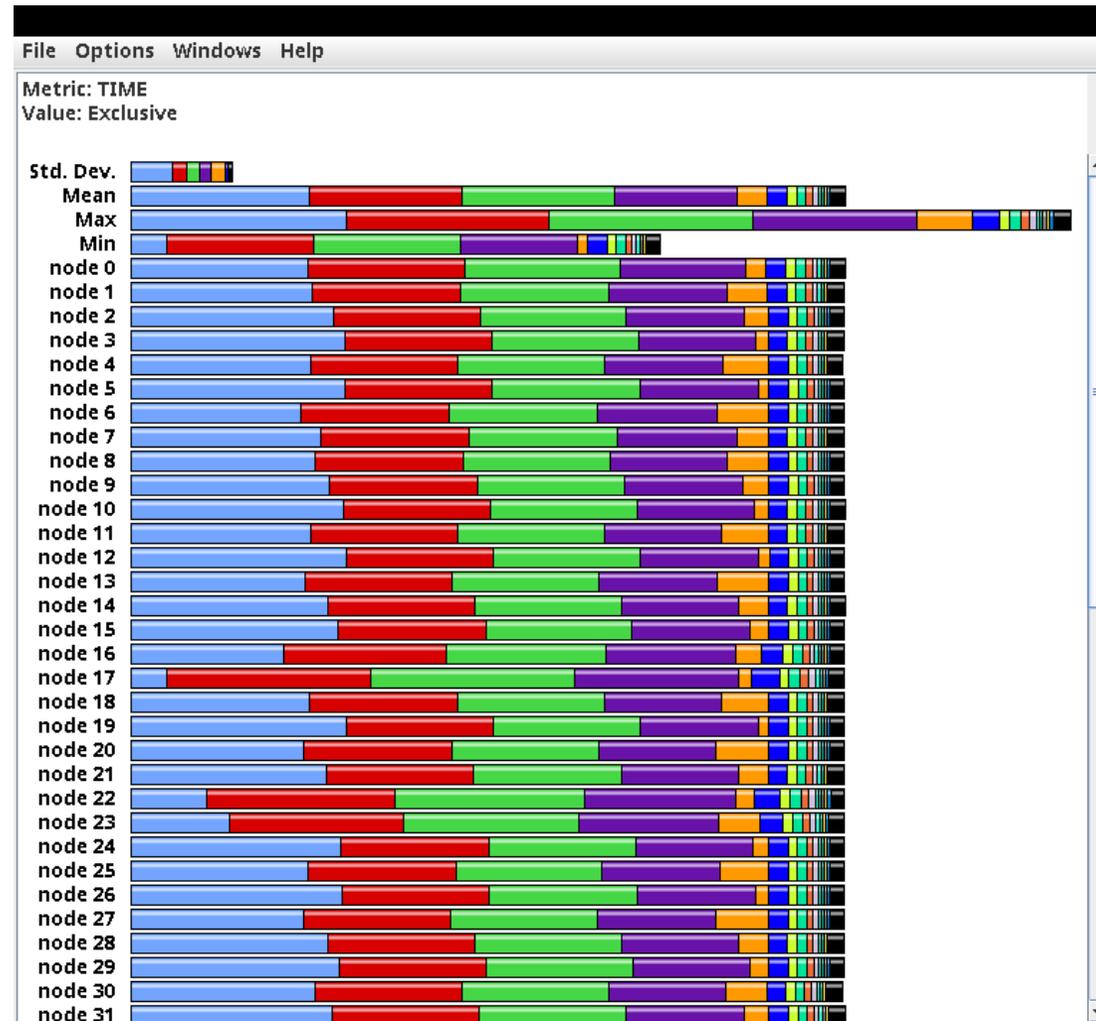
Corresponding to
/soft/perftools/tau/tau-2.31.1/craycn1/lib/Makefile.tau-intel-papi-ompt-mpi-pdt-openmp

-T mpi is chosen by default. Please use -T serial for non-mpi cases.
```

RUNTIME PRELOADING

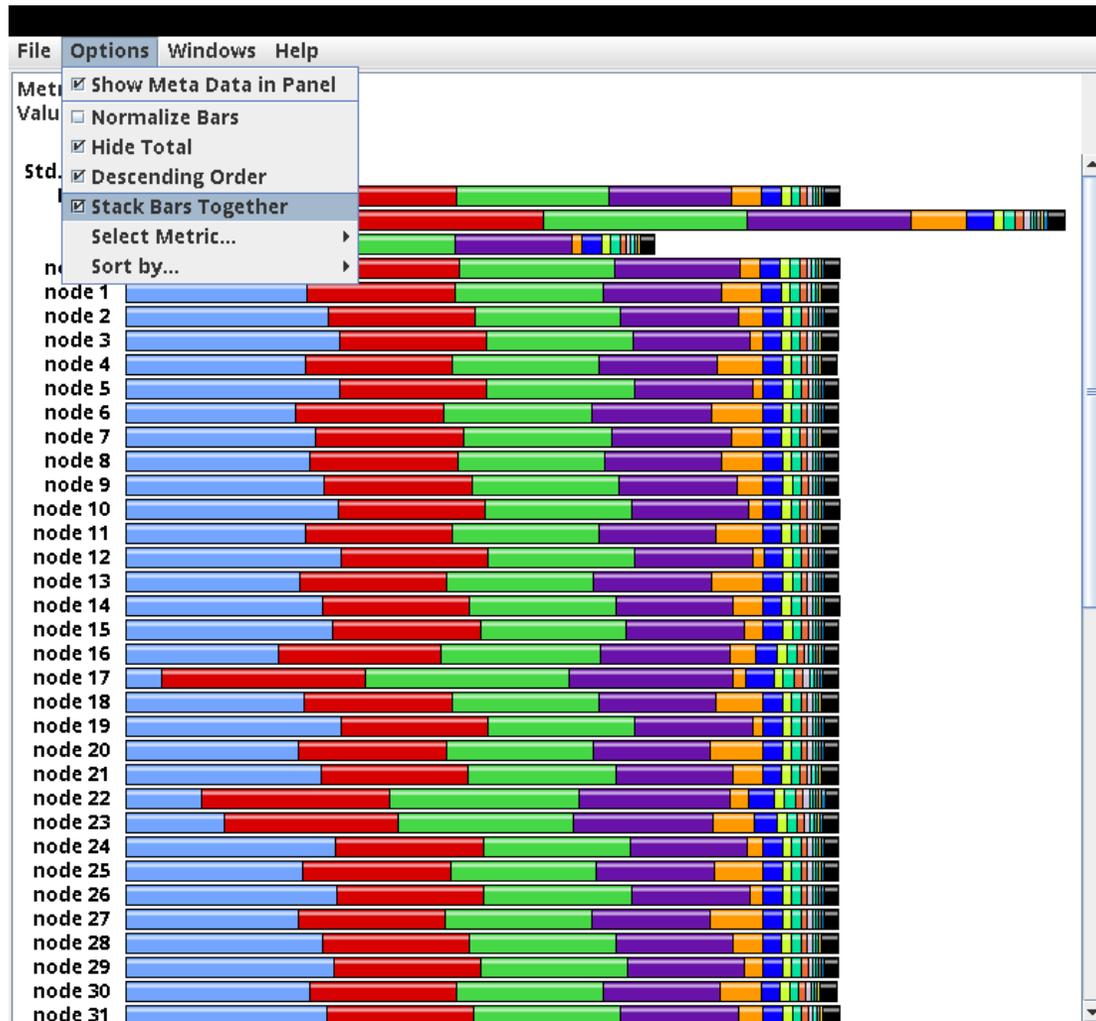
- Injects TAU DSO in the executing application
- Requires dynamic executables
- We must compile with `-dynamic -g`
- Use `tau_exec` while launching the application

ParaProf Profile Browser



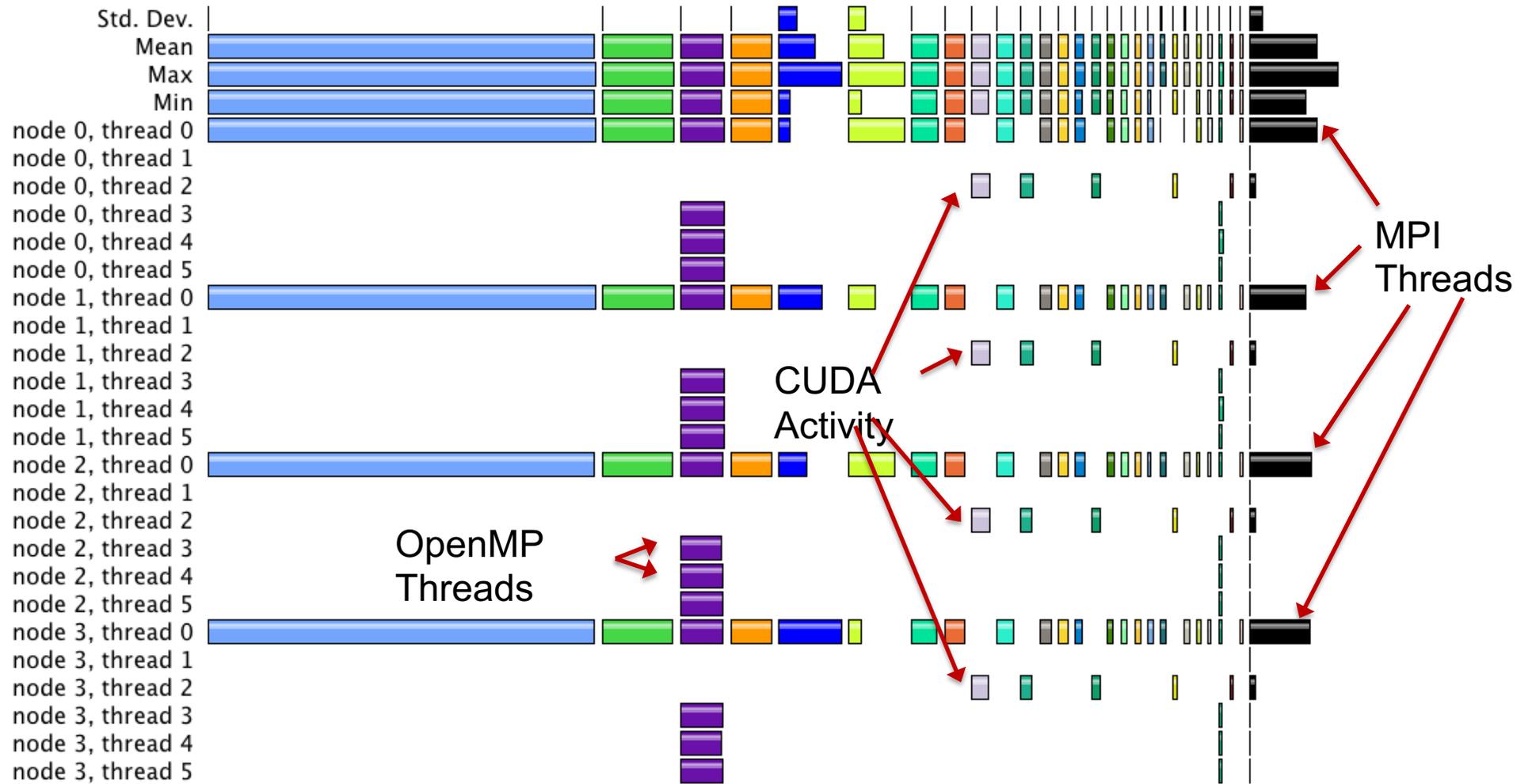
% paraprof

ParaProf Profile Browser

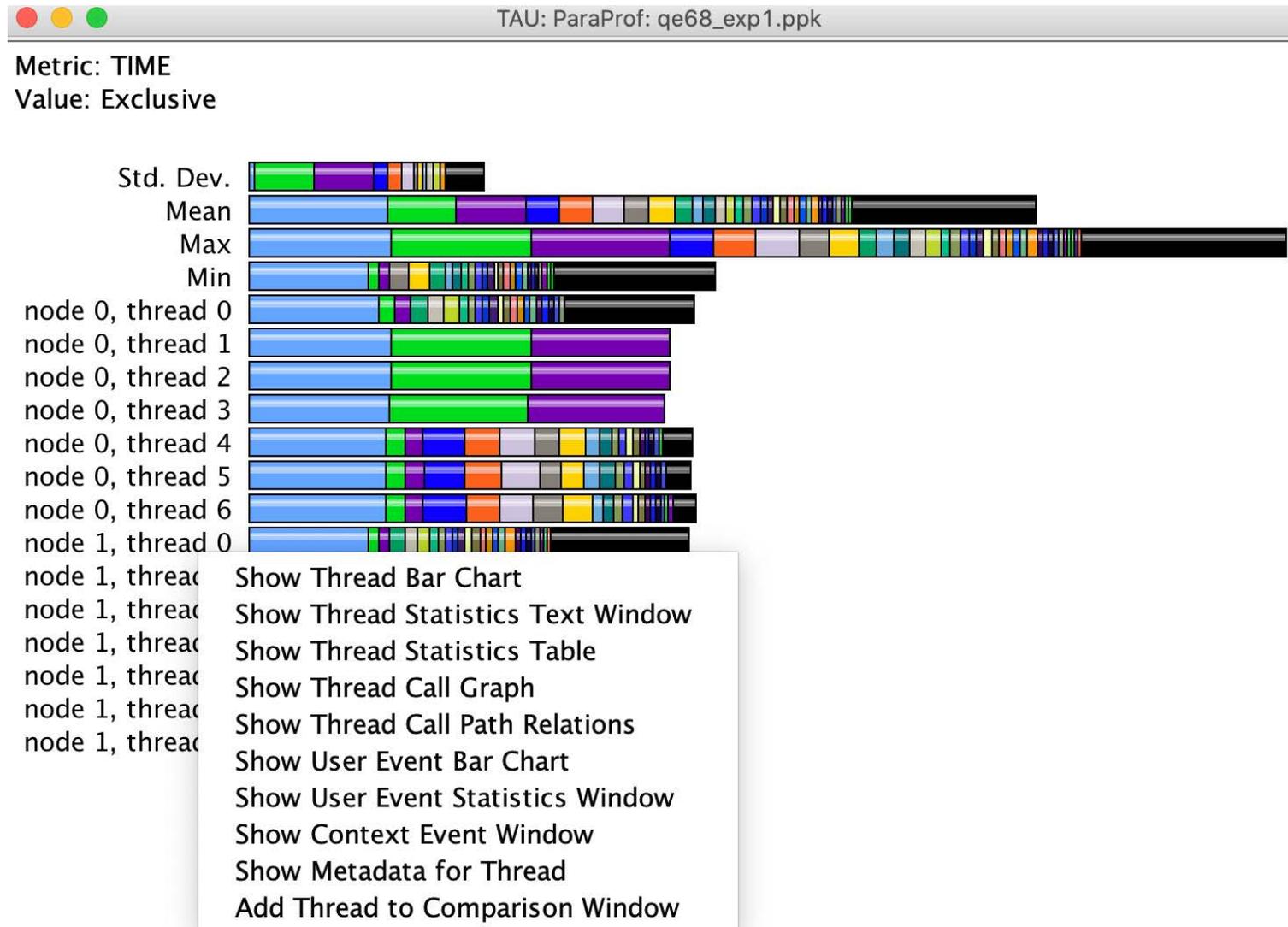


ParaProf Profile Browser

Metric: TAUGPU_TIME
Value: Exclusive



ParaProf Profile Browser: Choose Thread Statistics Window



ParaProf Thread Statistics Table

TAU: ParaProf: Statistics for: node 0, thread 0 - qe68_exp1.ppk

Name Δ	Exclusive TIME	Inclusive TIME	Calls	Child Calls
▾ .TAU application	12.111	13.341	1	26,524
▸ [CONTEXT] .TAU application	0	11.971	396	0
▸ MPI_Allreduce()	0.038	0.038	2,816	0
▾ MPI_Alltoall()	0.262	0.271	1,011	105
▾ [CONTEXT] MPI_Alltoall()	0	0.27	8	0
▸ [SAMPLE] .annobin_pthread_spin_lock.c [{pthread_spin_lock.c} {0}]	0.03	0.03	1	0
▸ [SAMPLE] PAMI_Context_trylock_advancev [{/m100/prod/opt/com]	0.09	0.09	2	0
▸ [SAMPLE] _ZN4PAMI8Protocol3Get13CompositeRGetINS1_4RGetES3	0.03	0.03	1	0
▸ [SAMPLE] __memcpy_power7 [{} {0}]	0.09	0.09	3	0
▸ [SAMPLE] opal_datatype_copy_content_same_ddt [{/m100/prod/op	0.03	0.03	1	0
▸ MPI_Barrier()	0.043	0.043	3,992	0
▸ MPI_Bcast()	0.004	0.004	875	5
▸ MPI_Comm_free()	0	0	11	0
▸ MPI_Comm_rank()	0.002	0.002	4,221	0
▸ MPI_Comm_size()	0.004	0.004	4,954	0
▸ MPI_Comm_split()	0.008	0.009	13	26
▸ MPI_Finalize()	0.399	0.416	1	37
▸ MPI_Gather()	0	0	3	0
▸ MPI_Get_count()	0	0	12	0
▸ MPI_Get_processor_name()	0	0	1	0
▸ MPI_Init_thread()	0.128	0.16	1	909
▸ MPI_Irecv()	0.002	0.002	1,212	0
▸ MPI_Isend()	0.024	0.024	1,212	4
▸ MPI_Recv()	0.001	0.001	24	0

Using sampling, TAU can explain 11.971 seconds out of 12.111 seconds using 396 samples.

ParaProf Thread Statistics Table

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Name	Exclusive ...	Inclusive ...	Calls	Child Calls
▼ .TAU application	12.111	13.341	1	26,524
▼ [CONTEXT] .TAU application	0	11.971	396	0
▶ [SUMMARY] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90}]	1.68	1.68	56	0
[SAMPLE] UNRESOLVED /usr/lib64/power9/libc-2.28.so	1.481	1.481	49	0
[SAMPLE] UNRESOLVED /usr/lib64/libcuda.so.450.51.06	1.466	1.466	49	0
▶ [SUMMARY] fft_scatter_2d_fft_scatter_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/FFTXlib/fft_s	0.749	0.749	24	0
[SAMPLE] t3bv_8 [t3bv_8.c] {0}	0.719	0.719	24	0
[SAMPLE] __c_mcopy8 [{/m100/prod/opt/compilers/hpc-sdk/2021/binary/Linux_ppc64le/21.5/compilers/lib/libnvc.so} {0}]	0.629	0.629	21	0
[SAMPLE] n1bv_9 [n1bv_9.c] {0}	0.6	0.6	20	0
[SAMPLE] t3fv_8 [t3fv_8.c] {0}	0.539	0.539	18	0
[SAMPLE] n1fv_9 [n1fv_9.c] {0}	0.51	0.51	16	0
[SAMPLE] fft_scalar_fft3_cft_1z_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/FFTXlib/fft_scala	0.3	0.3	9	0
[SAMPLE] __nv_exch_corr_cp_F1L518_1_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/ε	0.27	0.27	9	0
▶ [SUMMARY] xc_gcx__ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/XClib/xc_wrapper_gga.f90}]	0.21	0.21	7	0
[SAMPLE] __memcpy_power7 [{} {0}]	0.21	0.21	7	0
[SAMPLE] fftw_cpy2d [{/m100/prod/opt/libraries/fftw/3.3.8/gnu--8.4.0/lib/libfftw3.so.3.5.8} {0}]	0.21	0.21	7	0
[SAMPLE] fft_scalar_fft3_cft_2xy_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/FFTXlib/fft_scal	0.18	0.18	6	0
▶ [SUMMARY] fft_gradient_g2r_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/Modules/gradutils.f90	0.15	0.15	5	0
[SAMPLE] UNRESOLVED [vdso]	0.15	0.15	5	0
[SAMPLE] __GI__pthread_mutex_lock [{} {0}]	0.15	0.15	5	0
[SAMPLE] exch_corr_h_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {144	0.12	0.12	4	0
[SAMPLE] __memset_power8 [{} {0}]	0.119	0.119	4	0
[SAMPLE] __calloc [{} {0}]	0.09	0.09	3	0
[SAMPLE] fftw_cpy2d_pair [{/m100/prod/opt/libraries/fftw/3.3.8/gnu--8.4.0/lib/libfftw3.so.3.5.8} {0}]	0.09	0.09	3	0
[SAMPLE] __nv_drhov__F1L651_1_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/charged	0.09	0.09	3	0

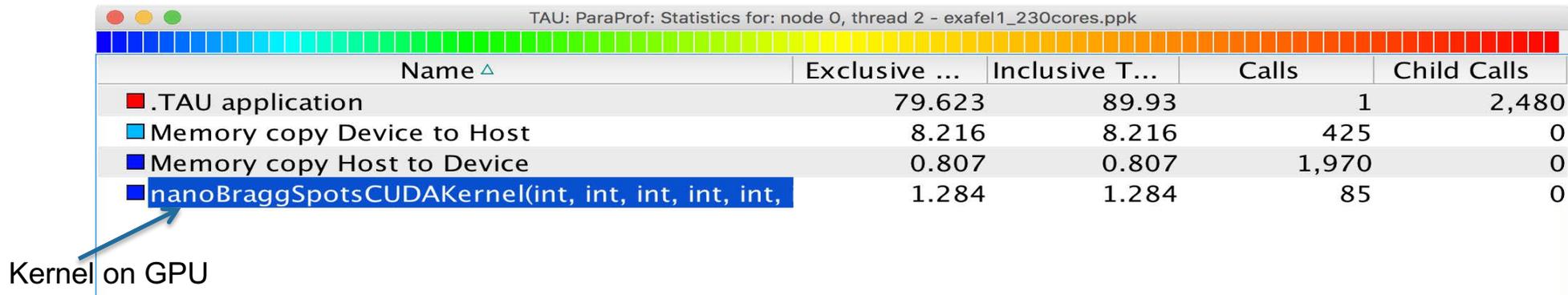
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▾ [CONTEXT] .TAU application	0	11.971	396	0
▾ [SUMMARY] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90}]	1.68	1.68	56	0
▣ [SAMPLE] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {339}]	0.66	0.66	22	0
▣ [SAMPLE] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {315}]	0.6	0.6	20	0
▣ [SAMPLE] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {344}]	0.18	0.18	6	0
▣ [SAMPLE] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {308}]	0.06	0.06	2	0
▣ [SAMPLE] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {353}]	0.06	0.06	2	0
▣ [SAMPLE] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {320}]	0.03	0.03	1	0
▣ [SAMPLE] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {325}]	0.03	0.03	1	0
▣ [SAMPLE] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {331}]	0.03	0.03	1	0
▣ [SAMPLE] gradh_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/exch_corr.f90} {303}]	0.03	0.03	1	0
▣ [SAMPLE] UNRESOLVED /usr/lib64/power9/libc-2.28.so	1.481	1.481	49	0
▣ [SAMPLE] UNRESOLVED /usr/lib64/libcuda.so.450.51.06	1.466	1.466	49	0
▸ [SUMMARY] fft_scatter_2d_fft_scatter_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/FFTXlib/fft_s	0.749	0.749	24	0
▣ [SAMPLE] t3bv_8 [/{t3bv_8.c} {0}]	0.719	0.719	24	0
▣ [SAMPLE] __c_mcopy8 [{/m100/prod/opt/compilers/hpc-sdk/2021/binary/Linux_ppc64le/21.5/compilers/lib/libnvc.so} {0}]	0.629	0.629	21	0
▣ [SAMPLE] n1bv_9 [/{n1bv_9.c} {0}]	0.6	0.6	20	0
▣ [SAMPLE] t3fv_8 [/{t3fv_8.c} {0}]	0.539	0.539	18	0
▣ [SAMPLE] n1fv_9 [/{n1fv_9.c} {0}]	0.51	0.51	16	0
▣ [SAMPLE] fft_scalar_fftw3_cft_1z_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/FFTXlib/fft_scala	0.3	0.3	9	0
▣ [SAMPLE] __nv_exch_corr_cp_F1L518_1_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/CPV/src/ε	0.27	0.27	9	0
▸ [SUMMARY] xc_gcx_ [{/m100_scratch/userinternal/mippolit/QE-code/NEW/qe_test_openacc/XClib/xc_wrapper_gga.f90}]	0.21	0.21	7	0
▣ [SAMPLE] __memcpy_power7 [/{ } {0}]	0.21	0.21	7	0
▣ [SAMPLE] fftw_cpy2d [/{m100/prod/opt/libraries/fftw/3.3.8/gnu--8.4.0/lib/libfftw3.so.3.5.8} {0}]	0.21	0.21	7	0

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.



```
% 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
▶ <code>__init__</code> [from_scatterers_fft.py}{13}}	20.036	20.362	303	10,914
▶ <code>run_sim2smv</code> [step5_pad.py}{138}}	16.78	134.9	1	1,066
▶ <code>__init__</code> [__init__.py}{150}}	11.669	15.909	101	1,010
▼ <code>channel_pixels</code> [step5_pad.py}{79}}	11.029	107.657	100	13,358
▼ [CONTEXT] <code>channel_pixels</code> [step5_pad.py}{79}}	0	9.345	312	0
■ [SAMPLE] <code>nanoBraggSpotsCUDA</code> [autofs/nccs-svm1_home1/iris/adse13_161/psana-legion/simtbx/sun	4.755	4.755	159	0
■ [SAMPLE] <code>simtbx::nanoBragg::nanoBragg::add_nanoBragg_spots_cuda()</code> [autofs/nccs-svm1_home1/iris/	4.08	4.08	136	0
■ [SAMPLE] <code>__memset_power8</code> [{} {0}}	0.3	0.3	10	0
■ [SAMPLE] UNRESOLVED <code>/usr/lib64/libc-2.17.so</code>	0.181	0.181	6	0
▶ [SUMMARY] <code>Tau_handle_driver_api_memcpy(void*, CUpti_CallbackDomain, unsigned int, CUpti_CallbackDz</code>	0.03	0.03	1	0
▶ <code>cuMemcpyDtoH_v2</code>	9.483	9.483	500	0
▶ <code>expand_to_p1_iselection</code> [__init__.py}{1376}}	7.349	7.35	101	606
▶ <code>load</code>	7.004	7.009	2	2,251
▶ <code>reset_wavelength</code> [util_fmodel.py}{121}}	6.197	6.553	100	47,550
▶ <code>is_unique_set_under_symmetry</code> [__init__.py}{790}}	5.913	5.915	202	808
▶ <code>__import__</code>	5.782	15.766	382	78
▶ <code>fp_fdp_at_wavelength</code> [fdp_plot.py}{44}}	5.616	5.723	800	1,600
■ <code>MPI_Init_thread()</code>	4.987	4.987	1	0
■ <code>cuDevicePrimaryCtxRetain</code>	4.735	4.735	2	0
▶ <code><module></code> [__init__.py}{1}}	4.255	23.888	85	756
■ <code>MPI_Finalize()</code>	3.829	3.829	1	1
▶ <code>match_bijvoet_mates</code> [__init__.py}{1032}}	3.146	3.684	101	707
▶ <code>bcast</code>	3.073	3.448	1	9
▶ <code>__init__</code> [__init__.py}{20}}	3.011	3.399	101	149,196
▶ <code>compute_f_mask</code> [__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 binvrchs
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] binvrchs_ [{} /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] binvrchs_ [{} /rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/ε	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

TAU: ParaProf: Statistics for: node 0 - /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/bin

File Options Windows Help



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/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.]	2.89	2.89	288	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {228}	0.14	0.14	14	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.]	0.09	0.09	9	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.]	0.09	0.09	9	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.]	0.06	0.06	6	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.]	0.06	0.06	6	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.]	0.06	0.06	6	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.]	0.06	0.06	6	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {244}	0.05	0.05	5	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {332}	0.05	0.05	5	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {275}	0.05	0.05	5	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {331}	0.04	0.04	4	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {445}	0.04	0.04	4	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {254}	0.04	0.04	4	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {314}	0.04	0.04	4	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {343}	0.04	0.04	4	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {403}	0.04	0.04	4	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {389}	0.03	0.03	3	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {415}	0.03	0.03	3	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {247}	0.03	0.03	3	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {300}	0.03	0.03	3	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {309}	0.03	0.03	3	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {444}	0.03	0.03	3	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {468}	0.03	0.03	3	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {242}	0.03	0.03	3	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f.] {407}	0.03	0.03	3	0
[SAMPLE] binvcrhs_ [{} /rwthfs/rz/cluster/work/hpclub17/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/sj	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/g	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 [@] begin_ [{ /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 [{ /t	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] GNI_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

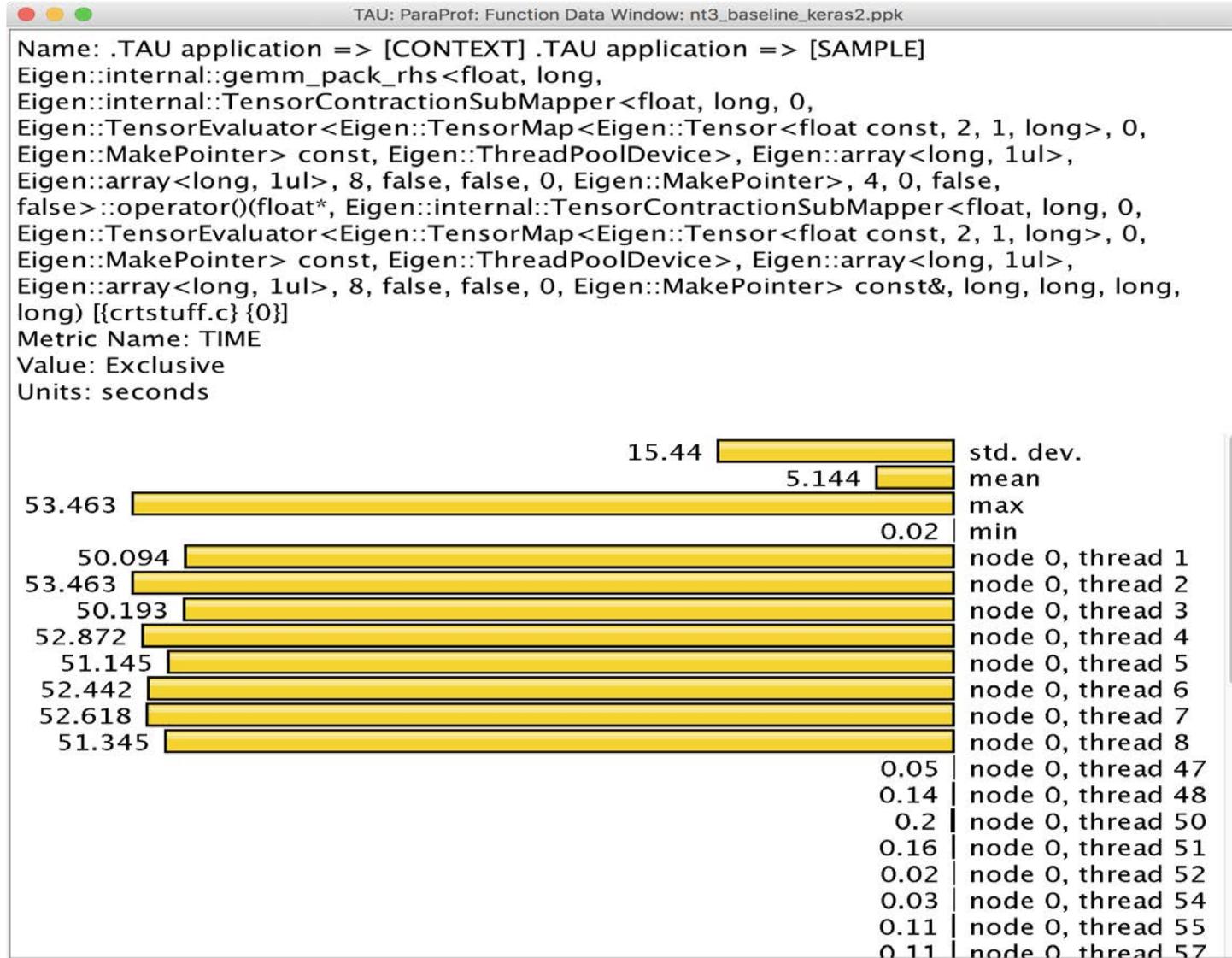
Deep Learning: Tensorflow

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

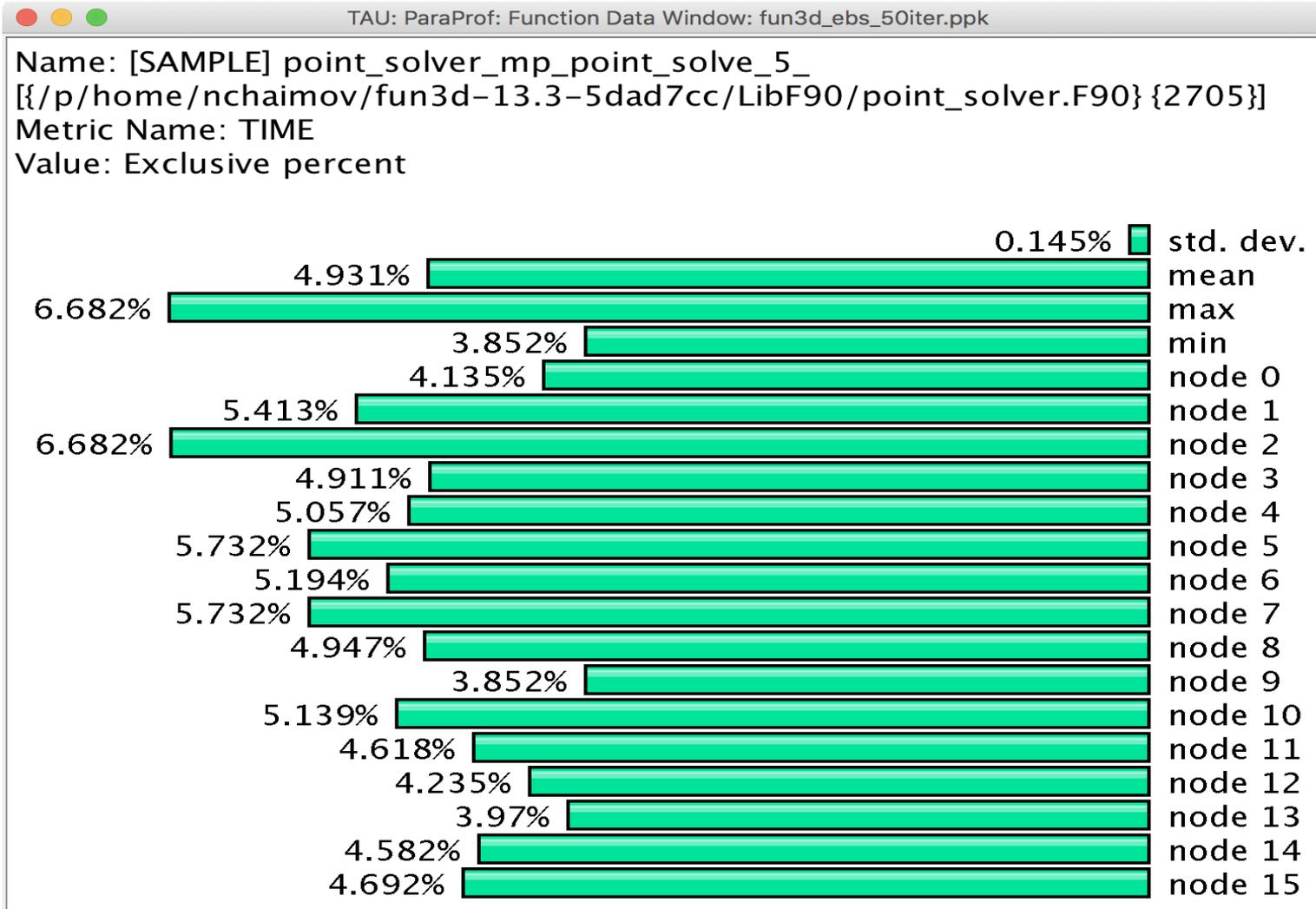
Name	Inclusiv...	Calls ▾
▼ .TAU application	519.211	1
▼ [CONTEXT] .TAU application	509.222	50,915
[SAMPLE] Eigen::internal::gebp_kernel<float, float, long, Eigen::internal::blas_data_mapper<float, long, 0, 0>,	240.632	24,089
[SAMPLE] __pthread_cond_wait [{} {0}]	86.384	8,634
[SAMPLE] Eigen::internal::gemm_pack_rhs<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<l	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<Eigen	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<l	2.91	291
[SAMPLE] std::_Function_handler<void (long, long), Eigen::internal::TensorExecutor<Eigen::TensorAssignOp<l	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<l	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::ptrtranspose(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)

Sampling Tensorflow



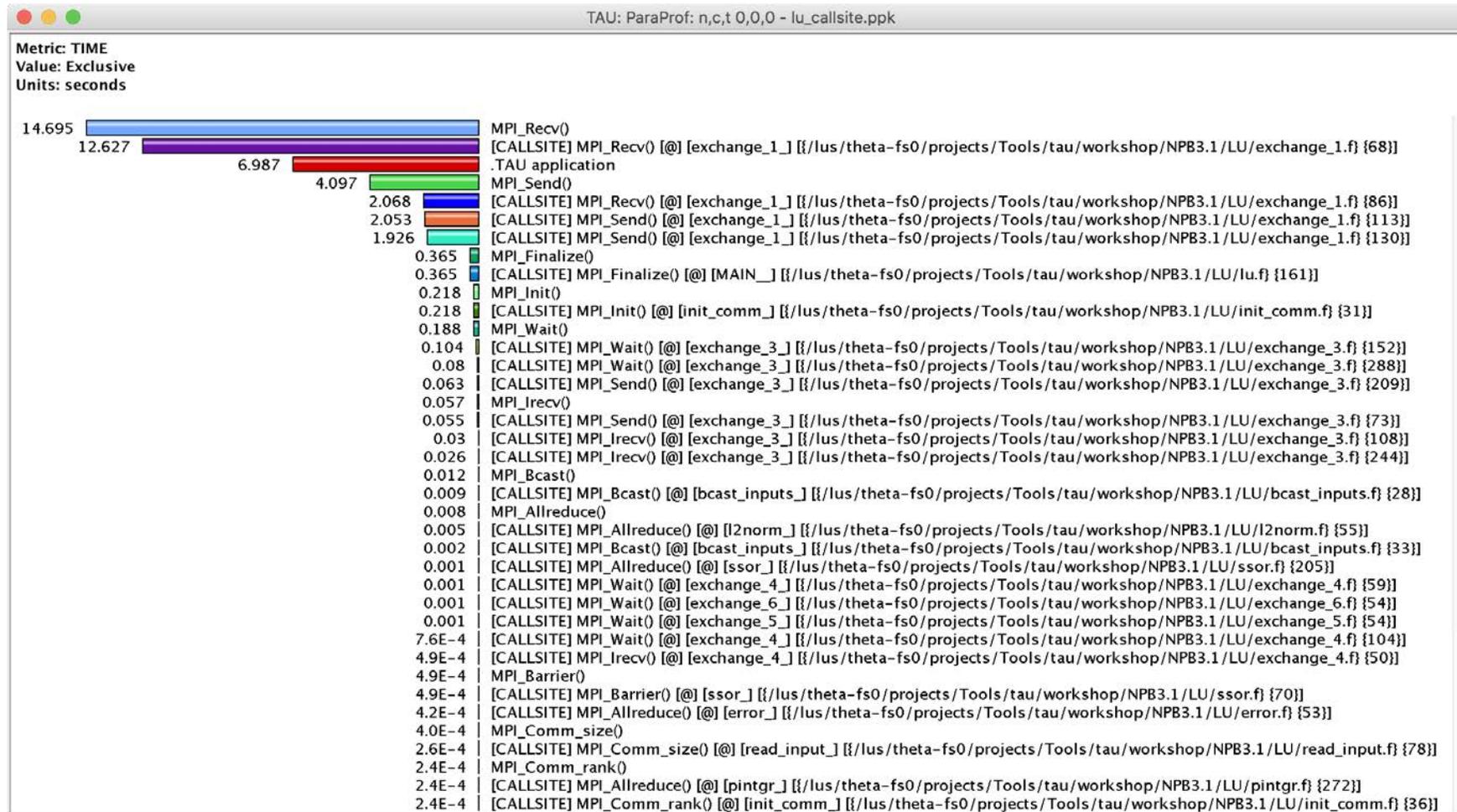
Event Based Sampling (EBS)



Uninstrumented!

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

Callsite Profiling and Tracing



% export TAU_CALLSITE=1

Identifying Collective Wait States: Thread Callpath Relations Window

TAU: ParaProf: Call Path Data n,c,t, 118,0,0 - 128_d3d.ppk

Metric Name: TIME
Sorted By: Exclusive
Units: seconds

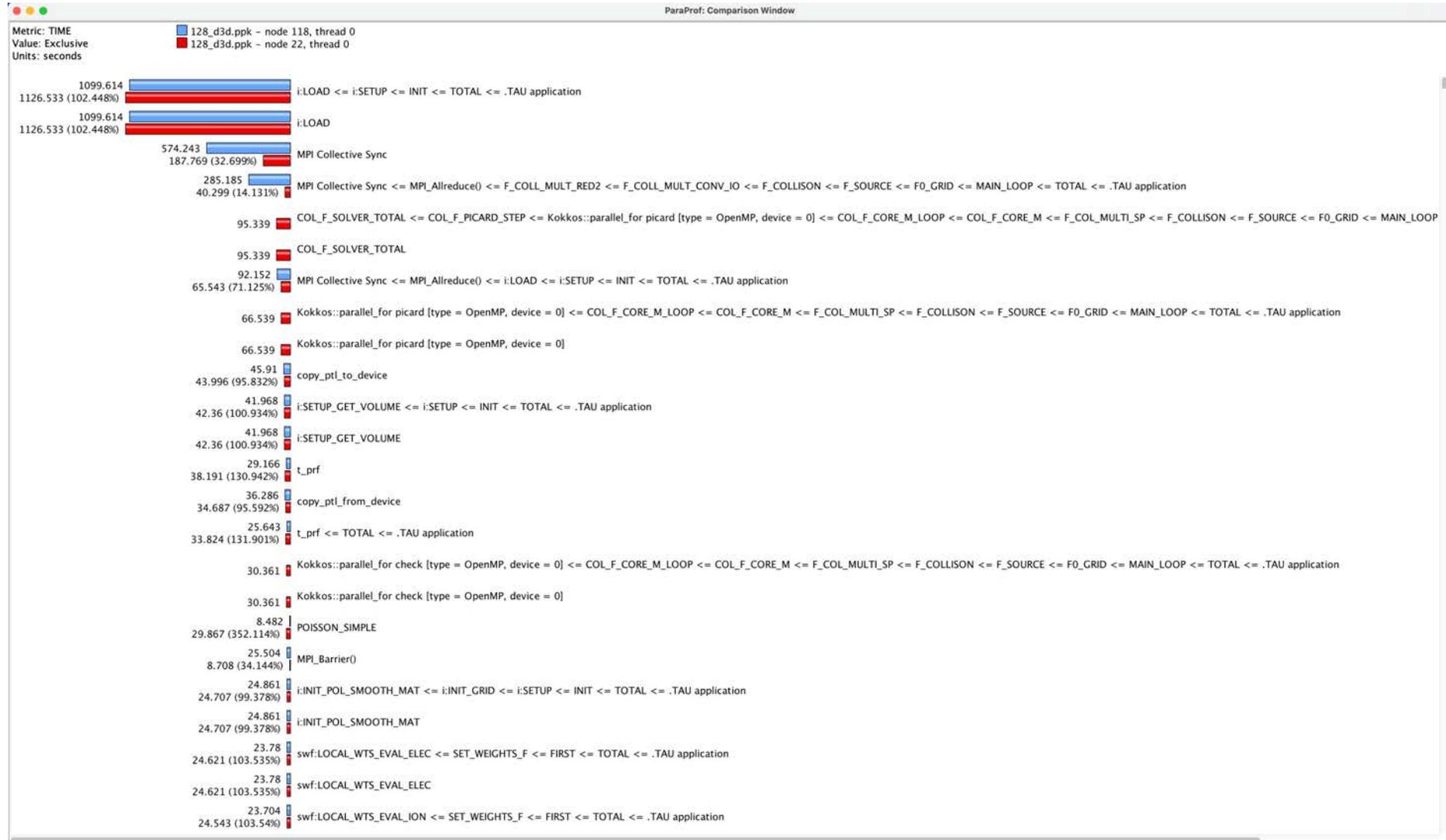
	Exclusive	Inclusive	Calls/Tot.Calls	Name[id]
	1099.614	1191.772	1/1	i:SETUP
-->	1099.614	1191.772	1	i:LOAD
	0.006	92.158	3/9543	MPI_Allreduce()
	9.8E-4	9.8E-4	11/15177	MPI_Gatherv()
	1.448	1.448	43/15177	MPI_Gather()
	15.353	15.353	46/15177	MPI_Alltoall()
	89.821	89.821	4311/15177	MPI_Bcast()
	6.777	6.777	195/15177	MPI_Allgather()
	68.678	68.678	991/15177	MPI_Reduce()
	9.179	9.179	12/15177	MPI_Comm_dup()
	0.125	0.125	25/15177	MPI_Allgatherv()
	382.861	382.861	9543/15177	MPI_Allreduce()
-->	574.243	574.243	15177	MPI Collective Sync
	2.507	2.508	10/186	DISTRIBUTE_F0G
	2.433	2.434	10/186	F_UPD_F0_SP
	5.156	5.158	20/186	F0_CHARGE_SEARCH_INDEX
	5.505	5.507	22/186	PULLBACK_WEIGHT
	24.86	24.872	102/186	UPDATE_PTL_WEIGHT
	0.473	0.473	2/186	MAIN_LOOP
	4.975	4.977	20/186	DIAG_f0_PORT1_PTL
-->	45.91	45.93	186	copy_ptl_to_device
	0.02	0.02	186/272	Kokkos::parallel_for set_buffer_particles_d [type = Cuda, device = 0]

MPI Collective Sync is the time spent in a barrier operation inside a collective

ParaProf Thread Comparison Window

Comparing Rank 118 with 22.

Right click on "node 118" -> Add node to comparison window



TAU – Context Events

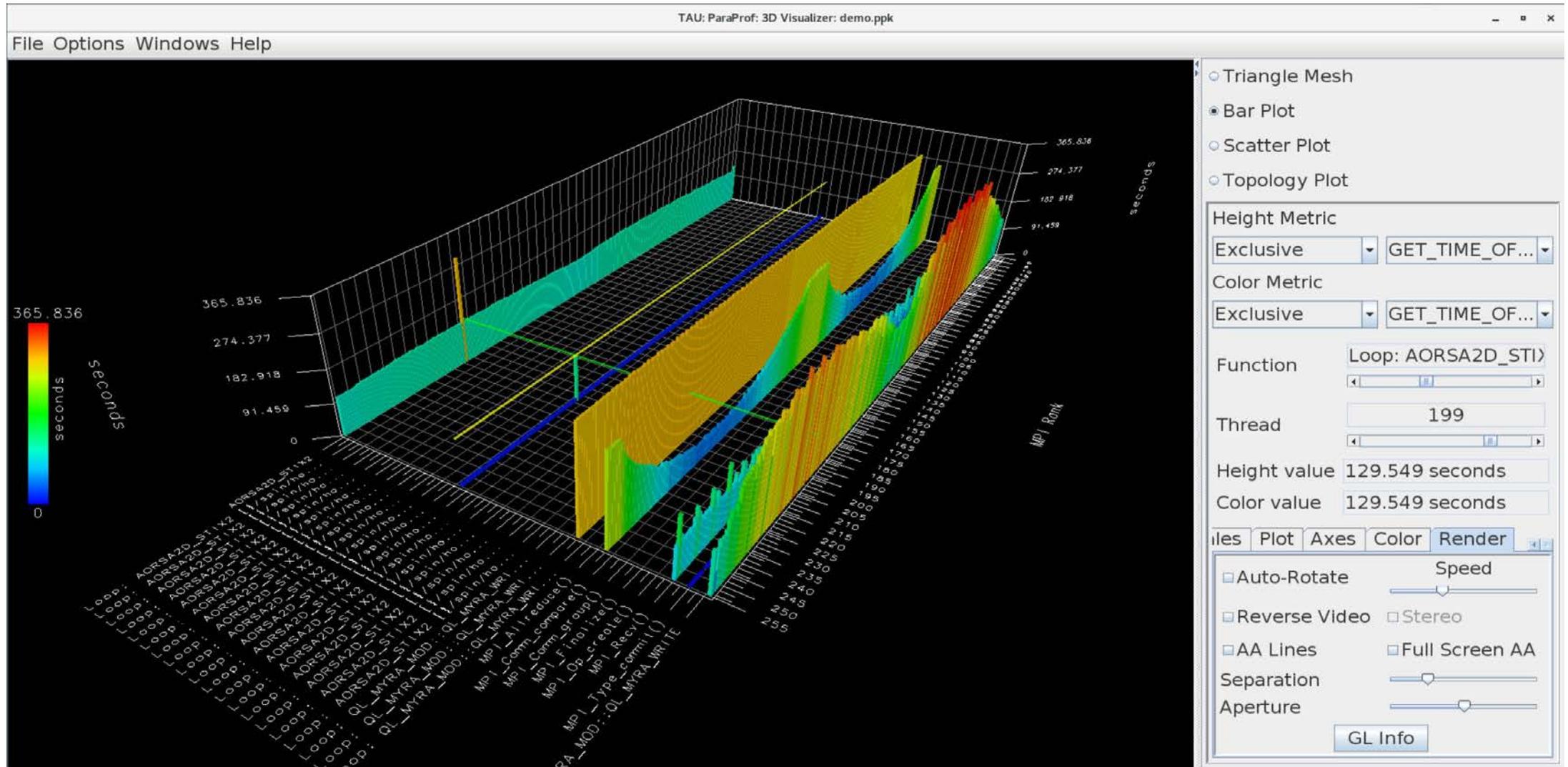
TAU: ParaProf: Context Events for thread: n,c,t, 1,0,0 – samarc_obe_4p_iomem_cp.ppk

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()						

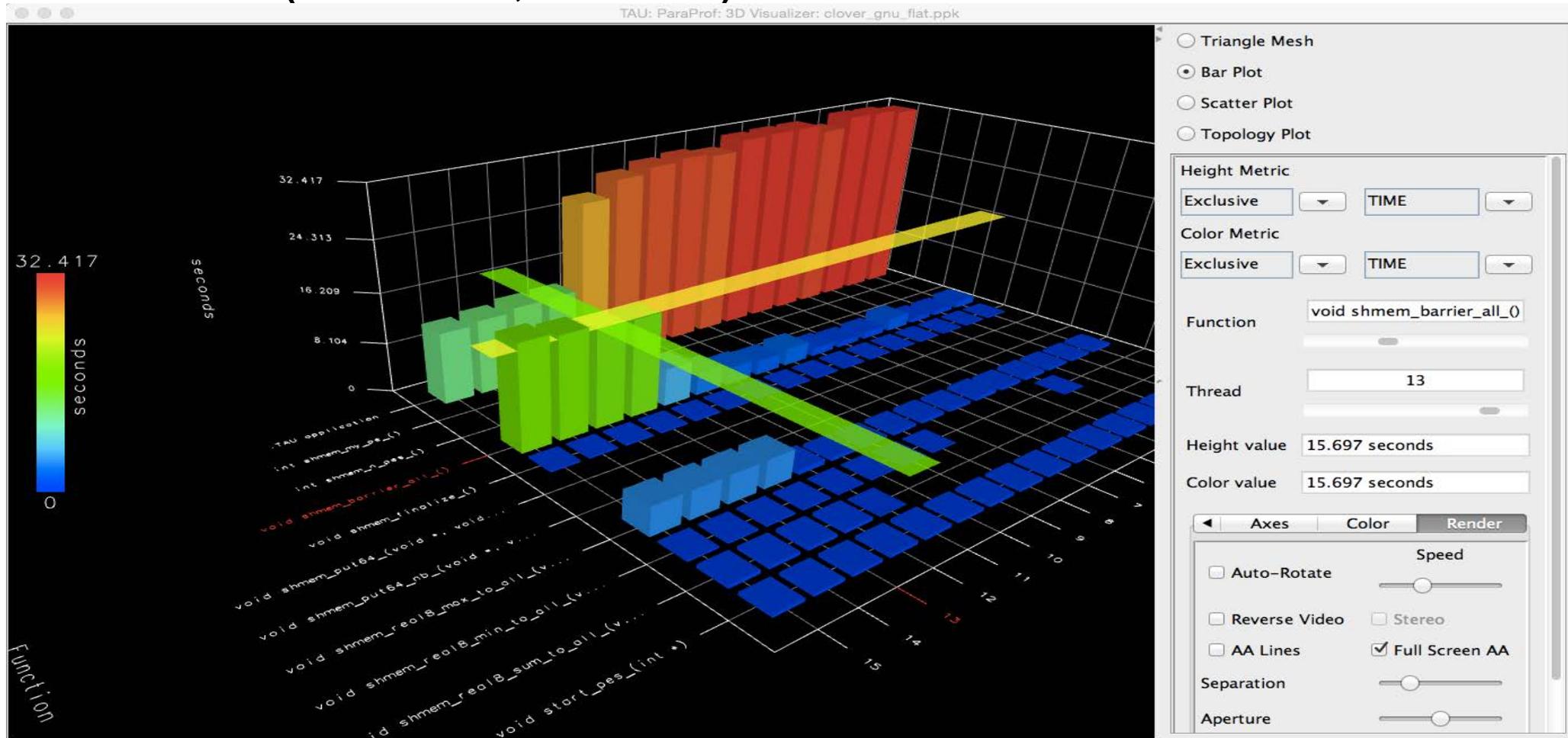
Write bandwidth per file

Bytes written to each file

ParaProf 3D Profile Browser: Bar Plot

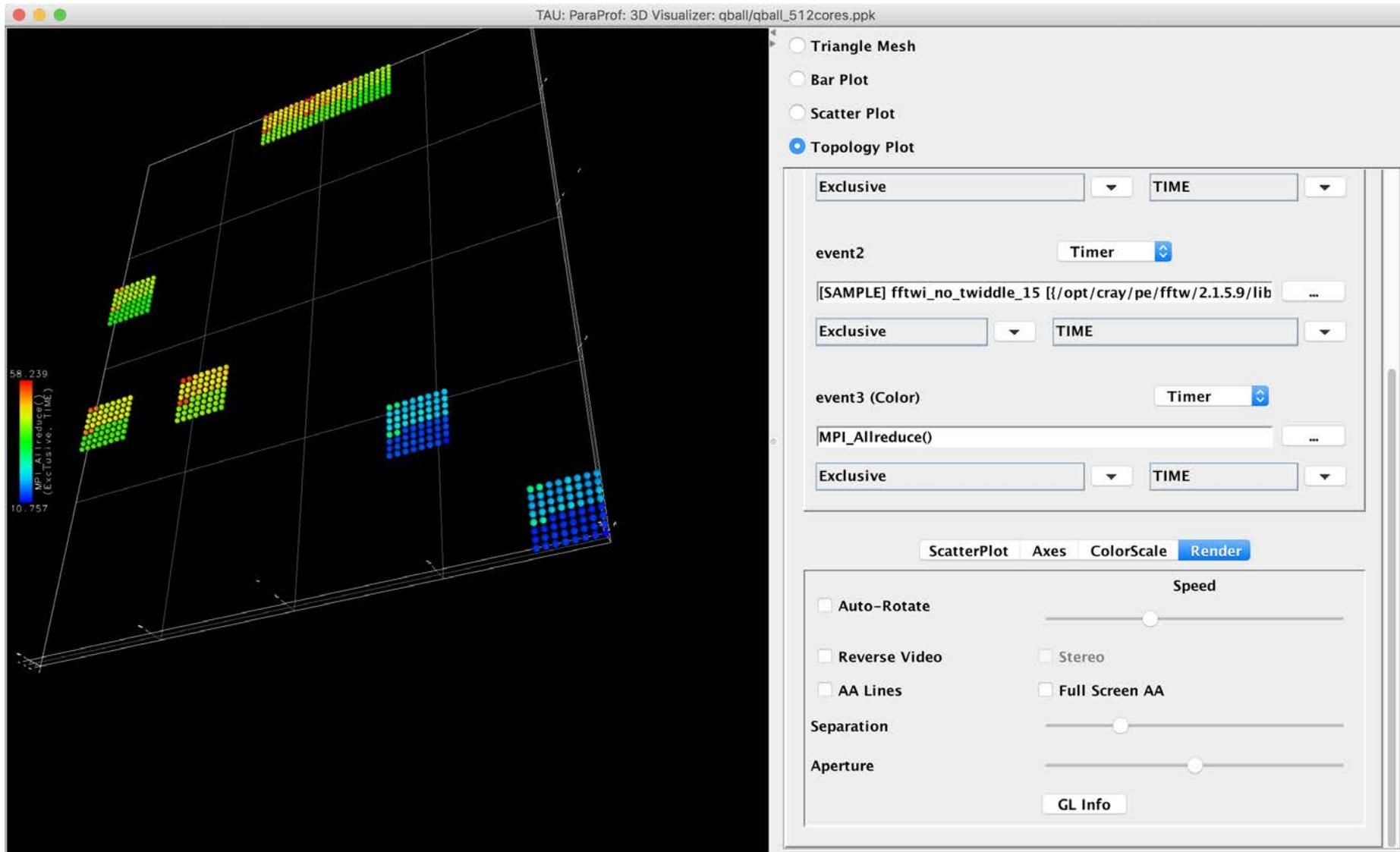


TAU – ParaProf 3D Visualization: Bar Plot using cross-hairs to zoom into a location (function, thread)

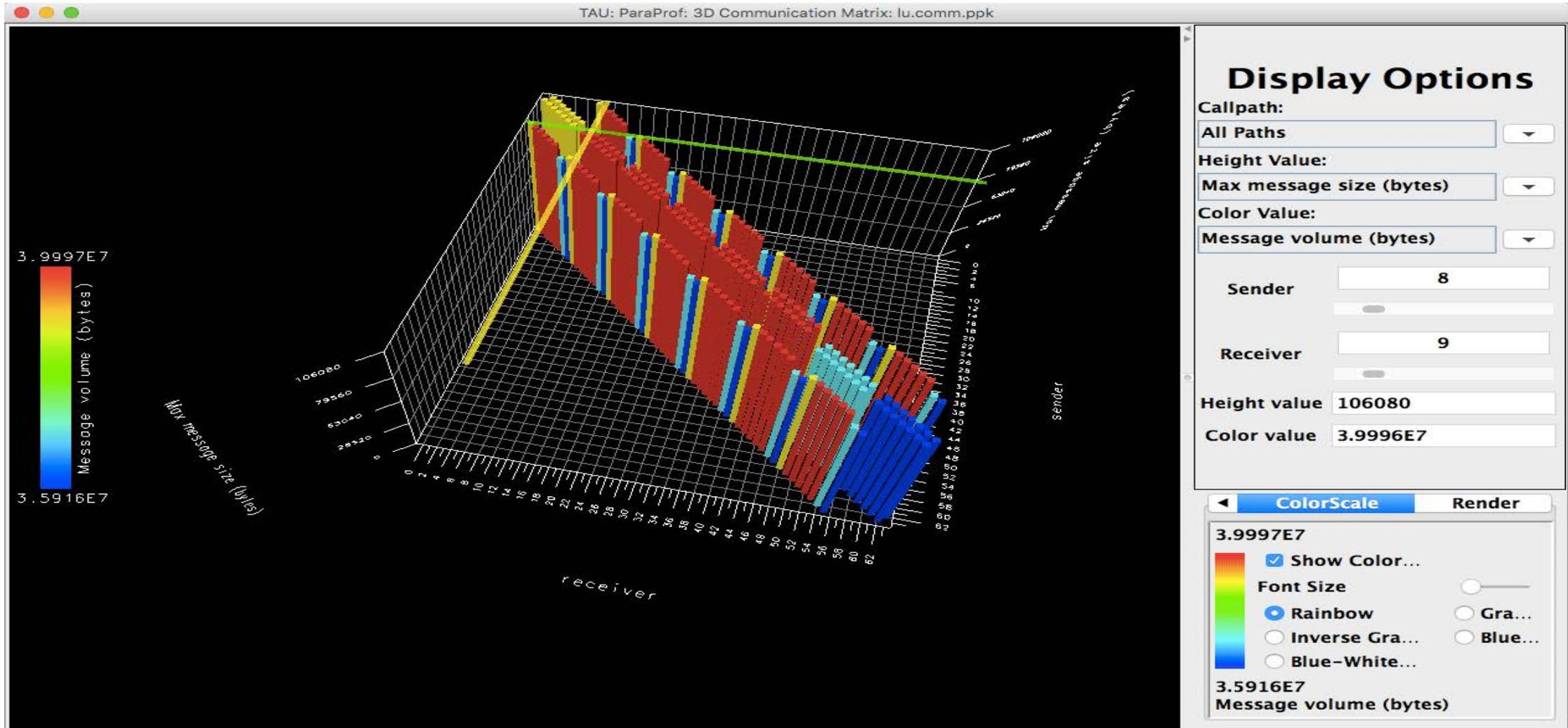


% paraprof app.ppk
Windows -> 3D Visualization -> Bar Plot (right pane)

TAU: ParaProf Topology Plot Window



TAU – 3D Communication Window

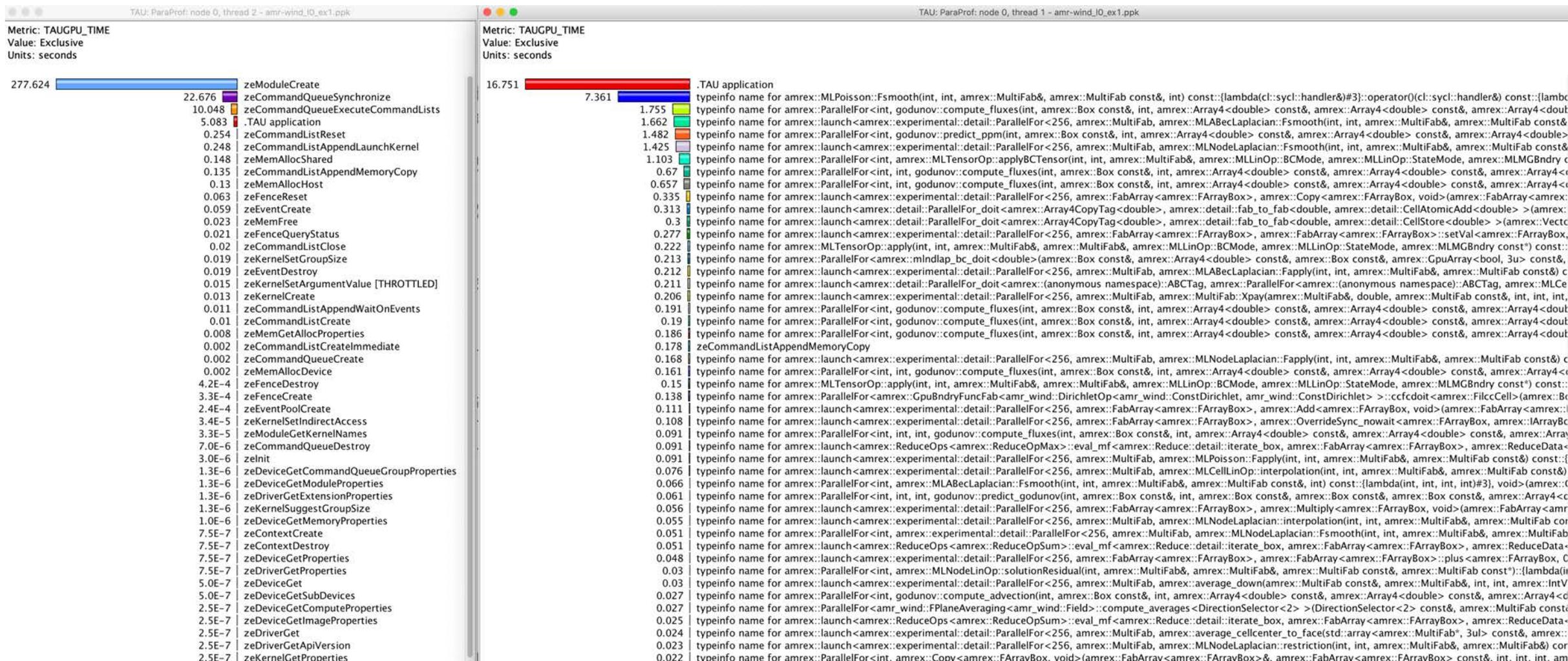


```
% export TAU_COMM_MATRIX=1; aprun ... tau_exec ./a.out  
% paraprof ; Windows -> 3D Communication Matrix
```

Using TAU on GPUs



TAU: Intel oneAPI DPC++ on an Intel Gen12LP or DG1 GPU



% tau_exec -T level_zero,serial -l0 ./a.out

TAU: Intel oneAPI DPC++ on an Intel Gen12LP or DG1 GPU

TAU: ParaProf: Statistics for: node 0, thread 1 - iso3dfd_dccpp.ppk

Name	Exclusive TAUGPU_TIME	Inclusive TAUGPU_TIME	Calls	Child Calls
.TAU application	0.18	22.279	1	10,002
_ZTSZZ13iso3dfdDeviceRN2c14sycl5queueEPFS3_S3_mmmmmmmjENKUIRT_E313_16clINS0_7handlerEEDaS5_EUIS4_E399_58	11.063	11.063	5,000	0
_ZTSZZ13iso3dfdDeviceRN2c14sycl5queueEPFS3_S3_mmmmmmmjENKUIRT_E313_16clINS0_7handlerEEDaS5_EUIS4_E407_58	11.033	11.033	5,000	0
zeCommandListAppendMemoryCopy	0.003	0.003	2	0

TAU: ParaProf: Statistics for: node 0, thread 0 - iso3dfd_dccpp.ppk

Name	Exclusive TAUGPU_TIME	Inclusive TAUGPU_TIME	Calls	Child Calls
pthread_create	0	0	1	0
.TAU application	22.73	22.73	1	1
[CONTEXT] .TAU application	0	22.71	729	0
[SAMPLE] std::_Sp_counted_ptr_inplace<cl::sycl::detail::event_impl, std::allocator<cl::sycl::detail::event_impl>, (_gnu_cxx::Lock_policy)2>	0.03	0.03	1	0
[SAMPLE] cl::sycl::detail::pi::emitFunctionEndTrace(unsigned long, char const*) [(crststuff.c) {0}]	0.09	0.09	2	0
[SAMPLE] cl::sycl::detail::Scheduler::GraphBuilder::cleanupCommandsForRecord(cl::sycl::detail::MemObjRecord*) [(crststuff.c) {0}]	0.03	0.03	1	0
[SAMPLE] cl::sycl::detail::LeavesCollection::push_back(cl::sycl::detail::Command*) [(crststuff.c) {0}]	0.03	0.03	1	0
[SAMPLE] cl::sycl::detail::ExecCGCommand::enqueueImp0 [(crststuff.c) {0}]	0.03	0.03	1	0
[SAMPLE] cl::sycl::detail::ExecCGCommand::SetKernelParamsAndLaunch(cl::sycl::detail::CGExecKernel*, _pi_kernel*, cl::sycl::detail::NDRDes	0.03	0.03	1	0
[SAMPLE] cl::sycl::detail::Command::addDep(cl::sycl::detail::DepDesc) [(crststuff.c) {0}]	0.03	0.03	1	0
[SAMPLE] _pi_device::getAvailableCommandList(_pi_queue*, _ze_command_list_handle_t**, _ze_fence_handle_t**) [(crststuff.c) {0}]	0.03	0.03	1	0
[SAMPLE] _gnu_cxx::__atomic_add(int volatile*, int) [(/usr/lib/gcc/x86_64-linux-gnu/9/../../../../include/c++/9/ext/atomicity.h) {53}]	0.03	0.03	1	0
[SAMPLE] UNRESOLVED UNKNOWN	0.06	0.06	2	0
[SAMPLE] UNRESOLVED /usr/lib/x86_64-linux-gnu/libze_intel_gpu.so.1.0.18513	0.509	0.509	17	0
[SAMPLE] UNRESOLVED /usr/lib/x86_64-linux-gnu/libstdc++.so.6.0.28	0.03	0.03	1	0
[SAMPLE] UNRESOLVED /usr/lib/x86_64-linux-gnu/libpthread-2.31.so	0.06	0.06	2	0
[SAMPLE] UNRESOLVED /usr/lib/x86_64-linux-gnu/libgic.so.1.0.5585	0.18	0.18	6	0
[SAMPLE] UNRESOLVED /usr/lib/x86_64-linux-gnu/libc-2.31.so	20.852	20.852	669	0
[SAMPLE] UNRESOLVED /usr/lib/x86_64-linux-gnu/ld-2.31.so	0.15	0.15	5	0
[SAMPLE] UNRESOLVED /home/shende/tau2/x86_64/lib/libTAUsh-level_zero-pthread.so	0.479	0.479	15	0
[SAMPLE] Initialize(float*, float*, float*, unsigned long, unsigned long, unsigned long) [(/home/users/sameer/samples/iso3dfd_dccpp/src	0.03	0.03	1	0

TAU: ParaProf: Statistics for: node 0, thread 2 - iso3dfd_dccpp.ppk

Name	Exclusive TAUGPU_TIME	Inclusive TAUGPU_TIME	Calls	Child Calls
.TAU application	2.738	22.592	1	290,467
zeCommandQueueExecuteCommandLists	19.073	19.073	10,002	0
zeModuleCreate	0.272	0.272	1	0
zeCommandListReset	0.165	0.165	10,002	0
zeEventHostSynchronize	0.118	0.118	22	0
zeCommandListAppendLaunchKernel	0.073	0.073	10,000	0
zeKernelSetArgumentValue [THROTTLED]	0.043	0.043	100,001	0
zeFenceQueryStatus [THROTTLED]	0.03	0.03	100,001	0
zeMemAllocHost	0.019	0.019	4	0
zeKernelSetGroupSize	0.012	0.012	10,000	0
zeCommandListClose	0.011	0.011	10,002	0
zeKernelGetProperties	0.01	0.01	10,000	0
zeEventCreate	0.007	0.007	10,002	0
zeMemFree	0.006	0.006	4	0
zeFenceReset	0.004	0.004	10,002	0
zeEventPoolDestroy	0.003	0.003	39	0
zeCommandListCreate	0.003	0.003	78	0
zeCommandListAppendMemoryCopy	0.002	0.002	2	0
zeEventPoolCreate	0.001	0.001	40	0
zeEventDestroy	0.001	0.001	10,002	0

% tau_exec -T level_zero,serial -l0 ./a.out

Intel Level Zero (TigerLake Gen12LP integrated CPUs or DG1)

TAU: ParaProf: Statistics for: node 0, thread 0 - ze_gemm_4096.ppk

Name	Exclusive TAUGPU_T...	Inclusive TAUGPU_TI...	Calls	Child Calls
TAU application	117,876	30,283,630	1	256
zeCommandQueueSynchronize	29,877,963	29,877,963	4	0
[CONTEXT] zeCommandQueueSynchronize	0	29,905,688	997	0
[SAMPLE] __GI__sched_yield [lib64/libc-2.26.so]	25,765,719	25,765,719	859	0
[SAMPLE] UNRESOLVED /soft/libraries/intel-level-zero	4,139,969	4,139,969	138	0
zeCommandQueueExecuteCommandLists	186,203	186,203	4	0
zeModuleCreate	98,896	98,896	1	0
zeCommandListAppendMemoryCopy	1,410	1,410	12	0
zeCommandQueueDestroy	321	321	4	0
zeDriverAllocDeviceMem	137	137	12	0
zeEventPoolDestroy	128	128	20	0
zeDriverFreeMem	96	96	12	0
zeCommandListCreate	89	89	4	0
zeCommandQueueCreate	82	82	4	0
zeCommandListDestroy	71	71	4	0
zeKernelSetArgumentValue	43	43	16	0
zeDeviceGetProperties	38	38	26	0
zeCommandListClose	35	35	4	0
zeEventCreate	30	30	4	0
zeEventDestroy	30	30	24	0
zeEventGetTimestamp	28	28	48	0
pthread_create	26	26	1	0
zeEventPoolCreate	20	20	4	0
zeKernelDestroy	20	20	1	0
zeModuleDestroy	17	17	1	0
zeCommandListAppendLaunchKernel	15	15	4	0
zeCommandListAppendBarrier	13	13	8	0
zeKernelSuggestGroupSize	12	12	4	0
zeEventQueryStatus	11	11	20	0
zeKernelCreate	11	11	1	0
zeKernelSetGroupSize	5	5	4	0
zeDeviceGet	2	2	2	0
zeInit	2	2	1	0
zeDriverGet	0	0	2	0

Units: microseconds

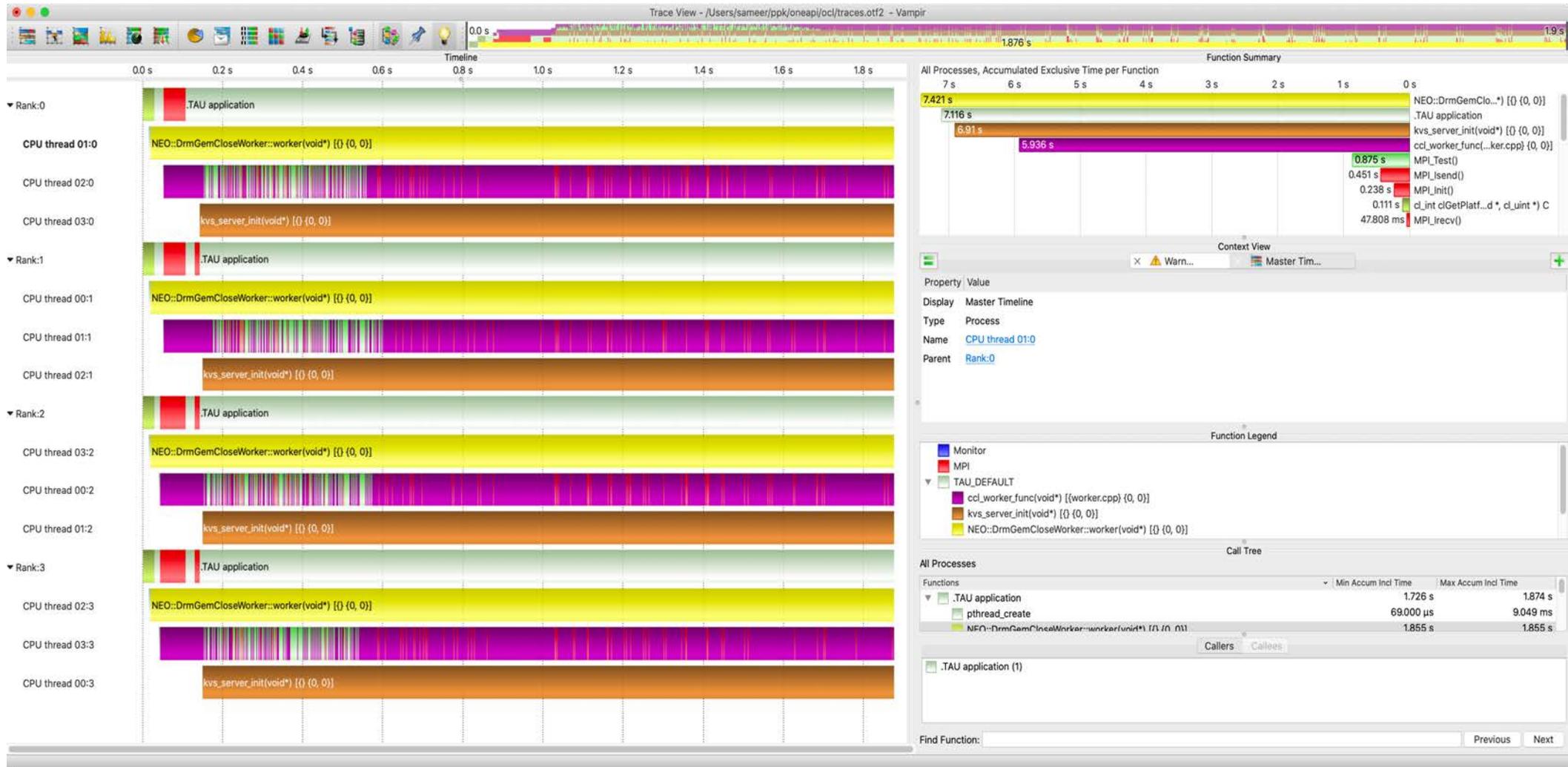
TAU: ParaProf: Statistics for: node 0, thread 2 - ze_gemm_4096.ppk

Name	Exclusive TAU...	Inclusive TAUG...	Calls	Child Calls
.TAU application	0.131	29.88	1	24
<Barrier>	0	0	8	0
<MemoryCopy>	0.049	0.049	12	0
GEMM	29.7	29.7	4	0

Units: seconds

Time spent in GEMM kernel

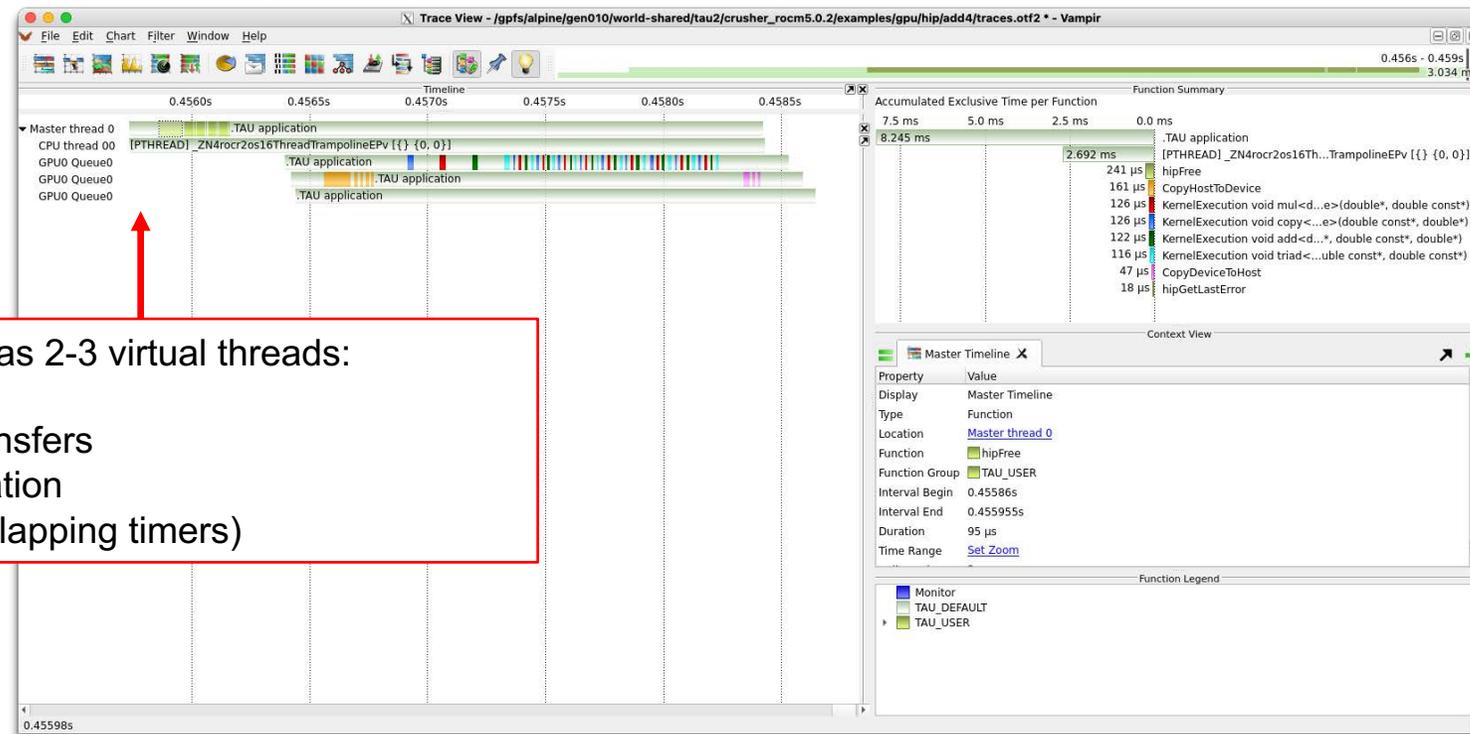
TAU and Vampir [TU Dresden]: Intel oneAPI OpenCL with MPI



```
% export TAU_TRACE=1; export TAU_TRACE_FORMAT=otf2
% mpirun -np 4 tau_exec -T level_zero -opencl ./a.out
```

Tracing support uses RocTracer

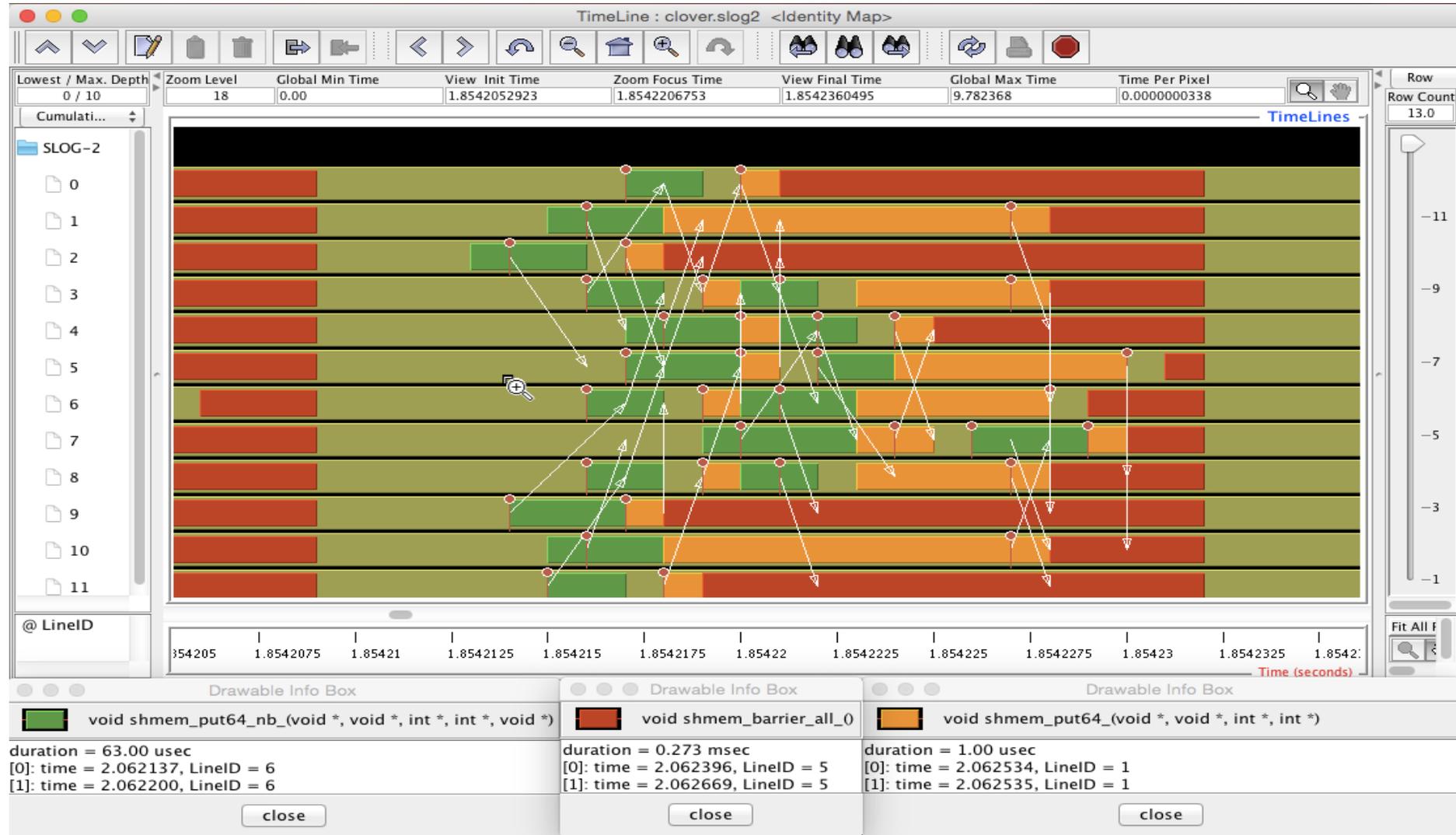
```
$ TAU_TRACE=1 TAU_TRACE_FORMAT=otf2 tau_exec -T serial,roctracer ./gpu-stream-hip
```



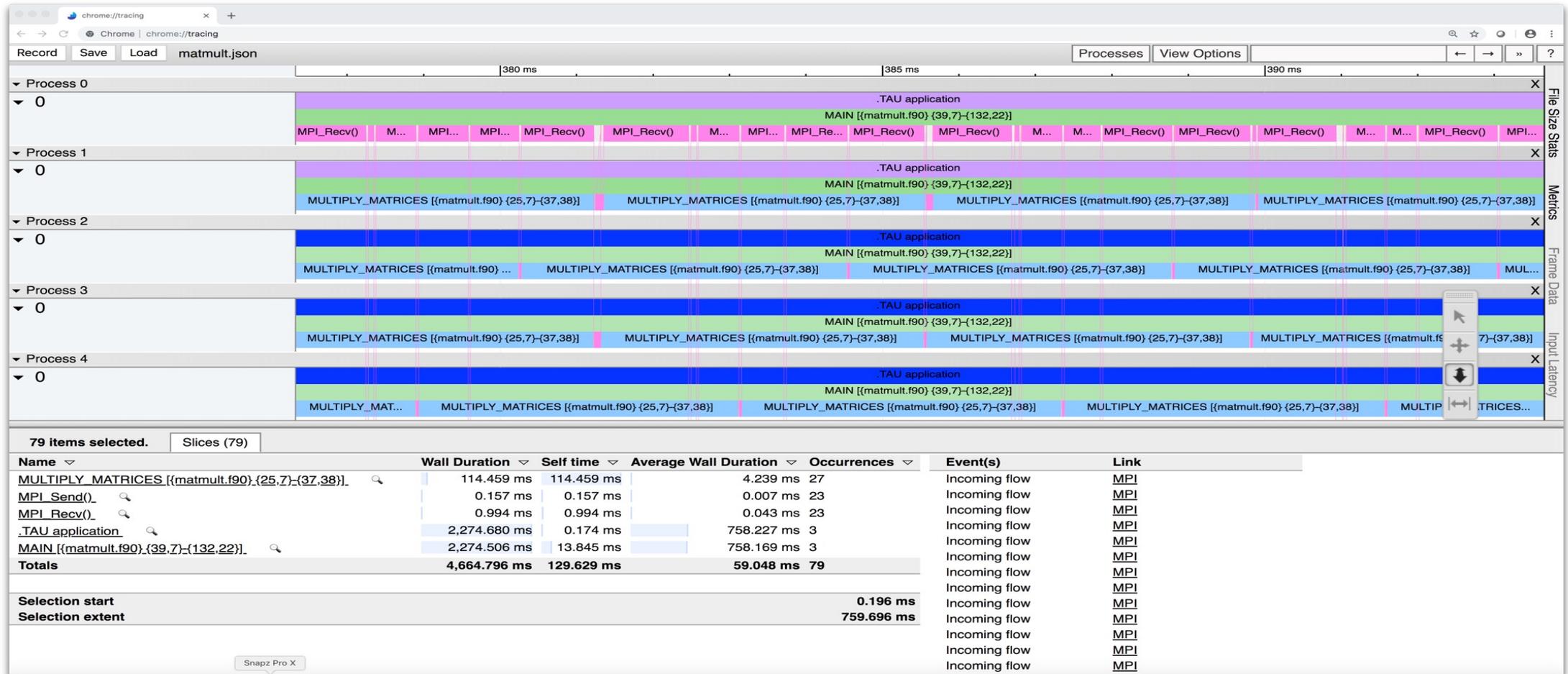
Each device has 2-3 virtual threads:
1) kernels,
2) memory transfers
3) synchronization
(prevents overlapping timers)

TAU output shown in Vampir

Tracing: Jumpshot (ships with TAU)



Tracing: Chrome Browser



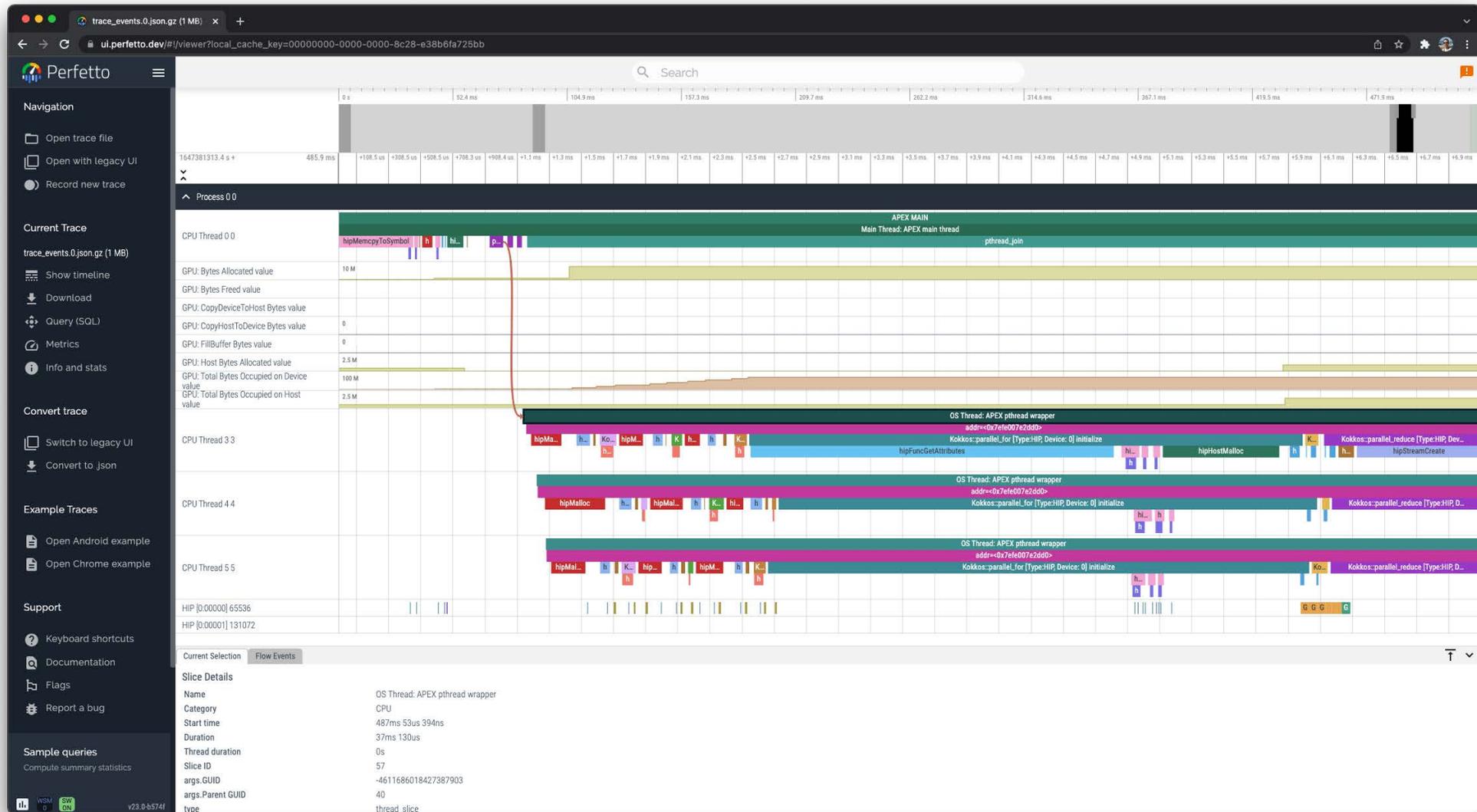
% export TAU_TRACE=1

% mpirun -np 256 tau_exec ./a.out

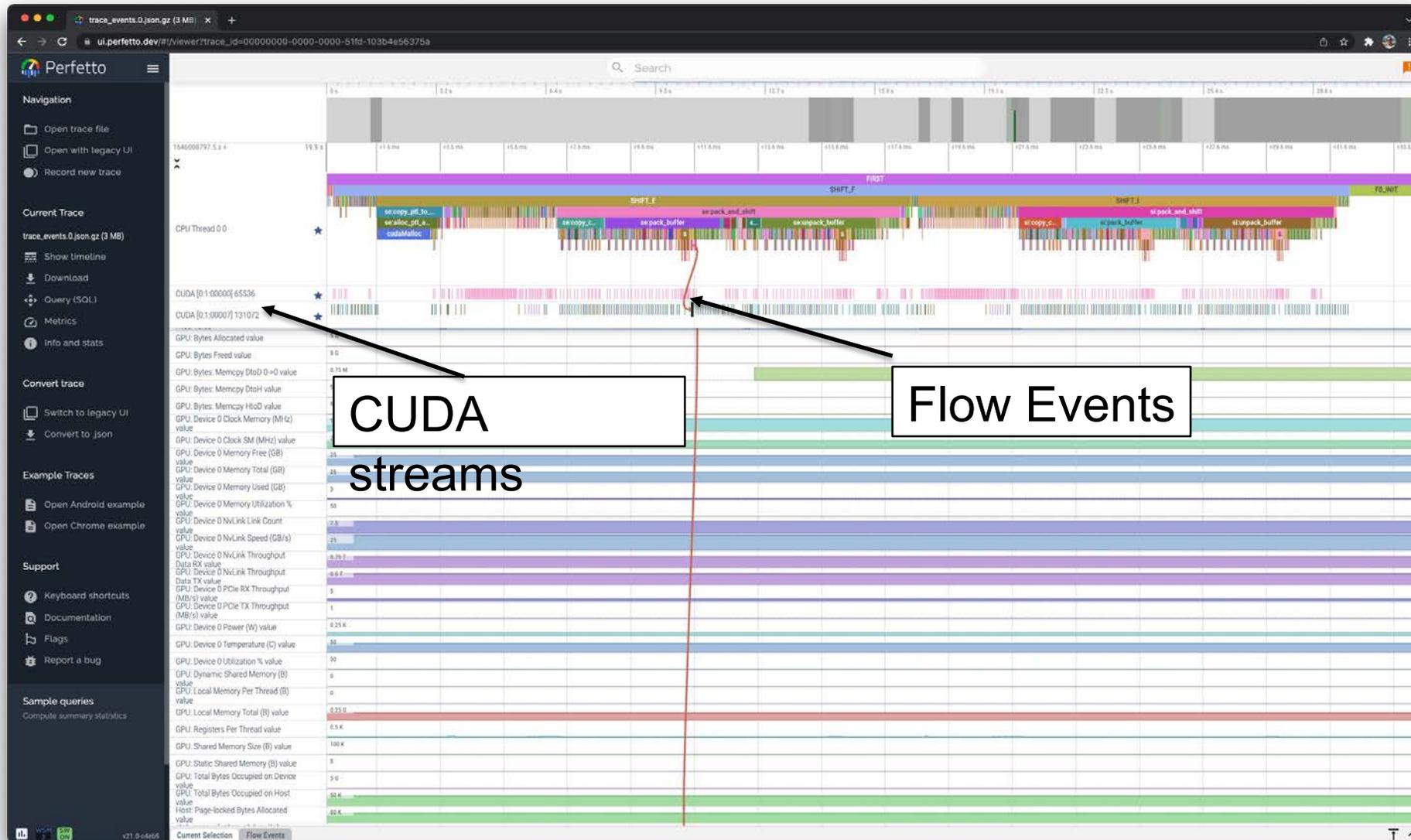
% tau_treemerge.pl; tau_trace2json tau.trc tau.edf -chrome -ignoreatomic -o app.json

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

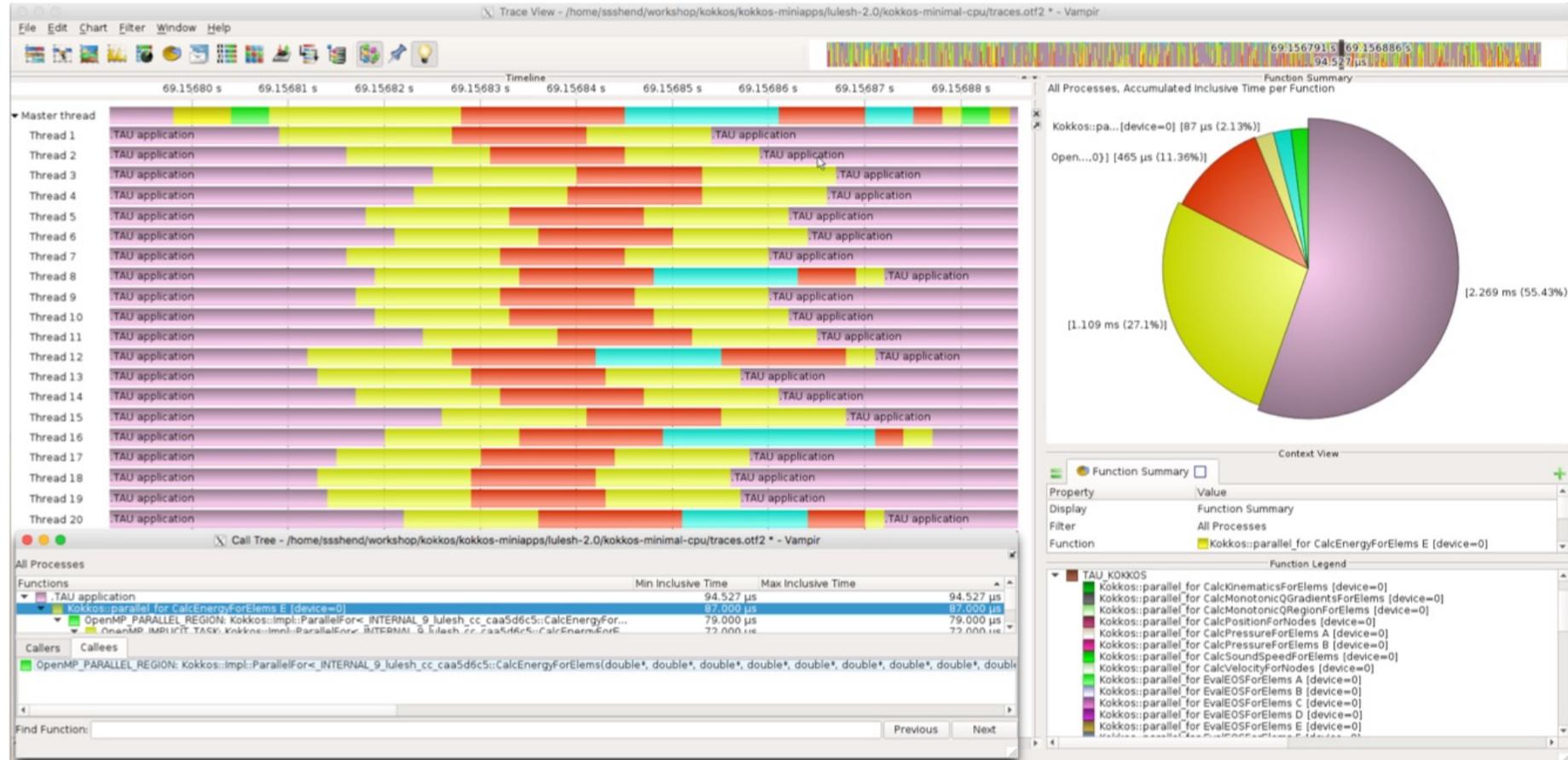
Perfetto.dev Trace Browser: Kokkos Example



Perfetto.dev Trace Browser



Vampir [TU Dresden] Timeline: Kokkos



```
% export TAU_TRACE=1; export TAU_TRACE_FORMAT=otf2
% tau_exec -T serial,ompt -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/ORNLD/DEMO/BUILD/ExaMiniMD-pthread/ExaMiniMD/src/comm_types (ssh)
void CommMPI::update_halo() {
    Kokkos::Profiling::pushRegion("Comm::update_halo"); ← 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::parallel_for
                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]; ← popRegion
    }

    Kokkos::Profiling::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<CommMF	0.489	0.489	190	0
OpenMP_Sync_Region_Barrier parallel_for<Kokkos::RangePolicy<CommMF	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



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>, void>::	0.03	0.03	1	0
└─ [SUMMARY] LAMMPS_RandomVelocityGeom::uniform0 [{} {/g/g20/reeve5/pr/CabanaMD/src/input.h}]	0.03	0.03	1	0
└─ [SAMPLE] LAMMPS_RandomVelocityGeom::uniform0 [{} {/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_Finalize0	0.367	0.369	1	68
└─ Comm::exchange_halo	0.026	0.351	6	4,772
└─ MPI_Init0	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_Allreduce0	0.082	0.082	39	0
└─ [CONTEXT] MPI_Allreduce0	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

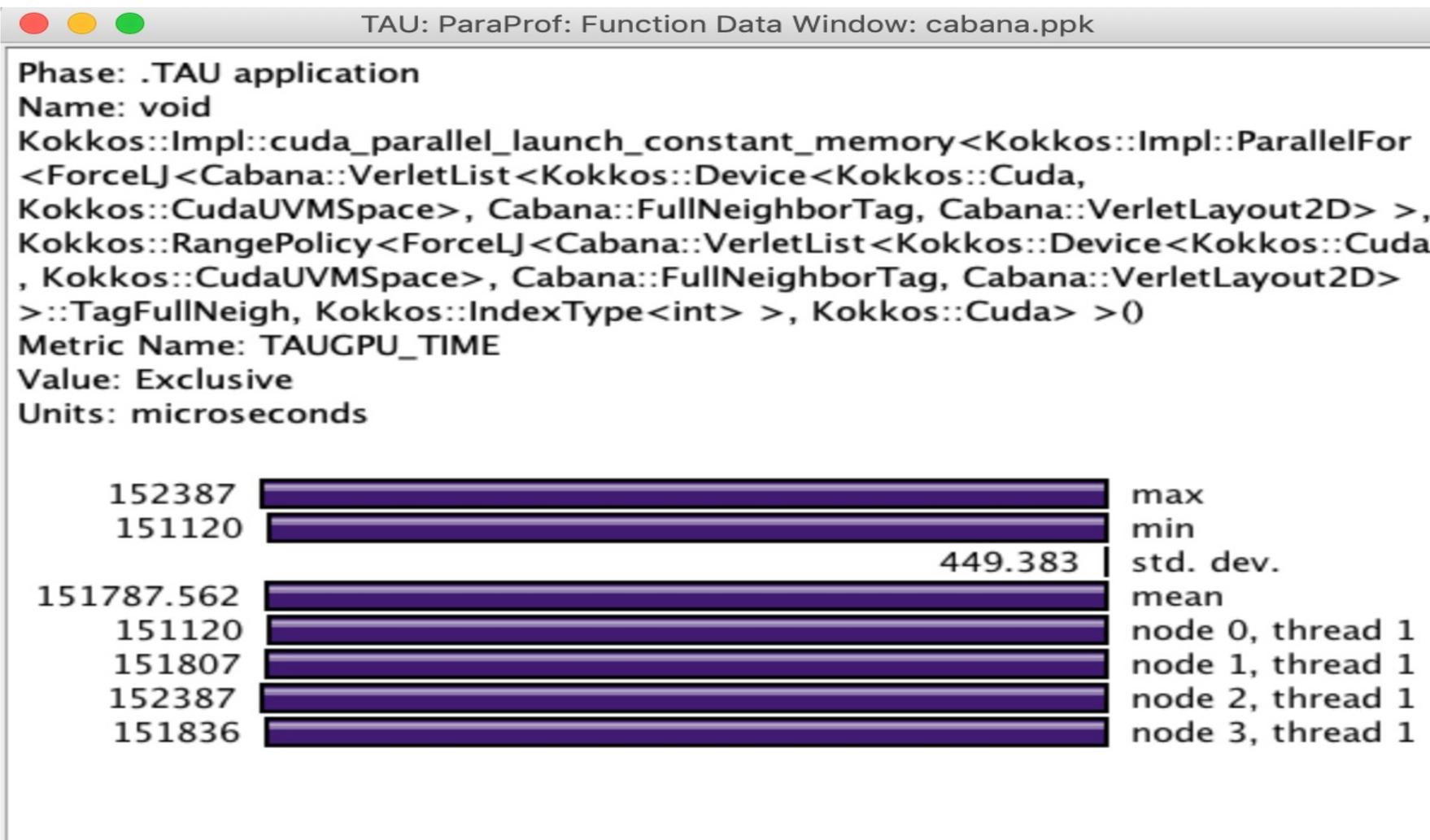
Kokkos sample within top-level application code

Instrumented Kokkos::parallel_for

Instrumented Kokkos::parallel_reduce

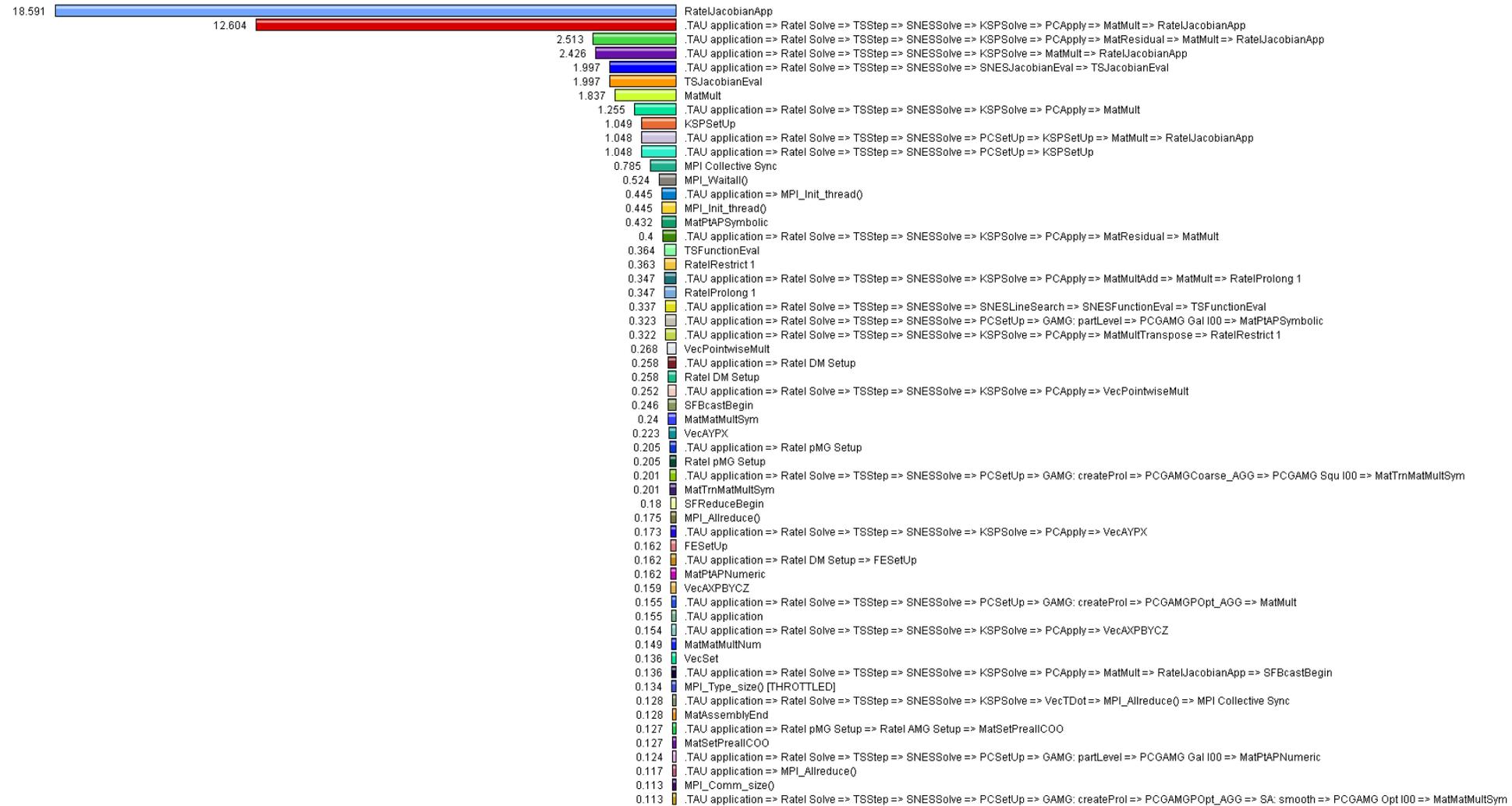
Event-based sampling (EBS) with Kokkos API

CabanaMD: CUDA Events



Mapping Events from PETSc using PerfStubs to TAU

Metric: TIME
Value: Exclusive
Units: seconds



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,intel,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
```



EXTRACTION
COMPUTING
PROJECT

```
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:

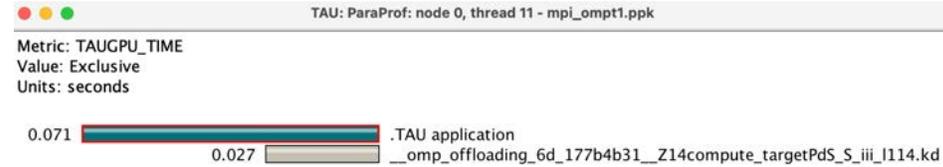
Tracks heap allocation/deallocation and memory leaks.

-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

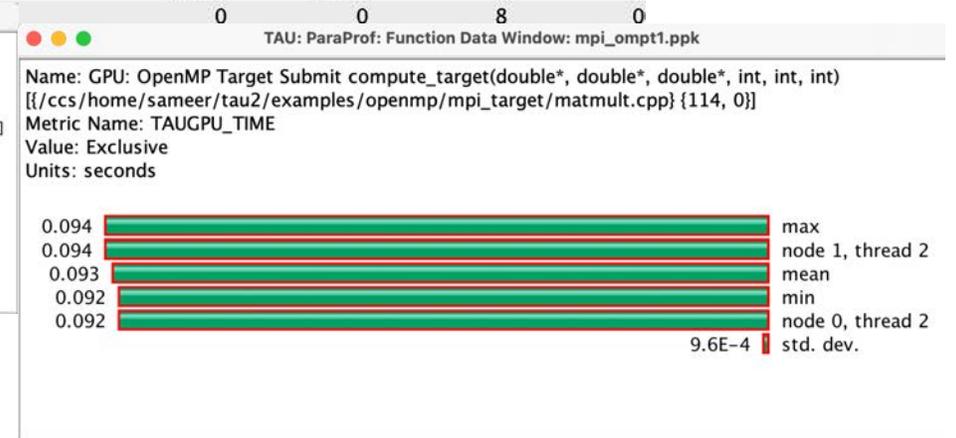
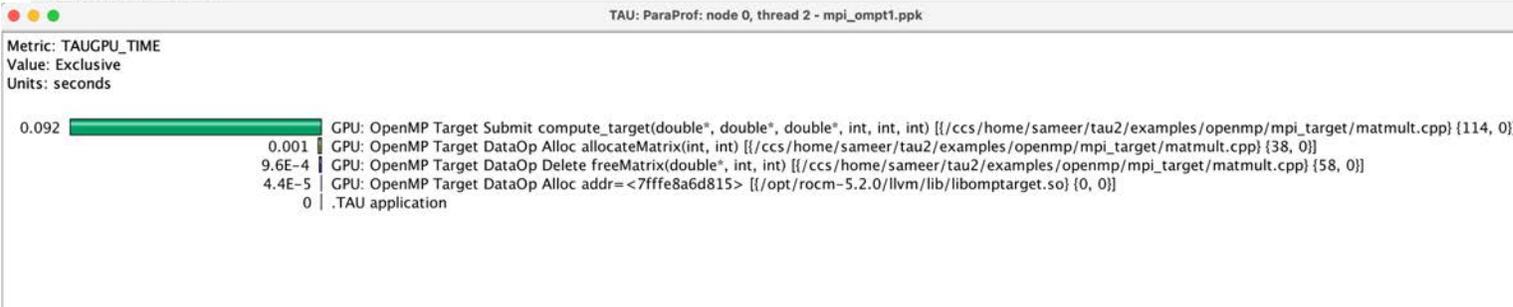
tau_exec can enable event based sampling while launching the executable using environment var **TAU_SAMPLING=1** or tau_exec **-ebs**

AMD HIPCC: OMPT Target Offload Support in TAU



TAU: ParaProf: Statistics for: node 0, thread 0 - mpi_ompt1.ppk

Name Δ	Exclusive...	Inclusive ...	Calls	Child Calls
.TAU application{{0}-{0xffffffff}}	1.566	1.829	1	124
MPI_Comm_rank()	0	0	1	0
MPI_Finalize()	0.01	0.01	1	1
MPI_Init()	0.118	0.118	1	0
OpenMP_Parallel_Region do_work() [{/autofs/nccs-svm1_home1/sameer/public/tau2/examples/openmp/mpi_target/matmult} {0, 0}]	0	0.025	20	47
OpenMP_Parallel_Region do_work() [{/ccs/home/sameer/tau2/examples/openmp/mpi_target/matmult.cpp} {148, 0}]	0	0.007	10	20
OpenMP_Sync_Region_Barrier_Implicit do_work() [{/autofs/nccs-svm1_home1/sameer/public/tau2/examples/openmp/mpi_target/matmult} {0, 0}]	0.023	0.023	20	0
OpenMP_Sync_Region_Barrier_Implicit do_work() [{/ccs/home/sameer/tau2/examples/openmp/mpi_target/matmult.cpp} {148, 0}]	0.006	0.006	10	0
OpenMP_Target allocateMatrix(int, int) [{/ccs/home/sameer/tau2/examples/openmp/mpi_target/matmult.cpp} {38, 0}]	0.007	0.007	30	1
OpenMP_Target compute_target(double*, double*, double*, int, int, int) [{/ccs/home/sameer/tau2/examples/openmp/mpi_target/matmult.cpp} {113, 0}]	0	0	20	0
OpenMP_Target compute_target(double*, double*, double*, int, int, int) [{/ccs/home/sameer/tau2/examples/openmp/mpi_target/matmult.cpp} {114, 0}]	0.094	0.094	10	0
OpenMP_Target freeMatrix(double*, int, int) [{/ccs/home/sameer/tau2/examples/openmp/mpi_target/matmult.cpp} {58, 0}]	0.001	0.001	30	0
OpenMP_Work_Loop .omp_outlined. [{/ccs/home/sameer/tau2/examples/openmp/mpi_target/matmult.cpp} {48, 0}]	0.002	0.002	30	0
pthread_create	0.001	0.001	9	0
	0	0	8	0



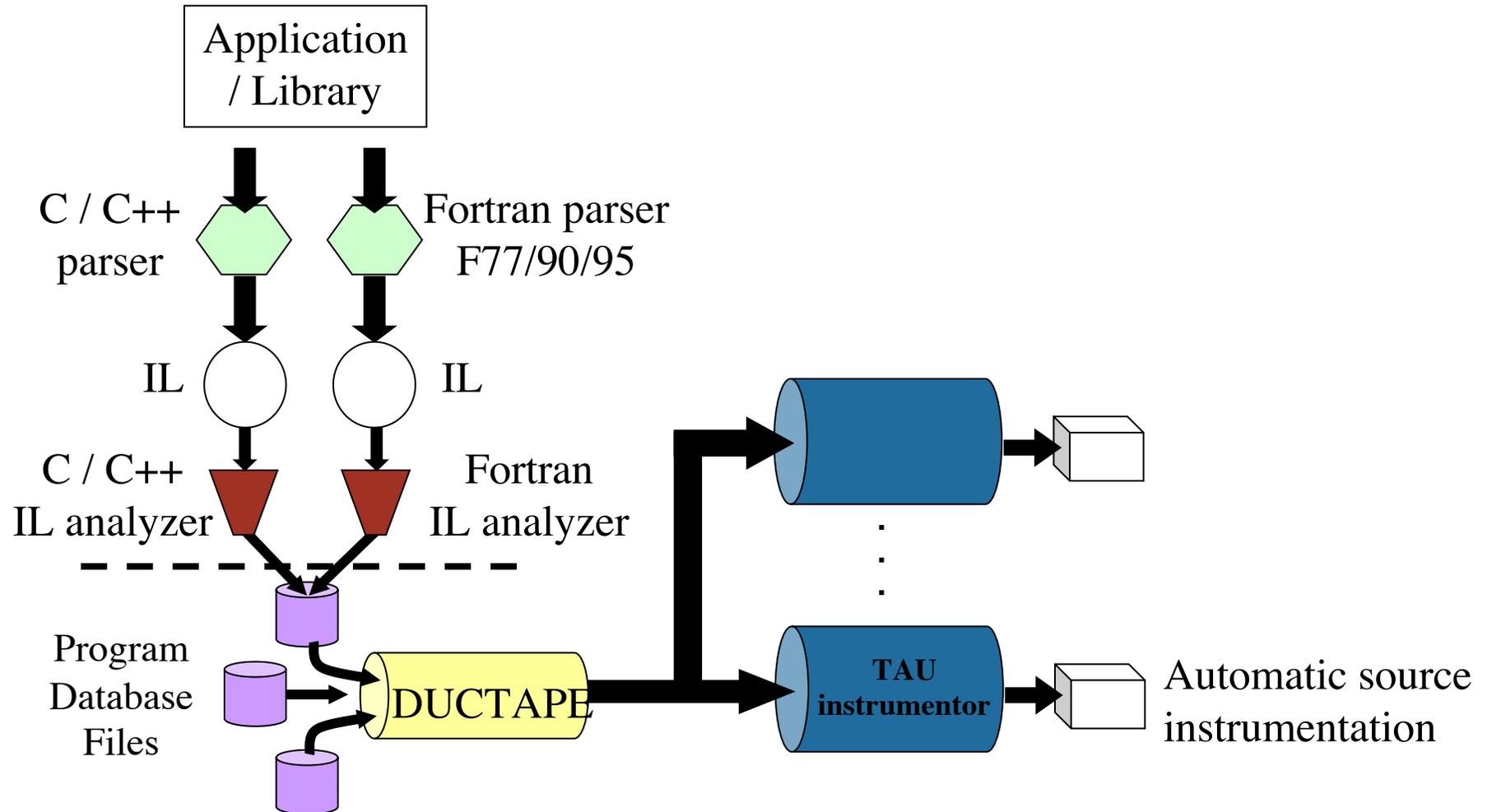
TAU Update for AMD

- TAU updated to support ROCm 5.2.0
- Support for AMD GPUs using Rocprofiler and Roctracer
 - Rocprofiler: sliding window algorithm (128k records)
- Released in TAU v2.31.1
- TAU and E4S available in Singularity container <https://e4s.io>
- Compiler-based instrumentation with hipcc
- TAU LLVM plugin for hipcc for selective instrumentation
 - TAU_COMPILER_SELECT_FILE=<file>
- TAU's support for OMPT for CPU side in OMPT v5.0
- Future: TAU's support for OpenMP GPU offloading with OMPT v5.1.
- TAU support for hipcc/clang for Crusher (PrgEnv-cray, PrgEnv-amd, mvapich2)
- Applications and outreach activities

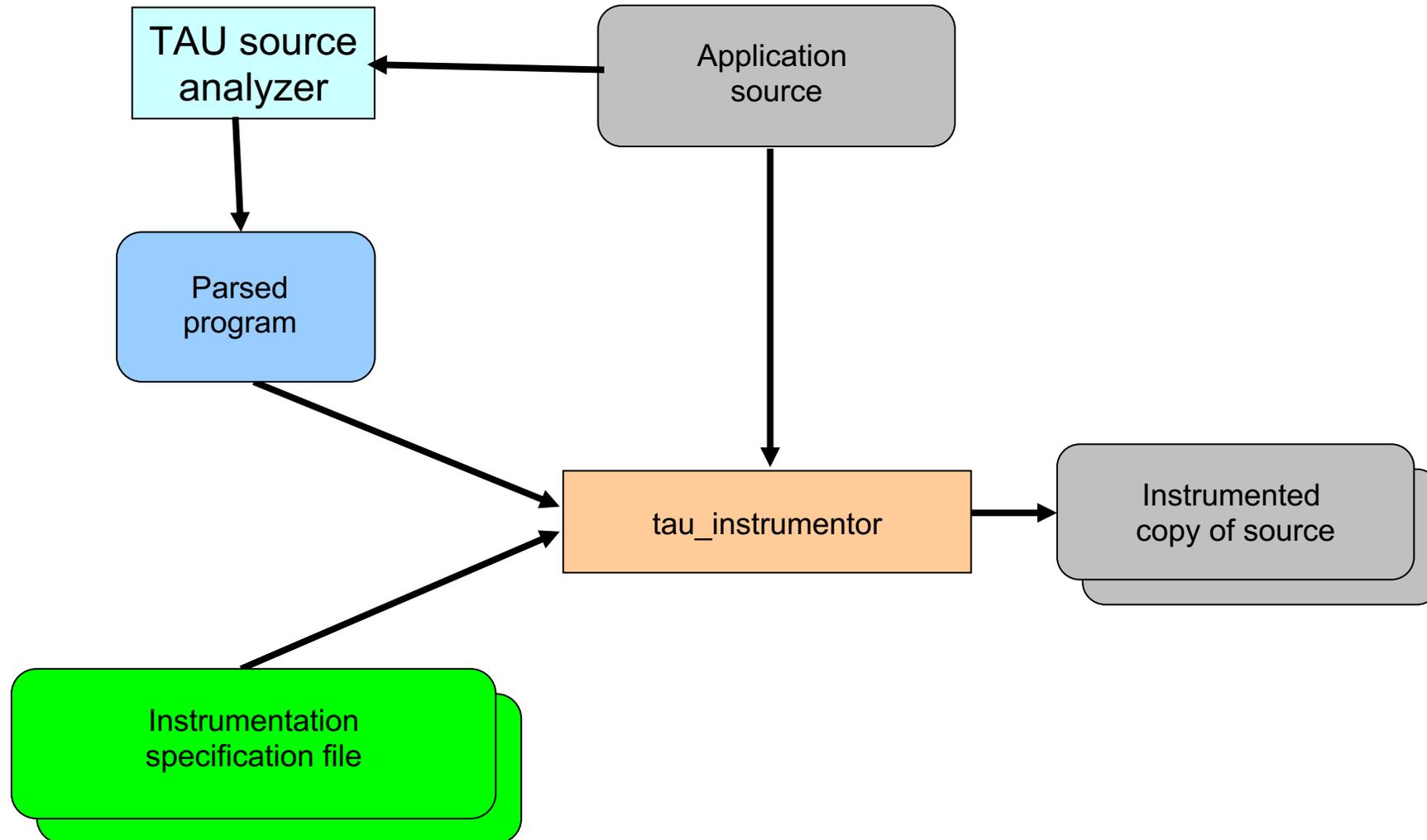
Automatic Source Instrumentation in TAU using PDT



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 corresponds 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/perf-tools/tau/tau-2.31.1/craycnl/lib/Makefile.tau-intel-papi-mpi-pdt
/soft/perf-tools/tau/tau-2.31.1/craycnl/lib/Makefile.tau-intel-papi-mpi-pthread-pdt
/soft/perf-tools/tau/tau-2.31.1/craycnl/lib/Makefile.tau-intel-papi-ompt-intel-mpi-pdt-
  openmp
/soft/perf-tools/tau/tau-2.31.1/craycnl/lib/Makefile.tau-intel-papi-ompt-intel-pdt-openmp
/soft/perf-tools/tau/tau-2.31.1/craycnl/lib/Makefile.tau-intel-papi-pthread-pdt
...
```

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= '-optComplnst -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
```

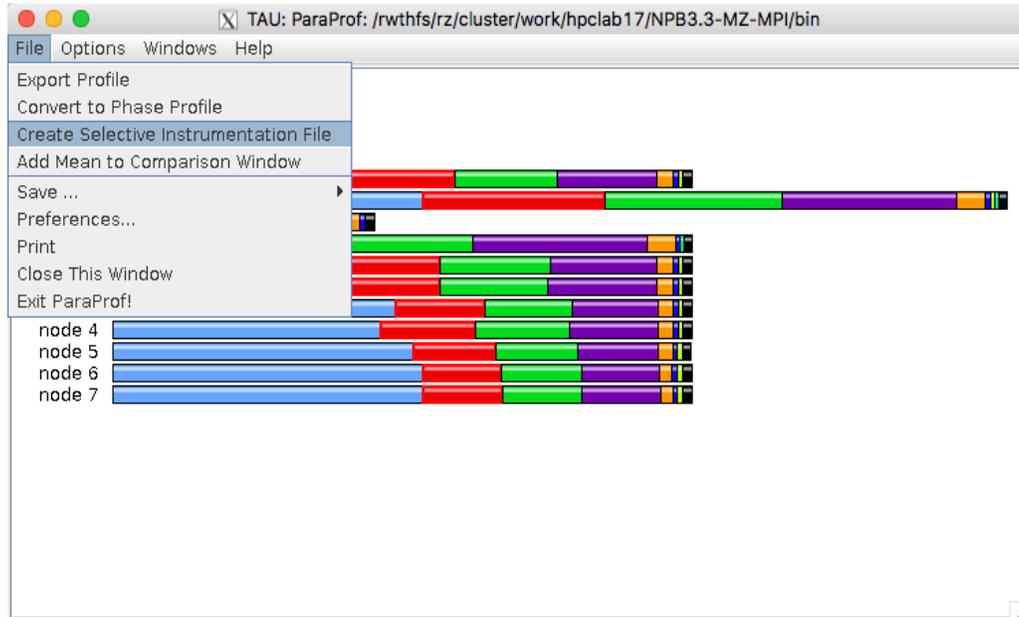
NOTE: paraprof can create this file from an earlier execution for you.

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



The screenshot shows the "TAU: ParaProf: Selective Instrumentation File Generator" dialog box. The "Output File" field is set to "/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/bin/select.tau". The "Exclude Throttled Routines" and "Exclude Lightweight Routines" checkboxes are checked. The "Lightweight Routine Exclusion Rules" section has "Microseconds per call:" set to 10 and "Number of calls:" set to 100000. The "Excluded Routines" list contains: lhsinit_, exact_solution_, matvec_sub_, matmul_sub_, binvrhs_, and binvrhs_. The "save" button is highlighted with an orange box. The "Merge" checkbox is checked, and the "close" button is visible in the bottom right corner.

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 <code>-otf=download</code>)
TAU_EBS_UNWIND	0	Setting to 1 turns on unwinding the callstack during sampling (use with <code>tau_exec -ebs</code> or <code>TAU_SAMPLING=1</code>)
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 <code>-optMemDbg</code> or <code>tau_exec -memory</code>)
TAU_EBS_SOURCE	TIME	Allows using PAPI hardware counters for periodic interrupts for EBS (e.g., <code>TAU_EBS_SOURCE=PAPI_TOT_INS</code> when <code>TAU_SAMPLING=1</code>)
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 <code>TAU_MEMDBG_PROTECT_*</code>)
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 <code>-optMemDbg</code> while building or <code>tau_exec -memory</code>)
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 <code>-optMemDbg</code> or <code>tau_exec -memory</code>)
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)



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 22.05 - May



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 [<https://spack.io>]
- Spack binary build caches for bare-metal installs
- 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
- E4S VirtualBox image with support for container runtimes
 - Docker
 - Singularity
 - Shifter
 - Charliecloud
- AWS and GCP images to deploy E4S

Extreme-scale Scientific Software Stack (E4S)



- E4S: HPC Software Ecosystem – a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures with support for GPUs from NVIDIA, AMD, and Intel in a single distribution
- Available from **source, containers, cloud, binary caches**
- Leverages and enhances SDK interoperability thrust
- Not a commercial product – an open resource for all
- Oct 2018: E4S 0.1 - 24 full, 24 partial release products
- Jan 2019: E4S 0.2 - 37 full, 10 partial release products
- Nov 2019: E4S 1.0 - 50 full, 5 partial release products
- Feb 2020: E4S 1.1 - 61 full release products
- Nov 2020: E4S 1.2 (aka, 20.10) - 67 full release products
- Feb 2021: E4S 21.02 - 67 full release, 4 partial release
- May 2021: E4S 21.05 - 76 full release products
- Aug 2021: E4S 21.08 - 88 full release products
- Nov 2021: E4S 21.11 - 91 full release products
- Feb 2022: E4S 22.02 – 100 full release products
- May 2022: E4S 22.05 – 101 full release products



<https://e4s.io>

Also include other products .e.g.,
AI: PyTorch, TensorFlow (CUDA, ROCm)
Co-Design: AMReX, Cabana, MFEM

Spack is a flexible package manager for HPC

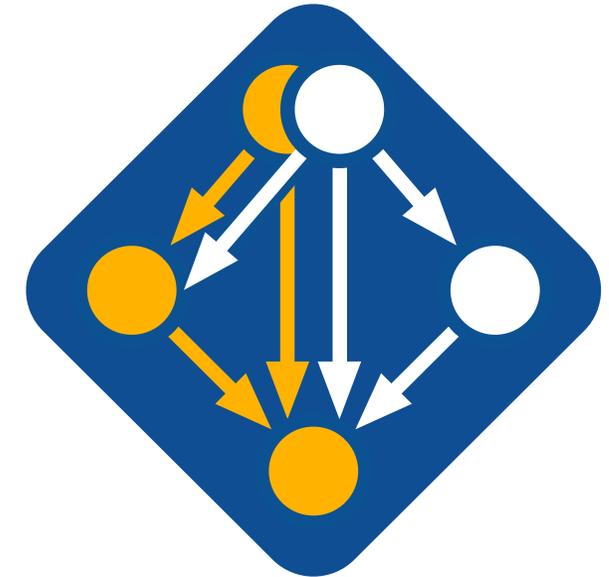
- How to install Spack (works out of the box):

```
$ 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](https://twitter.com/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@2.31.1 @ custom version
$ spack install tau@2.31.1 %gcc@9.3.0 % custom compiler
$ spack install tau@2.31.1 %gcc@9.3.0 +level_zero +opencl +/- build option
$ spack install tau@2.31.1 %gcc@9.3.0 +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

What are containers

A lightweight collection of executable software that encapsulates everything needed to run a single specific task

- Minus the OS kernel

- Based on Linux only

Processes and all user-level software is isolated

Creates a portable* software ecosystem

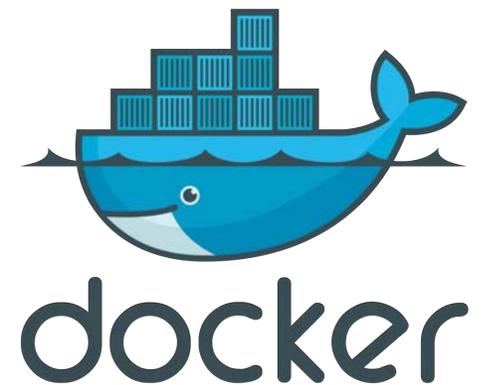
Think `chroot` on steroids

Docker most common tool today

- Available on all major platforms

- Widely used in industry

- Integrated container registry via Dockerhub



Hypervisors and Containers

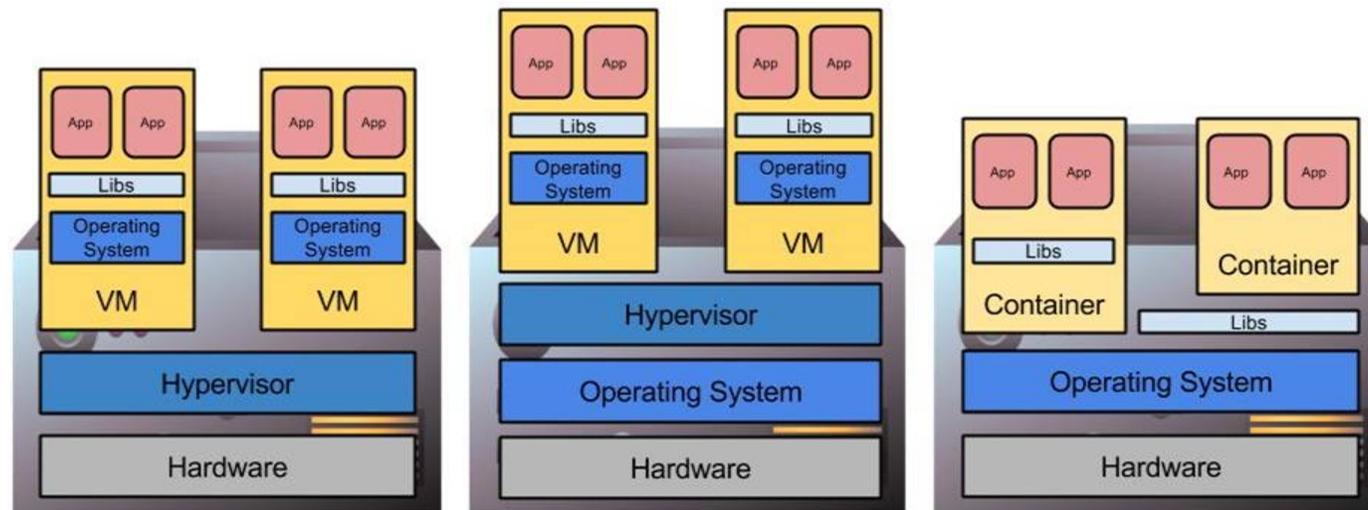
Type 1 hypervisors insert layer below host OS

Type 2 hypervisors work as or within the host OS

Containers do not abstract hardware, instead provide “enhanced chroot” to create isolated environment

Location of abstraction can have impact on performance

All enable custom software stacks on existing hardware

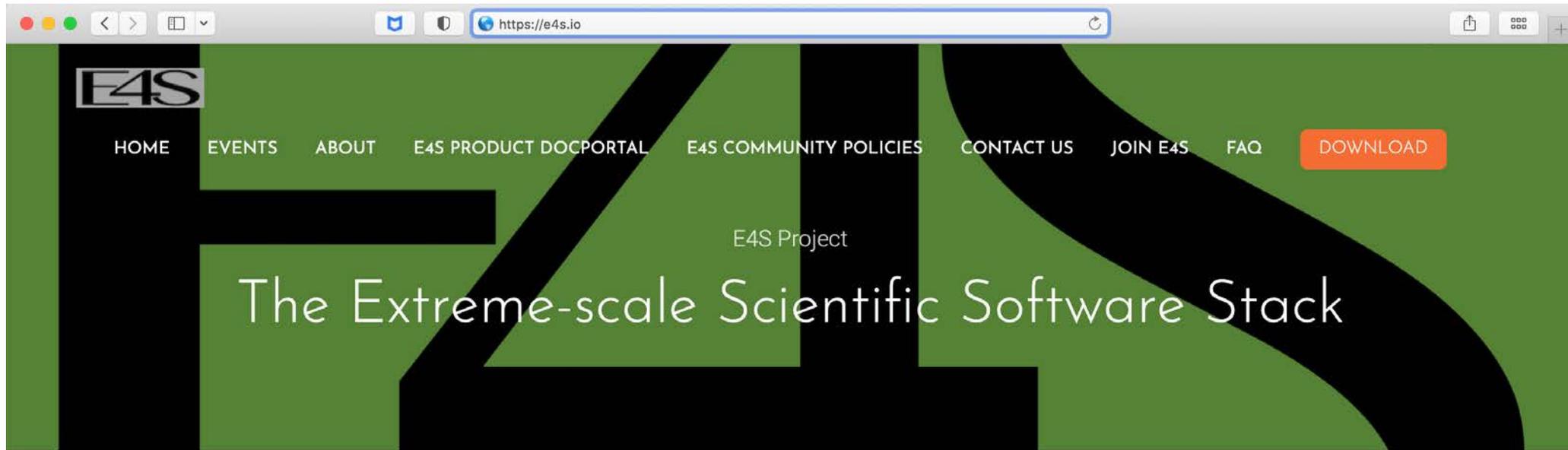


Type 1 Hypervisor

Type 2 Hypervisor

Containers

E4S Download from <https://e4s.io>



E4S 22.05 is now available!

See [Downloads](#) for more information.

What is E4S?

The Extreme-scale Scientific Software Stack (E4S) is a community effort to provide open source software packages for developing, deploying and running scientific applications on high-performance computing (HPC) platforms. E4S provides from-source builds and containers of a [broad collection of HPC software packages](#).

Download E4S 22.05 GPU Container Images: NVIDIA, AMD, Intel



Container Releases

⬇ Docker Downloads - CUDA

⬇ Docker Downloads - ROCm

⬇ Docker Downloads - OneAPI

⬇ Singularity x86_64 Download - CUDA

⬇ Singularity ppc64le Download - CUDA

⬇ Singularity x86_64 Download - ROCm

⬇ Singularity x86_64 Download - OneAPI

⬇ OVA Download



From source with Spack

🔗 Visit the Spack Project

Spack contains packages for all of the products listed in the E4S 22.05 Full Release category (see above Release Notes). General instructions for building software with Spack can be found at the Spack website. Questions concerning building those packages are deferred to the associated package development team.

- Separate full featured Singularity images for 3 GPU architectures
- GPU base images for
 - x86_64 (Intel, AMD, NVIDIA)
 - ppc64le
 - aarch64

Download E4S 22.05 GPU Container Images: NVIDIA, AMD, Intel

Note on Container Images

Container images contain binary versions of the Full Release packages listed above. Full-featured GPU-enabled container images are available from Dockerhub:

```
# docker pull ecpe4s/e4s-cuda:22.05
```

```
# docker pull ecpe4s/e4s-rocm:22.05
```

```
# docker pull ecpe4s/e4s-oneapi:22.05
```

E4S Full GPU Images

These images contain a full Spack-based deployment of E4S, including GPU-enabled packages for NVIDIA, AMD, or Intel GPUs.

These images also contain TensorFlow, PyTorch, and TAU.

AMD ROCm (x86_64)

ecpe4s/e4s-rocm:22.05  docker

e4s-rocm-22.05.sif  mirror 1

NVIDIA CUDA (x86_64, ppc64le)

ecpe4s/e4s-cuda:22.05  docker

e4s-cuda-x86_64-22.05.sif  mirror 1

e4s-cuda-ppc64le-22.05.sif  mirror 1

Intel OneAPI (x86_64)

ecpe4s/e4s-oneapi:22.05  docker

e4s-oneapi-22.05.sif  mirror 1

Download E4S 22.05 Base GPU Container Images

GPU Base Images

These images come with MPICH, CMake, and the relevant GPU SDK -- either AMD ROCm, NVIDIA CUDA Toolkit and NVHPC, or Intel OneAPI.

NVIDIA Multi-Arch (X86_64, PPC64LE, AARCH64)

ecpe4s/e4s-base-cuda:22.05  docker

e4s-base-cuda-x86_64-22.05.sif  mirror 1

e4s-base-cuda-aarch64-22.05.sif  mirror 1

e4s-base-cuda-ppc64le-22.05.sif  mirror 1

ROCM X86_64

ecpe4s/e4s-base-rocm:22.05  docker

e4s-base-rocm-22.05.sif  mirror 1

Intel OneAPI X86_64

ecpe4s/e4s-base-oneapi:22.05  docker

e4s-base-oneapi-22.05.sif  mirror 1

22.05 Release: 101 Official Products + dependencies (gcc, x86_64)

1: adios2	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/adios2-2.8.0-5fxpauervqbotprybps3mwkgh7t6jcbv
2: alquimia	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/alquimia-1.0.9-mkugz7joihpf4umcyidflg3dwik2nvlr
3: aml	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/aml-0.1.0-ogtuh4diyg4tq47tfjdpw7nue7sa5ka
4: amrex	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/amrex-22.05-7tgphdtmt3fmoijkfrfsnwbqzpxkxqfs
5: arborx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/arborx-1.2-a5j5wjdwqatoqsvs6xjckootv76g5h32
6: archer	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/archer-2.0.0-zurunmhys3lwqhqn3ffapnelmezog2gl
7: argobots	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/argobots-1.1-prj5il35vpp7sgcclenbh2thzqvrylwf
8: ascent	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ascent-0.8.0-qgivng4ownyfczct535vkvzle6irkjaq2
9: axom	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/axom-0.6.1-amuobdcyxxfsoyl7pyvbgvww3kysoaj
10: bolt	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/bolt-2.0-mb62bsxs7cvgisgkww4m46qffxvfkfz
11: bricks	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/bricks-r0.1-5qkeva7iiqimec7zwsugd33tz4mddslz
12: butterflypack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/butterflypack-2.1.1-fhncpxhwa4agoogz7magi6flubctqdp6
13: cabana	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/cabana-0.4.0-obd2epyboqn4pifoqwfiojyszqi6npoc
14: caliper	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/caliper-2.7.0-5scpuxjsztlwgbpcldgpw3kafmfvb3ub
15: chai	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/chai-2.4.0-l6nclfuapjlbctkriikyeo3mhdatl5l
16: charliecloud	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/charliecloud-0.26-wgnmvl3rceimjvrcstuogmhlzhelz466
17: conduit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/conduit-0.8.3-hm2j65mka5alpsg4uc4dswqvp7fusqvz
18: darshan-runtime	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/darshan-runtime-3.3.1-ausjp6wozamwgyhgxiv22qcsarxvoixy
19: datatransferkit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/datatransferkit-3.1-rc3-xd57qoqxv4ikmz7ypfowrmnboqtohwq4
20: dyninst	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/dyninst-12.1.0-du56qu4uijap4synulxijiwury3dni5h
21: faodel	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/faodel-1.2108.1-kvw27w57ny2achbuhpiu3cweudqin7h
22: flecsi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flecsi-1.4.2-fzhunvoffnf7l4sssl6l5ufukbrftc5u
23: flit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flit-2.1.0-j4naqyymm6h4mofj5id6sfit5ngr4xh6
24: flux-sched	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/flux-sched-0.22.0-nfljuuoxqlk4r7zx3yoepyzzjjfxsqz
25: fortrilinos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/fortrilinos-2.0.0-uobhjnniqweeclzx7awlhcvmxiktwo5
26: gasnet	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gasnet-2022.3.0-ep4xyqocdziblie475bojotd6qgpfpse
27: geopm	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/geopm-1.1.0-3bxmokyvkuh4gmymmu6b4iqhss5zq352
28: ginkgo	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/ginkgo-1.4.0-l6ahxdmshvwqrl6rmke7w4p3i5d5ehyd
29: globalarrays	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/globalarrays-5.8-y42lqtmfsq6nddv7vu5z3bjxbqz6yww
30: gotcha	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gotcha-1.0.3-cidwbtn2h7xjqzvajlks3idskhr3dcv
31: gptune	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/gptune-3.0.0-bjtlsqmggh24awymzp5g3fxt6wiequ3n
32: h5bench	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/h5bench-1.2-x5gqhbii26t7f4e3bpscw5wbhfg5qlhb
33: hdf5	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hdf5-1.12.2-75qn37lp7leuvlsrbizprz5o5yr3ekjo

22.05 Release: 101 Official Products + dependencies (gcc, x86_64)

34: heffte	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/heffte-2.2.0-hqigomw3nlexreke2rgquwvdazenvhb2
35: hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpctoolkit-2022.04.15-cqz4vlmjclq6qmxp4sonlrqiz4twl2sh
36: hpx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hpx-1.7.1-o7y77tofbg4jg2vcvfhjgdsqtckzhw3v
37: hypre	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/hypre-2.24.0-c7vk7oprzxpfs6njr42xn632tksu64ax
38: kokkos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/kokkos-3.6.00-fy3onzyijziq2x2laoxu7rttrwahaufj
39: kokkos-kernels	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/kokkos-kernels-3.6.00-gn7fvng67ekhwt324xo45lizuxea327n
40: lammps	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/lammps-20220107-pmr5l5hzxruzhpzkucukg7qqr6os5iir
41: legion	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/legion-21.03.0-g3tu5cdevxuzsrvcqinaxrgduik3ea54
42: libnrm	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libnrm-0.1.0-gjllhvje7in4rp3kvvaywywr7uyjprxj
43: libquo	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/libquo-1.3.1-2o7zqn3e2f7je3o3z4hcwsqgkn6bjmme
44: loki	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/loki-0.1.7-66nzpehhmoidzifzm6khyxhnbfgmppo
45: magma	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/magma-2.6.2-mmx2xmmz7cbcjbc2j3vn6eoxrwgivu24
46: mercury	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mercury-2.1.0-yzp4mkdsnmcf5dgsein4ek2co7eag763
47: metall	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/metall-0.20-6o2ewhyu2ilxbo74j5qqdeunqjkmgt
48: mfem	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mfem-4.4.0-cra7q4353kgqdw7futlc5vik5hf4bu6
49: mpich	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpich-4.0.2-ssbmd2ccbzxkxk7fzrlekupe23rokw2
50: mpifileutils	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/mpifileutils-0.11.1-zvlai7bnjegicp5dzelnvwmvu6sye5j
51: netlib-scalapack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/netlib-scalapack-2.2.0-l2chii6rgvnp6rswldzqxza7trgpd kib
52: nccmp	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nccmp-1.9.0.1-ef6vn4ls3rj7wieuygnpf5c2i4trzpvo
53: nco	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nco-5.0.1-xlix5wvr6bprihee7rryknegskv4sjho
54: nrm	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/nrm-0.1.0-cyiqhjsurt3q4bkn37u2ylvzhgdtmuu
55: omega-h	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/omega-h-9.34.1-3d4zvshz6tj7twd3nqcnbls4zwryrv
56: openpm�-api	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openpm�-api-0.14.4-6ktbupm7eqmq73vflxkjiapn3kanomm4
57: openmpi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/openmpi-4.1.3-p5q2yggpo7lhc2n26deo25ymx3thdwt
58: papi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papi-6.0.0.1-fxfxybh2varhxhnu6jcrqsg5ixrrcxp2
59: papyrus	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/papyrus-1.0.2-r2wef2ldj24dluqgd43hjn23fxowxet2
60: parallel-netcdf	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parallel-netcdf-1.12.2-7ruhgcy35hofq4goi6c3d42tteuhqlwl
61: paraview	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/paraview-5.10.1-ohruf5tnfp2yeywlslszty5jfbq6pjw7
62: parsec	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/parsec-3.0.2012-dcaz2iwq6nrz7l6kcwpsbftpb3urv6
63: pdt	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pdt-3.25.1-d5jyjfrocerrcl5cxqwsfrbv5l776d7r
64: petsc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/petsc-3.17.1-vffv6b2ykyi3a4lxuoe7dzi4zggbrdq
65: phist	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/phist-1.9.5-vxmwjbn3kywtogpldhhmouoehgi7d2m
66: plasma	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plasma-21.8.29-hwpchnbrscxsmzgyioeepsjwddgnunxm

22.05 Release: 101 Official Products + dependencies (gcc, x86_64)

67: plumed	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/plumed-2.6.3-g6dn67baochvycvcicgeltwijnvotgjk2
68: precice	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/precice-2.4.0-orye5yx46n4mm2zey7xeg5k5i222twiw
69: pruners-ninja	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pruners-ninja-1.0.1-hn6y2kevr5hgmllykfverjadgbgkppcn
70: pumi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/pumi-2.2.7-zkipah7wz3a4eksedht2syqpx3tcg6ki
71: py-cinemasci	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-cinemasci-1.7.0-77yj2xigharoeq6lciw4mzngexnegxmc
72: py-jupyterhub	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-jupyterhub-1.4.1-3cebk5prfze6najqsdabftwxgqkccmwm
73: py-libensemble	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-libensemble-0.9.1-noalxjfvdyidhsvps4zn7mhu4j5hf2wo6
74: py-parsl	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-parsl-1.1.0-ul2cthsh524nmpv6zrseklzodp6ej4en
75: py-radical-saga	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/py-radical-saga-1.11.1-naxx4rp2e6wr7oo24jw3catzys26loya
76: qthreads	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/qthreads-1.16-v7vcyz7vakzdyzpa3mjdbnov4s55a6vw
77: raja	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/raja-0.14.0-edjvff74mwc27fngfj4qlatppls5vzl
78: rempi	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/rempi-1.1.0-yoa3gfri6iafv2l2avkhg25pzzpgiftwg
79: scr	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/scr-3.0rc2-miby3jm6nkm4gg7ovpbwe4kpwxnwou6
80: slate	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/slate-2021.05.02-6krdeny5oeki4o2slafxstn7wa6vgmlq
81: slepc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/slepc-3.17.1-fzx6e3h2jqmsvhgbeclbwuirgrax7hkl
82: stc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/stc-0.9.0-vd4xaiuv4ryo4tzqzqvnsr4qwtndyyxq
83: strumpack	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/strumpack-6.3.1-du3qimqp3yrjcso22pw2zsbbswgrtsay
84: sundials	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/sundials-6.2.0-5iz6lim5mabrkkukic63lipmz5r6lmbv
85: superlu-dist	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/superlu-dist-7.2.0-2jp6torp4rjf44hhffm56glemlegfoyb
86: swig	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/swig-4.0.2-fortran-fjva3hwpow4b3dmrmguisinqdrt2ixyk
87: sz	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/sz-2.1.12-kzqvvd05fvv2s6sgheei7ikwgsbsd7m
88: tasmanian	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tasmanian-7.7-5q6657fcerfpwshuhdmrowzvxpoo25tt
89: tau	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tau-2.31.1-ikx2r2pk34hej3rmjqoam5ma6rvzbuqm
90: trilinos	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/trilinos-13.2.0-hmpjtr4o7fnpffc6m6b4pl73ipr422e
91: turbine	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/turbine-1.3.0-aztpwwbbjeogl5bwiznmpx2lcyos64cz
92: umap	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/umap-2.1.0-blwc2edy5e3lkrylgbrwfd55slyuuy4s
93: umpire	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/umpire-6.0.0-gwbap637zehqkvjwmetuqcgjtkwhzzlo
94: unifyfs	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/unifyfs-0.9.2-hcid7bugnj4vzetl4oh4zfnah2gzscfb
95: upcxx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/upcxx-2022.3.0-fpv2zorgjpac5iuqibffz57h6x3xhrjr
96: variorum	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/variorum-0.4.1-fcfi26hd2dfvnwe5gehtv4iqx36hafj7
97: veloc	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/veloc-1.5-avca7jodby7efy3be63siav4mqao2big
98: vtk-m	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/vtk-m-1.7.1-hbilfvhsgkelno7jrvr6fffyn6guusxf
99: wannier90	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/wannier90-3.1.0-vzfixrlicq5jrtzj2wpd6bg7nbkqdit6
100: warpx	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/warpx-22.05-gtg2e5dwy3l3r53t7fsyzscbj25gzu2m
101: zfp	/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/zfp-0.5.5-3cc5y5ffuvxtdsiurtrt4blcbodbxj2p

GPU runtimes

- Intel (oneAPI)
 - 2022.1.0
- AMD (ROCm)
 - 5.1.1
- NVIDIA (CUDA)
 - 11.4
- NVHPC
 - 22.3

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1: adios2	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/adios2-2.8.0-l3uoqxbcqtdw6acjkm2mkilrsz4cplhn
2: alquimia	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/alquimia-1.0.9-uur6z7y5odoyby6umwxdorfo2nbbnohw
3: aml	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/aml-0.1.0-zfgeqmb6632fta22ytmomo4mu2fw3lwb
4: amrex	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/amrex-22.05-km2isnpb7l3muxey6hnbnoju2llw5hjo
5: arborx	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/arborx-1.2-rm7wnlzo3wcam6briglal22oyrictnb5
6: archer	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/archer-2.0.0-vsljqh3qhilsqgpqnqkgmeld267kgkrd
7: argobots	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/argobots-1.1-53v35i6gn2swvvr17bxa1wzuc2tq3ty
8: ascent	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ascent-0.8.0-y3gnx7ztjofbiwwgc537bmnix32dho4
9: axom	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/axom-0.6.1-g552mnzr43bnkz6pnozqplpqqc77qtk
10: bolt	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/bolt-2.0-nbievusty3ohurw66gybj3ylsx57wrex
11: butterflypack	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/butterflypack-2.1.1-6cfpnjkfjtyrcrkr5uds3utwgdiun4rh
12: cabana	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/cabana-0.4.0-qtngrrdxuwr2dvcfw6cq7ooi5itfw5sp
13: caliper	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/caliper-2.7.0-6yob3cnulacurei4r74wqywbiddi2zqx
14: chai	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/chai-2.4.0-gdjlgtnw37djx77ub6loueiozpwyrwz4
15: charliecloud	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/charliecloud-0.26-gfvv4zs2da4lmjry5pcv7bgiulq53dkh
16: conduit	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/conduit-0.8.3-nt23fkfvsdc7vvgphhzugk5k3fr5hry7
17: darshan-runtime	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/darshan-runtime-3.3.1-3tri6deqymvo5l2yb5dpeyya7qy52p3
18: datatransferkit	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/datatransferkit-3.1-rc3-34axhs5y4fphnqrxqeoatq23xmfhy64y
19: dyninst	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/dyninst-12.1.0-qjucc4hbzk73utkjer2u6iauookgc5xk
20: exaworks	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/exaworks-0.1.0-j4oyws2l6b3oa3ehiph7hr3qsu3xwcn
21: faodel	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/faodel-1.2108.1-5uvp7odssmdoy3u3kwcyb4imvhsifkpc
22: flecsi	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flecsi-1.4.2-w6mhu5bfumqzg27v4nw4nu35l7xkbbeq
23: flit	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flit-2.1.0-4mnc1if2iiayhwkhndemxo24ligjzq7v
24: flux-sched	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flux-sched-0.22.0-rfqrabahnjutfgmss7377d7rtmhhknf2
25: fortrilinos	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/fortrilinos-2.0.0-xqopkkdcnj32t6ujpkpia5s5i5fj3dkz
26: gasnet	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gasnet-2022.3.0-rtr5lpjjrbzca6fdbvfxsmhqsymbixhc
27: ginkgo	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ginkgo-1.4.0-zhjkhwzcfthnzc57o7fex57m4ausb7l
28: globalarrays	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/globalarrays-5.8-n4sze7tqf4ty3x65a6vnyoos6ninzuzf
29: gotcha	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gotcha-1.0.3-ygplgppszeiftecygig3zpnk34m7nva
30: gptune	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gptune-3.0.0-rf7kag2a4ntxlqp5geggyqrodosmad7
31: h5bench	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/h5bench-1.2-f4dxdpplnt5i6ll3pxwqobm24vpr5fhy
32: hdf5	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hdf5-1.12.2-np7u5ivkhh2dljmeboekev5mgalipou7
33: heffte	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/heffte-2.2.0-jshdo5of5p6nzqyurrtovgv4ymntx7iw

22.05 Release: 101 Official Products + dependencies (gcc, ppc64le)

34: hpctoolkit	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpctoolkit-2022.04.15-yfhefus2qk7nb2dpvcnfljud5wimyl5
35: hpx	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpx-1.7.1-ubdtwy7do6h3awjh2wyiaddui2yxz5sx
36: hypre	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hypre-2.24.0-v7hkiurnu6bo2dz5zfhhbb77xztik6c4
37: kokkos	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-3.6.00-4asspnluai7wx5mmerralzei6xtba6eud
38: kokkos-kernels	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-kernels-3.6.00-rna5swth72aqfwag2a62icyg5gxqdahc
39: lammps	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/lammps-20220107-i4wdut62blpbwr6kitptivbyapb525f2
40: legion	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/legion-21.03.0-kp4fz7au7ttb2cfoqsvt3t2wdfgjy4i2
41: libnrm	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libnrm-0.1.0-nn7mpcrk7fdevym4zpeeha6m7nqg3cis
42: libquo	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libquo-1.3.1-cv3vcijmffuutay6rkidwmbh7eajc4x6
43: loki	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/loki-0.1.7-k52kcywvu6ftfymw3lvqqldrwcwmy2
44: magma	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/magma-2.6.2-c3oionxxjnja35pbkriliexlncqocmpk
45: mercury	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mercury-2.1.0-hzpxw73vc6p5cuyn5echuh63emzio5nv
46: metall	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/metall-0.20-wcjaceek46d6jgk3kaz3rlkppugvfmhr
47: mfem	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mfem-4.4.0-noytuh65o4hmxcgtojvufel35yrdpp4m
48: mpark-variant	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpark-variant-1.4.0-m5m6aixgdol2wyqw3jicr55zipd3dkut
49: mpich	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpich-4.0.2-66lytwzbos3xsv5ulxlauggcggunxli
50: mpifileutils	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpifileutils-0.11.1-vfp3xeqlizyp2fxbgzdwum5yuxczqcpa
51: netlib-scalapack	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/netlib-scalapack-2.2.0-qf2uni4wwakywf2to6bcs2v6o5ezeryp
52: nccmp	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nccmp-1.9.0.1-avgfvcvac7k2hq7cpv7zjgkwh5eontgk
53: nco	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nco-5.0.1-zizmp6sgjstd5rrtuu6oayuuzcrxmeoi
54: nrm	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nrm-0.1.0-ea2gwqxrymwiszsb36uz2iprgc5oi4zt
55: omega-h	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/omega-h-9.34.1-c5gj526wkjvrmjzywtc4lmgrqh6ewvly
56: openpm�-api	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openpm�-api-0.14.4-wdkkdo2v2xnzshojxl4p5ytqiyelxbmf
57: openmpi	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openmpi-4.1.3-s3g3qrtiqwjrxj5bnosfngquuc3vs5x
58: papi	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papi-6.0.0.1-vghyjh55fu6mmal6czcaqciaboserw5e
59: papyrus	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papyrus-1.0.2-vsxqqctyjyifgpazqdsyjkubkecmwj
60: parallel-netcdf	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parallel-netcdf-1.12.2-zagedvigmexckbaqhfhhi5c5py526
61: parsec	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parsec-3.0.2012-77zuv5ioe5schjyba55dsd2fhgxfmzk
62: pdt	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pdt-3.25.1-hdxejnf32dsvceukljn4orbehsw7ble
63: petsc	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/petsc-3.17.1-pbri2lcnrritfkk6xx3qvg4tqalo77fu
64: plasma	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plasma-21.8.29-ow5ip3dmcfwjj2bg34hllruotrdrdlr
65: plumed	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plumed-2.6.3-yw57pgxlhdwgnabprd235yv2q43gb4j4
66: precice	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/precice-2.4.0-brfbvpkoo6vdtewk542jw2amzqilycxa

22.05 Release: 101 Official Products + dependencies (gcc, ppc64le)

67: pruners-ninja	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pruners-ninja-1.0.1-xri4wt2pkvv54tsto3zl2njriblfnqei
68: pumi	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pumi-2.2.7-5uqwy4a5b7p372ptvekosyeadl5bqno
69: py-cinemasci	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-cinemasci-1.7.0-ovv4qw4vp6ao3ukyt7yffqo2dr76hcix
70: py-jupyterhub	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-jupyterhub-1.4.1-jloxcbs7x6hsbzktls25mqv3p4nfn26
71: py-libensemble	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-libensemble-0.9.1-5bs6ugzqcdrh2cuwjkbuydd2j rutwpg
72: py-opentuner	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-opentuner-0.8.7-xqcv6l6vmpmp7p5nw4nl47vlshoogl4w
73: py-parsl	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-parsl-1.1.0-hqnojotjauv4o5na5yhnyqs7eodedd4r
74: py-radical-pilot	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-pilot-1.11.2-tieorl4fju5za2n2vdtbkquqjxphw6ui
75: py-radical-saga	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-saga-1.11.1-sjv4nhrhvlvhgtku2lat27fmvf7kveyd
76: qthreads	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/qthreads-1.16-md7z53zbdffm3zmgpqi4tcno7aqo6bb
77: raja	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/raja-0.14.0-fmvdypdhro2n7k6xovmfgmkc26aekdof
78: rempi	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/rempi-1.1.0-bultj4j7ef7qsdffo3gapameeyftjx4n
79: scr	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/scr-3.0rc2-xip4gfjzkzjar73urcab7mqwp6p3lqn2
80: slate	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slate-2021.05.02-rvxg3qm3bc4orccwvnnfxt6j35i5tuws
81: slepc	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slepc-3.17.1-bur33hbhnuumsk6uktqhg4tjco6sdmri
82: stc	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/stc-0.9.0-vcqy4zscq5mktfdxsk36j5www6wbl55l
83: strumpack	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/strumpack-6.3.1-4i5oyjylpm27o4zecxegpn7imrhok5lb
84: sundials	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sundials-6.2.0-h4xo2zqezj6ef5y7v3727srlratiqs5l
85: superlu-dist	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/superlu-dist-7.2.0-6rwclsr7fo5rfybu3mylfjowblydznu
86: swig	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/swig-4.0.2-fortran-zpsyg6fhwuekaff4fqyvnd7cypnevcjs
87: sz	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sz-2.1.12-xobq2pz6l25htimluokwqvtggwxgfs
88: tasmanian	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tasmanian-7.7-a2rk5ujjed542bqp3vpmo235532qzdqk
89: tau	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tau-2.31-fym3ff54vwf6bw53rj2ntvakfbwirgcj
90: trilinos	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/trilinos-13.2.0-mmz5acf7trnptodope3jv3lucnugylcd
91: turbine	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/turbine-1.3.0-df2lqm4bnlo6vvjbutnzpayfspaee4m
92: umap	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umap-2.1.0-6nh3hjzgbisu2wcigrwqusvdugkzvxxg
93: umpire	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umpire-6.0.0-2phff7zj3b4sht6qkdtb3im46nzoe774
94: unifyfs	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/unifyfs-0.9.2-h33e2ceufqjlvqopz456vluituxlrfor
95: upcxx	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/upcxx-2022.3.0-hfzxejrtpjvvgg5p3ndjphkuh5y4cl65
96: veloc	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/veloc-1.5-sy2ht5e34kry5gqamq2i5eiba4baz54
97: vtk-m	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/vtk-m-1.7.1-vjkewsjwisjtnrhjqgee72krlu2takbl
98: wannier90	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/wannier90-3.1.0-4xbesxrnwafmset7hv3ydunlpwjfeyqx
99: warpx	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/warpx-22.05-33bd7p6hkoc13iayodejy3fua77wfpb5
100: yaksa	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/yaksa-0.2-32f626altdcxrvpeukiigbpy7ibtgkd
101: zfp	/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/zfp-0.5.5-mcame7nbb22fh27n44nkimbokt6azel6

GPU runtimes

- NVIDIA (CUDA)
 - 11.0
- NVHPC
 - 22.3

E4S 22.05 Release: Support for AMD GPUs

```
Singularity> python
Python 3.9.7 (default, Sep 16 2021, 13:09:58)
[GCC 7.5.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
```

```
>>> import tensorflow
>>> tensorflow.__version__
'2.8.0'
```

```
>>> import torch
>>> torch.__version__
'1.11.0+rocm4.5.2'
```

```
>>>
```

```
Singularity> which hipcc
/opt/rocm/hip/bin/hipcc
```

```
Singularity> spack find -l amdgpu_target=gfx90a +rocm
==> 17 installed packages
```

```
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 -----
357tvji amrex@22.05      egwwklq ginkgo@1.4.0    pmri64c petsc@3.17.1      t2bsxuz umpire@6.0.0
uawks2x arborx@1.2       m75ci6i heffte@2.2.0        aoo762y raja@0.14.0          tboqlrc upcxx@2022.3.0
2h2jniil camp@0.2.2       ddpp5a7 hpx@1.7.1           w3wwqzx slepc@3.17.1
uh7nqyy chai@2.4.0       aegedco kokkos@3.6.00       dvyddsb strumpack@6.3.1
c2pvxtt gasnet@2022.3.0 zwsqooc magma@2.6.2        ypavztb superlu-dist@7.2.0
```

```
Singularity> spack find -l amdgpu_target=gfx908 +rocm
==> 17 installed packages
```

```
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 -----
5rbk2or amrex@22.05      wsnjv4  ginkgo@1.4.0    w67sm7w petsc@3.17.1      oijpipf umpire@6.0.0
3n5fwfv arborx@1.2       6bksj3x heffte@2.2.0    qbdnr3o raja@0.14.0        yuzwxoy upcxx@2022.3.0
yuk323w camp@0.2.2       kxqzrjt hpx@1.7.1       te425aa slepc@3.17.1
sntvjjs chai@2.4.0       vmsecny kokkos@3.6.00   x3yv3xj strumpack@6.3.1
afhffop gasnet@2022.3.0 bsj3ldg magma@2.6.2     q25hplz superlu-dist@7.2.0
```

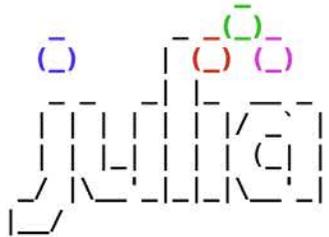
```
Singularity> █
```

E4S 22.05 Release: Support for NVIDIA GPUs

```
Singularity> python
Python 3.9.7 (default, Sep 16 2021, 13:09:58)
[GCC 7.5.0] :: Anaconda, Inc. on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow as tf
>>> tf.__version__
'2.9.1'
>>> tf.config.list_physical_devices('GPU')
[PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU'), PhysicalDevice(name='/physical_device:GPU:1', device_type='GPU')]
>>> import torch
>>> torch.__version__
'1.11.0+cu113'
>>> torch.cuda.get_device_name(torch.cuda.current_device())
'NVIDIA A100-PCIE-40GB'
>>>
Singularity> spack find -l +cuda cuda_arch=80
==> 27 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 -----
5fxpau adios2@2.8.0 hqigomw heffte@2.2.0 mmx2xmm magma@2.6.2 fzx6e3h slepc@3.17.1 gwmap63 umpire@6.0.0
a5j5wd arborx@1.2 o7y77to hp@1.7.1 cra7q43 mfem@4.4.0 du3qimq strumpack@6.3.1 hbilfvh vtk-m@1.7.1
5scpxj caliper@2.7.0 c7vk7op hypre@2.24.0 dcaz2iw parsec@3.0.2012 5iz6lim sundials@6.2.0 3cc5y5f zfp@0.5.5
5nftkwe camp@0.2.2 kn4ult3 kokkos@3.6.00 mvt3juo petsc@3.17.1 2jp6tor superlu-dist@7.2.0
l6nclfu chai@2.4.0 fy3onzy kokkos@3.6.00 edjvff7 raja@0.14.0 5q6657f tasmanian@7.7
l6ahxdm ginkgo@1.4.0 gn7fvng kokkos-kernels@3.6.00 6krdeny slate@2021.05.02 hmpjtr4 trilinos@13.2.0
Singularity> spack find -l +cuda cuda_arch=70
==> 27 installed packages
-- linux-ubuntu20.04-x86_64 / gcc@9.4.0 -----
mvzqvvg adios2@2.8.0 zz33g5c heffte@2.2.0 7ddf6kl magma@2.6.2 td7e334 slepc@3.17.1 hjgbyxh umpire@6.0.0
2wllnpi arborx@1.2 zrpfbiq hp@1.7.1 hyuvayy mfem@4.4.0 66zzxrb strumpack@6.3.1 stzpxgb vtk-m@1.7.1
xb3ix2x caliper@2.7.0 m735zlc hypre@2.24.0 37dtmme parsec@3.0.2012 ykvyvrc sundials@6.2.0 ldaf46p zfp@0.5.5
etalgqv camp@0.2.2 dmru53c kokkos@3.6.00 2lsmpfg petsc@3.17.1 7bbqseb superlu-dist@7.2.0
rjky53t chai@2.4.0 xwt7ck4 kokkos@3.6.00 ttunttv raja@0.14.0 r7artq7 tasmanian@7.7
36fsm5m ginkgo@1.4.0 k47b42d kokkos-kernels@3.6.00 yearhs slate@2021.05.02 qpycht6 trilinos@13.2.0
Singularity> █
```

E4S 22.05 Release: GUI Tools

```
Singularity> module load paraview
Singularity> which paraview
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/paraview-5.10.1-ohruf5tnfp2yeywlslszty5jfbq6pjw7/bin/paraview
Singularity> module load visit
Singularity> which visit
/usr/local/visit/bin/visit
Singularity> which paraprop
/spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-9.4.0/tau-2.31.1-ikx2r2pk34hej3rmjqoam5ma6rvzbuqm/bin/paraprop
Singularity> module load julia
Singularity> julia
```



Documentation: <https://docs.julialang.org>

Type "?" for help, "!" for Pkg help.

Version 1.7.3 (2022-05-06)

Official <https://julialang.org/> release

julia>

```
Singularity> nvidia-smi
Tue May 31 23:33:39 2022
```

NVIDIA-SMI 470.57.02 Driver Version: 470.57.02 CUDA Version: 11.4							
GPU	Name	Persistence-M	Bus-Id	Disp.A	Volatile Uncorr. ECC	GPU-Util	Compute M.
Fan	Temp	Perf	Pwr:Usage/Cap	Memory-Usage			MIG M.
0	NVIDIA A100-PCI...	Off	00000000:25:00.0	Off	0	0%	Default Disabled
N/A	42C	P0	37W / 250W	0MiB / 40536MiB			
1	NVIDIA A100-PCI...	Off	00000000:E1:00.0	Off	0	32%	Default Disabled
N/A	38C	P0	37W / 250W	0MiB / 40536MiB			

E4S 22.05 Release: Intel oneAPI with support for Intel GPUs

```
Singularity> which clinfo
/usr/bin/clinfo
Singularity> clinfo -l
Platform #0: Intel(R) FPGA Emulation Platform for OpenCL(TM)
  -- Device #0: Intel(R) FPGA Emulation Device
Platform #1: Intel(R) OpenCL
  -- Device #0: Intel(R) Xeon(R) Gold 6348H CPU @ 2.30GHz
Platform #2: Intel(R) OpenCL HD Graphics
  -- Device #0: Intel(R) Iris(R) Xe MAX Graphics [0x4905]
Singularity> spack find -dl -v kokkos+sycl
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / oneapi@2022.1.0 -----
rdujf3d kokkos@3.6.00~aggressive_vectorization~compiler_warnings~cuda~cuda_constexpr~cuda_lambda~cuda_ldg_intrinsic~cuda_relocatable_d
evice_code~cuda_uvm~debug~debug_bounds_check~debug_dualview_modify_check~deprecated_code+examples~explicit_instantiation~hpx~hpx_async
_dispatch~hwloc~ipo~memkind~numactl+openmp~pic+profiling~profiling_load_print~pthread~qthread~rocm+serial+share+sycl+tests~tuning~wra
pper build_type=RelWithDebInfo std=17
xoj37yl      cmake@3.23.1~doc+ncurses+ownlibs~qt build_type=Release
az4hpr4      ncurses@6.2~symlinks+termlib abi=none
uycnlmy      pkgconf@1.8.0
w4cv7zw      openssl@1.1.1o~docs~shared certs=system
uqtpe2z      perl@5.34.1+cpanm+shared+threads
sngm6aa      berkeley-db@18.1.40+cxx~docs+stl patches=b231fcc
ndilfw       bzip2@1.0.8~debug~pic+shared
yzcfxcb      diffutils@3.8
zf2ftv4      libiconv@1.16 libs=shared,static
4hns3dz      gdbm@1.19
s63k2n3      readline@8.1
nxdjy7n      zlib@1.2.12+optimize+pic+shared patches=0d38234

Singularity> ls /spack.yaml
/spack.yaml
Singularity> which dpcpp
/opt/intel/oneapi/compiler/2022.1.0/linux/bin/dpcpp
Singularity> which mpiicpc
/opt/intel/oneapi/mpi/2021.6.0/bin/mpiicpc
```

E4S Validation Test Suite

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

Branch: master | testsuite / validation_tests / magma /

File	Commit Message	Time
..		
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.

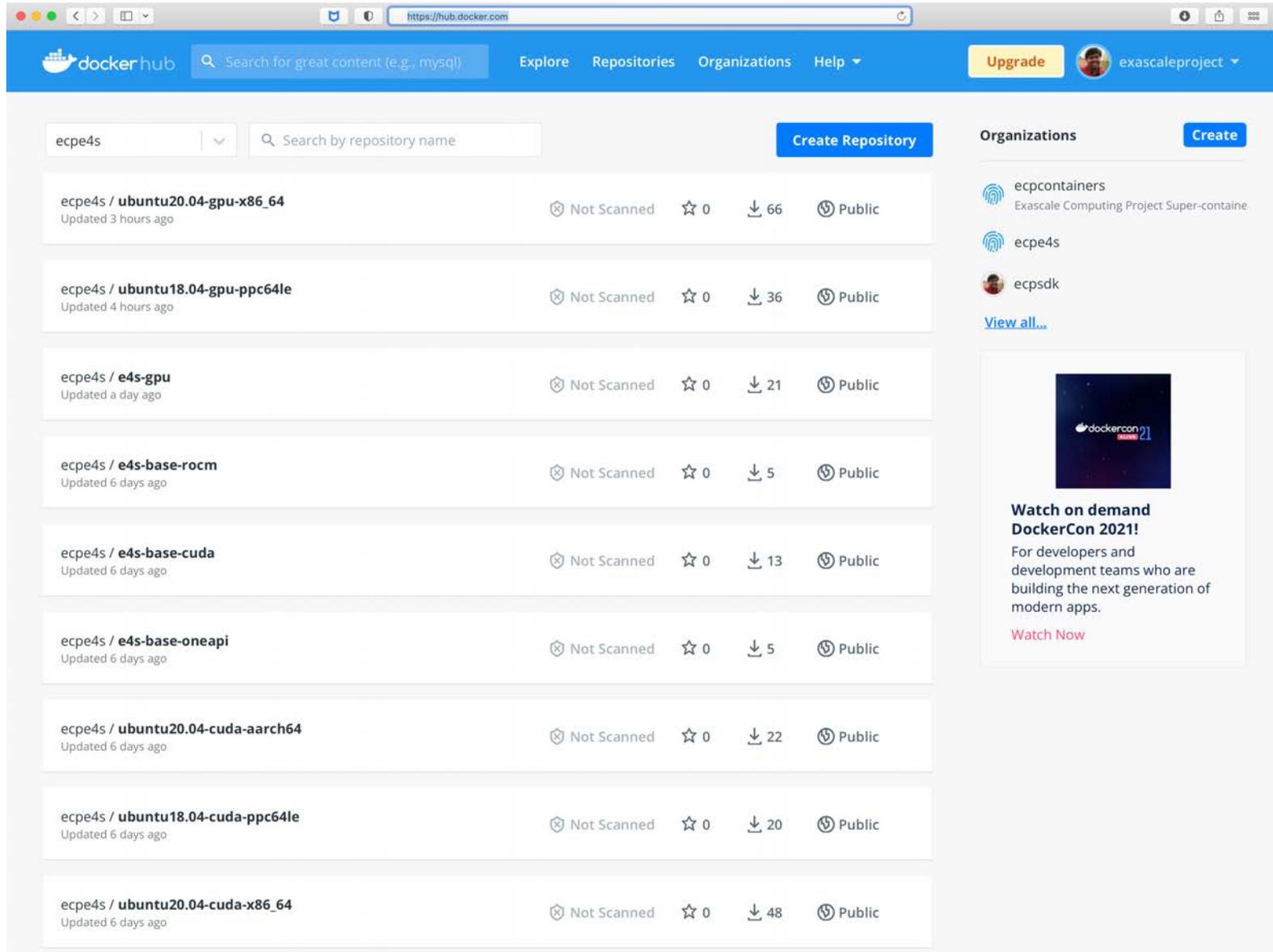
Include the MAGMA header:

```
#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 Base Container Images for x86_64, ppc64le, and aarch64



- Hub.docker.com
- ecpe4s
- Platforms:
 - x86_64
 - Ppc64le
 - aarch64
- GPU runtimes:
 - Cuda
 - ROCm
 - oneAPI

E4S 22.05 AWS image: US-West2 (OR)

The screenshot displays a Linux desktop environment with the following components:

- ParaView 5.9.0:** A 3D visualization of a pressure field on a rectangular domain. The color scale ranges from 0.0e+00 (blue) to 1.2e-38 (red).
- Terminal Window:** Shows the execution of the Singularity command: `singularity run --/ecp.sing`. The output lists available modules, including `amrex/21.11-rocm-6cm`.
- TAU Performance Statistics:** A table showing the breakdown of execution time for various operations. The total time is 218.852 seconds.

Name	Exclusive TIME	Inclusive TIME
.TAU application	8.784	218.852
Belos: Operation Op*x	0.629	0.706
Belos: PseudoBlockGmresSolMgr total solve time	0.615	65.591
Belos: ICGS[2]: Orthogonalization	0.22	18.854
Belos: Operation Op*x	1.672	2.32
Belos: Operation Prec*x	7.617	43.327
Ifpack2::Chebyshev::apply	4.76	25.865
Kokkos::parallel_for Kokkos::View::initialization [DualV	0.003	0.003
Kokkos::parallel_for Kokkos::View::initialization [MV::D	0.004	0.004
Kokkos::parallel_for Kokkos::View::initialization [export	0.002	0.002
Kokkos::parallel_for Kokkos::View::initialization [import	0.002	0.002

E4S 22.05 AWS

- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- Trilinos 13.2.0
- OpenFOAM
- ParaView
- TAU
- Docker
- Shifter
- Charliecloud
- E4S Singularity...

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 and Wi4MPI [CEA] for OpenMPI replacement.
- 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.
 - e4s-cl init --backend [singularity|shifter] --image <file> --source <startup_cmds.sh>
 - e4s-cl mpirun -np <N> <command>

- Usage:

```
./opt/intel/oneapi/setvars.sh
```

```
e4s-cl init --backend singularity --image ~/images/e4s-gpu-x86.sif --source ~/source.sh
```

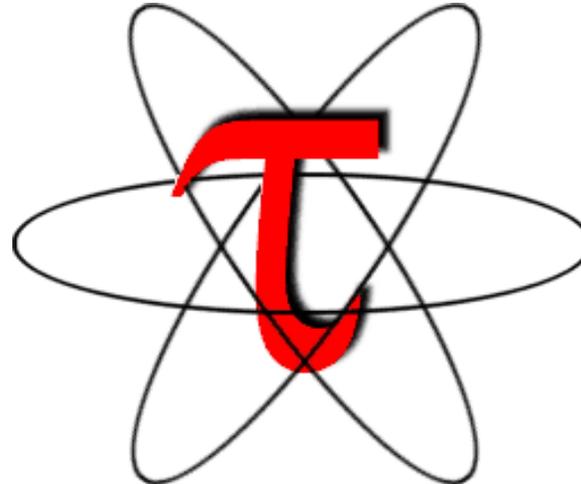
```
cat ~/source.sh
```

```
./spack/share/spack/setup-env.sh  
spack load trilinos+cuda cuda_arch=80  
spack unload mpich
```

```
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



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Hands-on session: TAU



Login to AWS instance and follow instructions in README file

- Reserve a unique host by entering your contact info at the Google Doc:

- <https://e4s.io/tutorial>

- Use a web browser for DCV (remote desktop) software



[https://\[hostname\]:8443/#e4s](https://[hostname]:8443/#e4s)

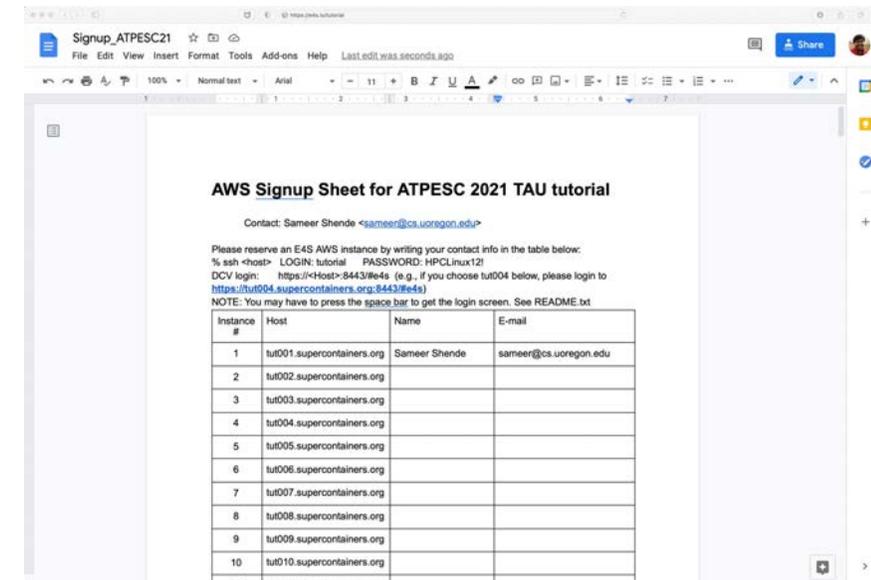
(e.g., <https://tut032.supercontainers.org:8443/#e4s>

if you reserved instance #32 or tut032.supercontainers.org)

login: tutorial

password: HPCLinux12!

press space bar, reenter password if necessary; open terminal window; click on README.txt



% cd; cat README

Login to Theta from AWS:

- Open a gnome-terminal window

```
ssh -Y theta.alcf.anl.gov -l <loginid>
% qsub -I -n 1 -A ATPESC2022 -q ATPESC2022 -t 59
% tar xf /soft/perftools/tau/workshop.tgz
% cd workshop/CoMD/src-mpi; make clean; make ; cd ../bin
% cat ./r.sh; ./r.sh
% cat rt.sh; ./rt.sh
% module load tau
% paraprof &
```



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 ATPESC2022 -q ATPESC2022 -t 59
% 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,intel,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 &
```

TAU Breakout Session – CoMD on Theta

- Setup preferred program environment compilers (check instructions for launching jobs)
 - 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/CoMD/src-openmp;  
% make clean  
% make  
% cd ../bin; cat rompt.sh  
In a second window:  
% qsub -I -n 1 -A ATPESC2022 -q ATPESC2022 -t 50 -q debug-cache-quad  
  
% cd workshop/CoMD/bin; ./romp.sh  
% ./rompt.sh  
% paraprof --pack ex1.ppk  
In the first window:  
% paraprof ex1.ppk &
```

TAU Breakout Session – MPI on ThetaGPU

- Setup preferred program environment compilers (check instructions for launching jobs)
- NOTE: On Ubuntu please link with `-no-pie` option for sampling.

```
% ssh -Y theta.alcf.anl.gov
% module load cobalt/cobalt-gpu; qsub -I -n 1 -A ATPESC2022 -q single-gpu -t 50
% module use ~sameer/modulefiles; module load tau;
% tar xzf ~sameer/alcf22/workshop.tgz
% cd workshop/matmult
% make clean
% make
% mpirun -np 4 ./matmult
% mpirun -np 4 tau_exec -ebs ./matmult
% paraprof --pack mm.ppk
Bring ppk file to your desktop:
% paraprof mm.ppk &
```

TAU Breakout Session – CUDA on ThetaGPU

- Setup preferred program environment compilers (check instructions)

```
% ssh -Y theta.alcf.anl.gov
% module load cobalt/cobalt-gpu; qsub -I -n 1 -A ATPESC2022 -q single-gpu -t 50
% module use ~sameer/modulefiles; module load tau;
% tar zxf /soft/perftools/tau/workshop.tgz
% cd workshop/cuda;
% make clean
% make
% ./matmult
% cat ./rt
% ./rt
% pprof -a | more
% paraprof --pack cupti_ex.ppk
Bring ppk file to your desktop:
% paraprof cupti_ex.ppk &
```

TAU Breakout Session – CUDA with MPI on ThetaGPU

- Setup preferred program environment compilers (check instructions)

```
% ssh -Y theta.alcf.anl.gov
% module load cobalt/cobalt-gpu; qsub -I -n 1 -A ATPESC2022 -q single-gpu -t 50
% module use ~sameer/modulefiles; module load tau;
% tar zxf /soft/perftools/tau/workshop.tgz
% cd workshop/CloverLeaf/CloverLeaf_CUDA;
% make clean
% make -j
% mpirun -np 3 ./clover_leaf
% mpirun -np 3 tau_exec -T cupti,mpi -cupti ./clover_leaf
% pprof -a | more
% paraprof --pack cupti_ex.ppk
Bring ppk file to your desktop:
% paraprof cupti_ex.ppk &
```

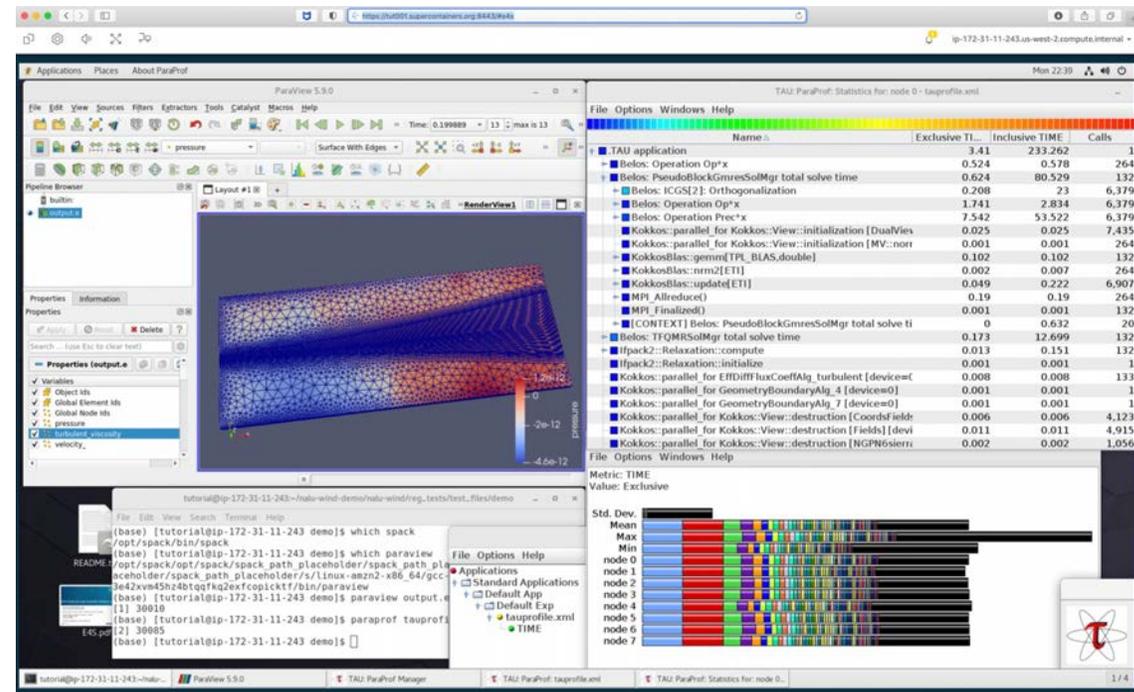
AWS: Using TAU's Kokkos Profiling Interface in an ECP Application

```
% cat ~/README
```

```
% cd nalu-wind-demo; cat demo.sh; ./demo.sh
```

```
% cd nalu-wind/reg_tests/test_files/demo
```

```
% paraprof tauprofile.xml &
```



Using E4S on ThetaGPU

- Setup preferred program environment compilers (check instructions)

```
% ssh -Y theta.alcf.anl.gov
% module load cobalt/cobalt-gpu; qsub -I -n 1 -A ATPESC2022 -q single-gpu -t 50
% singularity run --nv ~sameer/scr/e4s/ecp.simg
Singularity> conda activate cuda
Singularity> cd /opt/demo/python_tests
Singularity> python ./f2.py
Singularity> spack find
```

