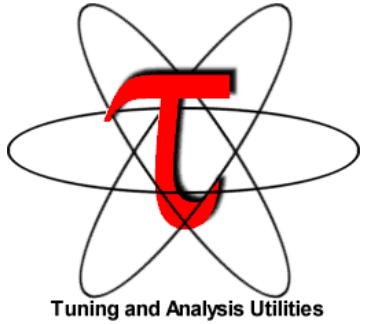
TAU Performance System®

ALCF Computational Performance Workshop 2022
May 23, 2022 10:15am – 11:15am CDT

Sameer Shende
Research Associate Professor and Director,
Performance Research Laboratory, OACISS, University of Oregon
President and Director, ParaTools, Inc.
http://tau.uoregon.edu/TAU_ALCF22.pdf



ParaTools

ECP EXASCALE COMPUTING PROJECT
NNSA National Nuclear Security Administration
U.S. DEPARTMENT OF ENERGY | Office of Science

Agenda

- Motivation and challenges
- Introduction to the TAU Performance System®
- Intel oneAPI integration
- Summary

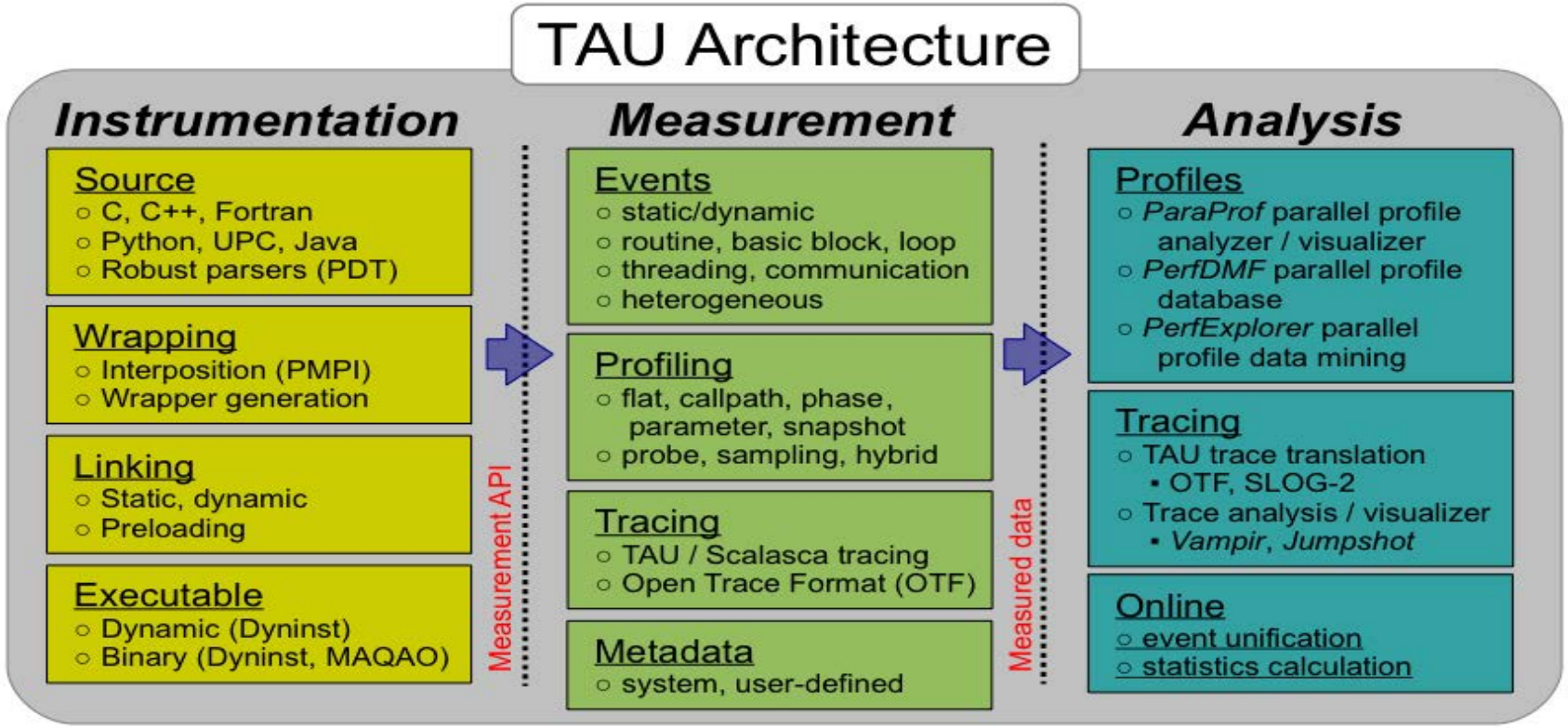
Motivation and Challenges

- With growing hardware complexity, it is getting harder to accurately measure and optimize the performance of our HPC and AI/ML workloads.
- TAU Performance System®:
  - Deliver a scalable, portable, performance evaluation toolkit for HPC and AI/ML workloads.
  - http://tau.uoregon.edu
- As our software gets more complex, it is getting harder to install tools and libraries correctly in an integrated and interoperable software stack.
- Extreme-scale Scientific Software Stack (E4S)
  - Curated, Spack based software distribution of HPC & AI/ML packages includes Intel oneAPI and features binary build-caches and containers.
  - https://e4s.io

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

Measurement and analysis support
- MPI (MVAPICH2, Intel MPI), OpenSHMEM, ARMCI, PGAS, DMAPP
- Supports Intel oneAPI compilers
- pthreads, OpenMP, OMPT interface, hybrid, other thread models
- GPU: OpenCL, oneAPI DPC++/SYCL (Level Zero), OpenACC, Kokkos, RAJA
- Parallel profiling and tracing

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

TAU integration with Intel oneAPI

Instrumentation in TAU

- Intel oneAPI DPC++, C++, C, Fortran source and compiler-based instrumentation
- Intel oneAPI Clang compiler integration and instrumentation (-finstrument-functions)
- Intel oneAPI OpenMP Tools Interface (OMPT v5.0)
- Level Zero integration for DPC++ runtime events
- DPC++ symbol demangling support (-fno-sycl-unnamed-lambda)
- OpenCL performance instrumentation
- Intel MPI profiling interface in Intel HPCToolkit
- Intel Python instrumentation, support for Intel AI Toolkit for Tensorflow/PyTorch
- Intel Exascale Laboratory MAQAO binary instrumentation
- Intel PIN integration
- PAPI [UTK] and LIKWID [FAU] performance counter library integration for Intel CPUs

The only vendor toolchain that provides comprehensive language support for instrumentation at the above levels for transparently observing key events during execution!

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 many instructions are executed in these code regions?
  Floating point, Level 1 and 2 *data cache misses*, hits, branches taken? What is the extent of vectorization for loops?
- What is the memory usage of the code? When and where is memory allocated/de-allocated? Are there any memory leaks? What is the memory footprint of the application? What is the memory high water mark?
- How much energy does the application use in Joules? What is the peak power usage?
- What are the I/O characteristics of the code? What is the peak read and write *bandwidth* of individual calls, total volume?
- How does the application *scale*? What is the efficiency, runtime breakdown of performance across different core counts?

Instrumentation

Add hooks in the code to perform measurements

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

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
- *Intel® OneAPI*
  - Level Zero
  - Track time spent in kernels executing on GPU
  - Track time spent in OneAPI runtime calls
- *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 + pthread*
  - PMPI + pthread interfaces
- *MPI + Intel ® oneAPI DPC++/SYCL*
- PMPI + Level Zero interfaces
- *OpenCL + Python*
  - OpenCL + Python instrumentation interfaces
- *Kokkos + OpenMP*
  - Kokkos profiling API + OMPT to transparently track events
- *Kokkos + pthread + MPI*
  - Kokkos + pthread wrapper interposition library + PMPI layer
- *MPI + OpenCL*
  - PMPI + OpenCL profiling interfaces

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

```
% mpirun -np 256  ./a.out
```

Track GPU operations

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

Track MPI performance

```
% mpirun -np 256   tau_exec ./a.out
```

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

```
% mpirun -np 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;
% mpirun –np 256  tau_exec –T ompt,mpi  -ompt  ./a.out
```

Track memory operations

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

Use event based sampling (compile with –g)

```
% mpirun –np 256 tau_exec –ebs ./a.out
Also  export TAU_METRICS=TIME,PAPI_L1_DCM…  -ebs_resolution=<file | function | line>
```

Non-MPI execution: use –T serial

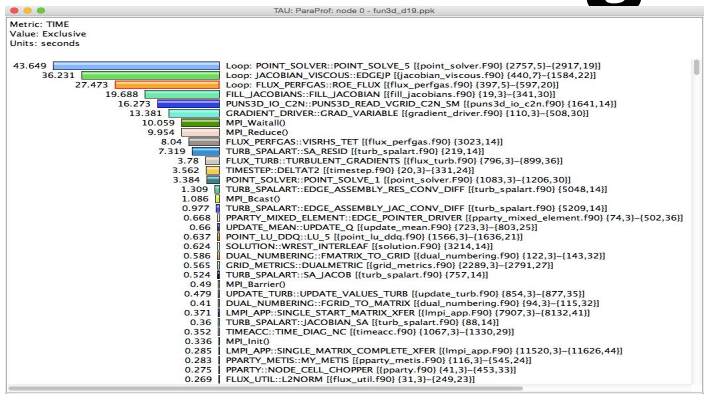
```
% tau_exec –T serial,level_zero –l0 –ebs ./a.out
```

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/craycnl/lib/Makefile.tau-intel-papi-mpi-pdt
/soft/perftools/tau/tau-2.31.1/craycnl/lib/Makefile.tau-intel-papi-mpi-pthread-pdt
/soft/perftools/tau/tau-2.31.1/craycnl/lib/Makefile.tau-intel-papi-ompt-mpi-pdt-openmp
/soft/perftools/tau/tau-2.31.1/craycnl/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/craycnl/lib/shared-intel-papi-ompt-mpi-pdt-openmp/

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

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

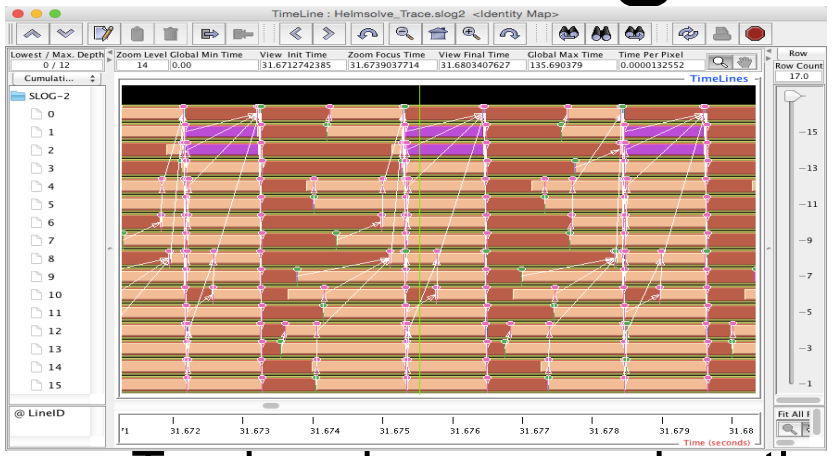
Profiling and Tracing

Profiling



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

Tracing



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

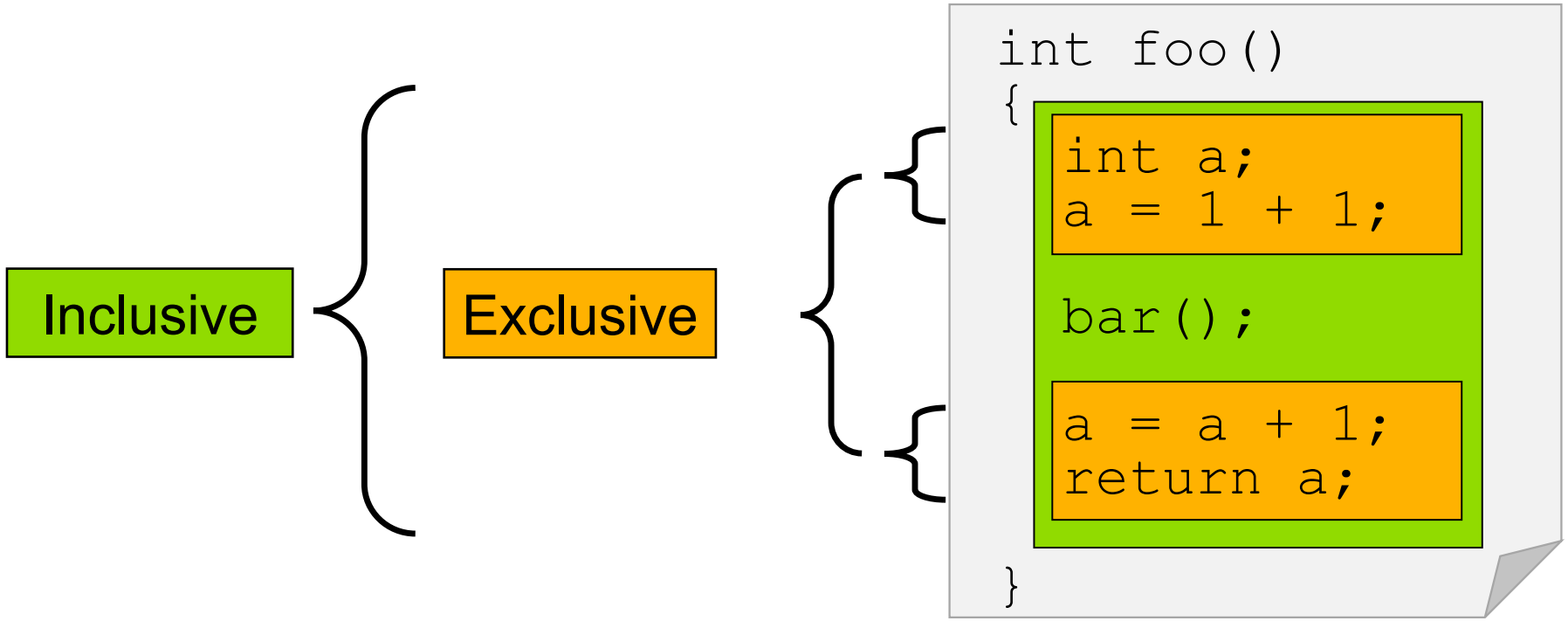
- Profiling and tracing

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

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

Inclusive vs. Exclusive values

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



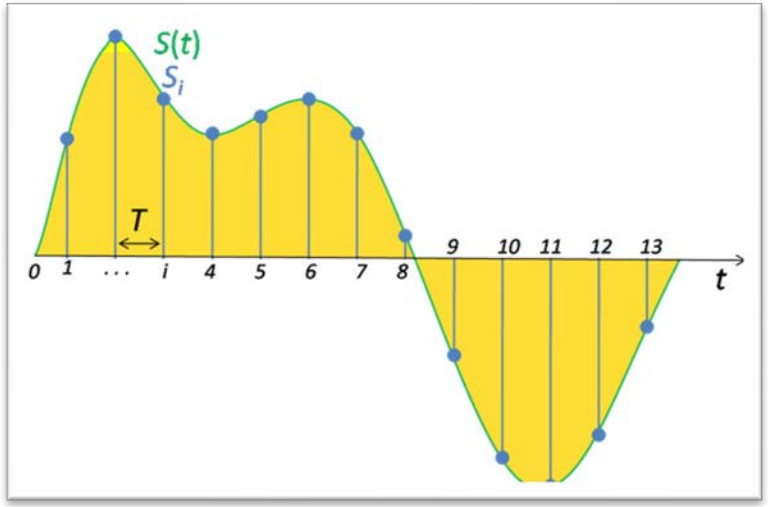
Performance Data Measurement

Direct via Probes

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

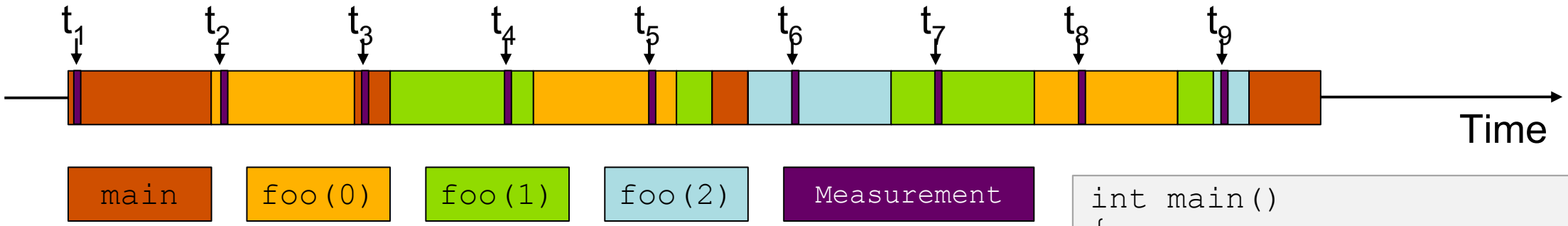
- Exact measurement
- Fine-grain control
- Calls inserted into code

Indirect via Sampling



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

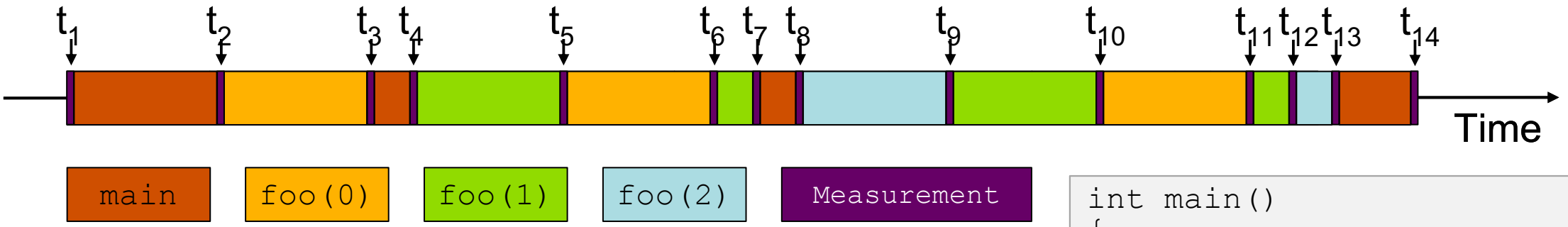
Event-Based Sampling (EBS)



- 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:

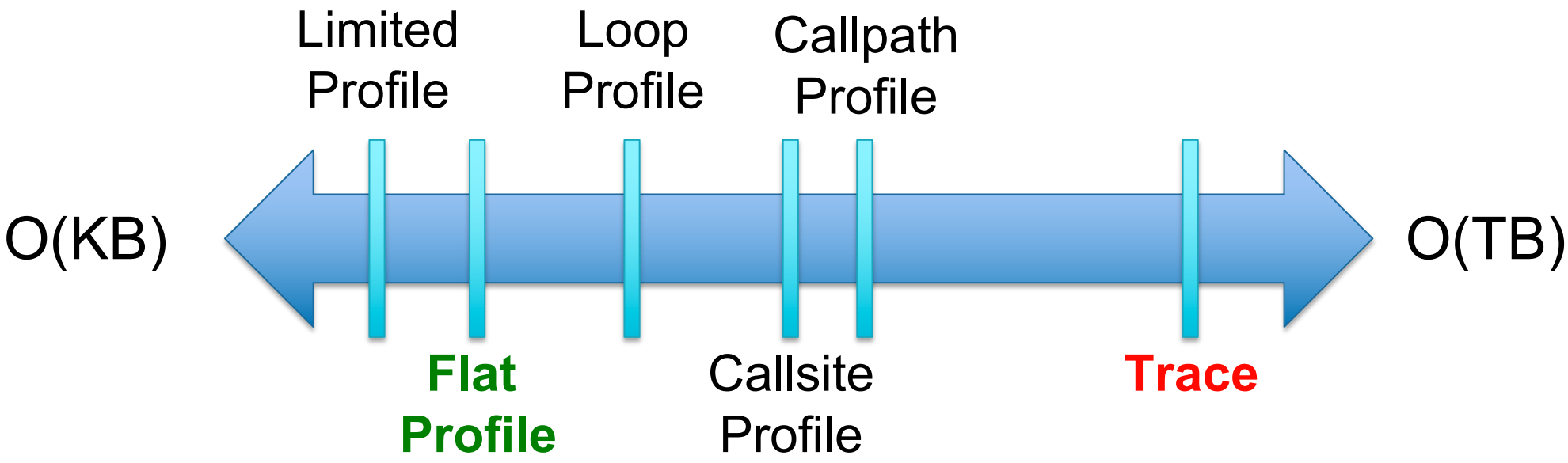
- Much more detailed information

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");
}
```

How much data do you want?



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: Quickstart Guide

Setup:

- `% module load tau`

Profiling with an un-instrumented application:

- `MPI:` `% mpirun -np 64 tau_exec -ebs ./a.out`
- `MPI+OpenMP with Clang 9+:` `% export TAU_OMPT_SUPPORT_LEVEL=full;`
  `% mpirun -np 64 tau_exec -T ompt,mpi -ompt ./a.out`
- `Pthread:` `% mpirun -np 64 tau_exec -T mpi,pthread -ebs ./a.out`
- `Python+MPI+Sampling:` `% mpirun -np 64 tau_python -ebs ./a.py`
- `Python+MPI+CUDA+Sampling:` `% mpirun -np 64 tau_python -cupti -ebs ./a.py`
- `Python+CUDA (no MPI):` `% tau_exec -T cupti,serial -cupti ./a.py`

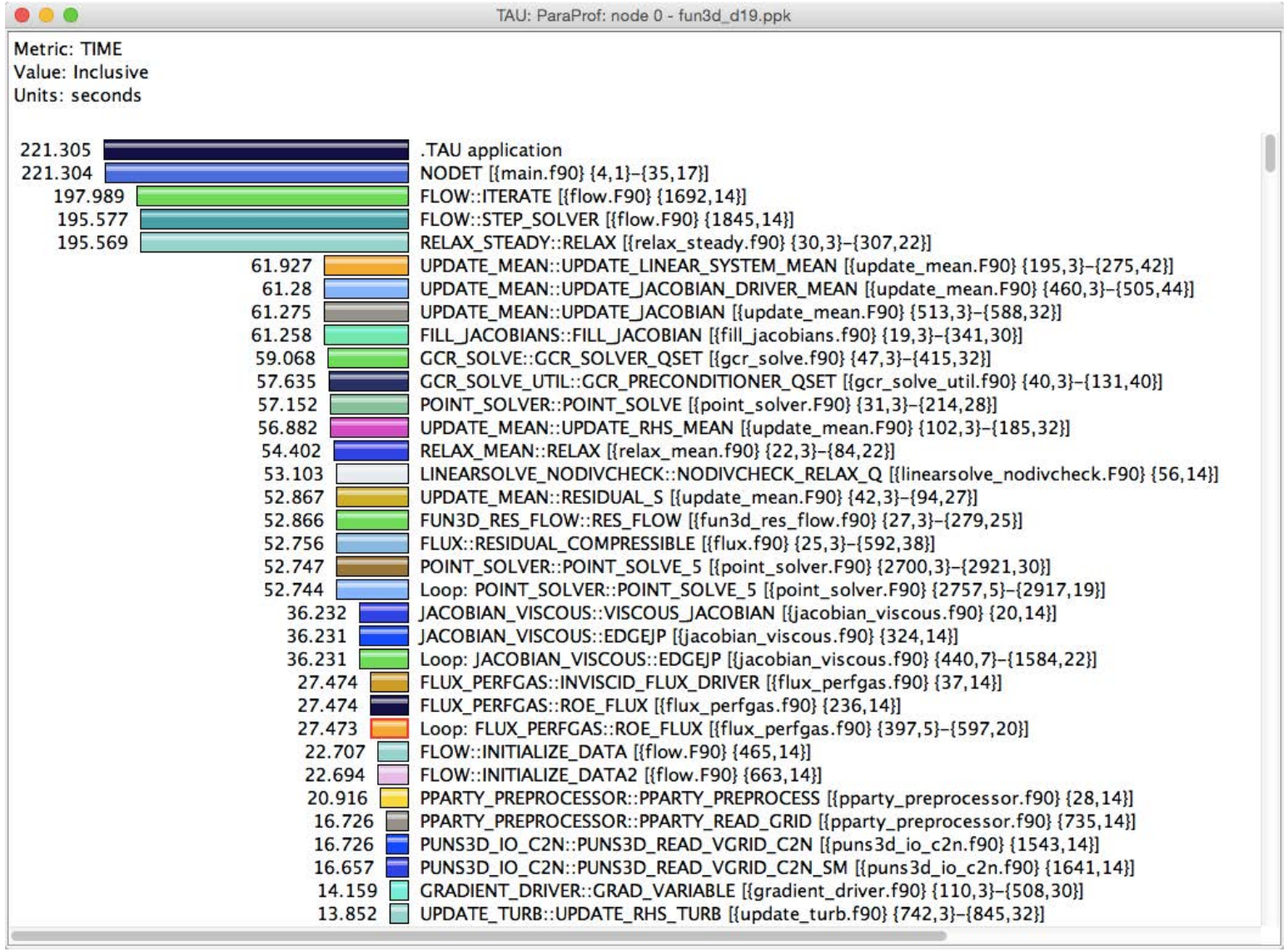
Analysis: `% pprof -a -m | more;  % paraprof (GUI)`

Tracing:

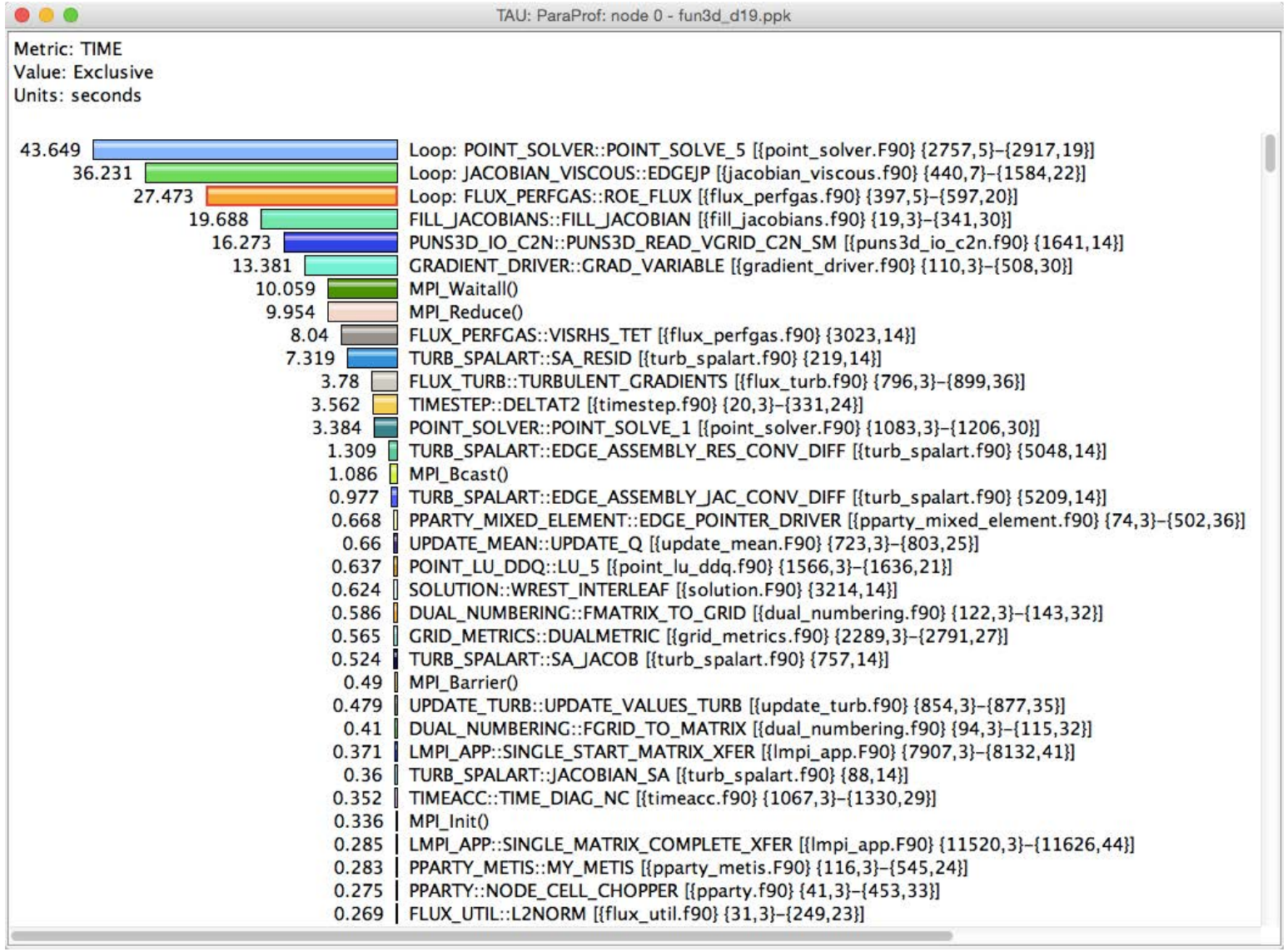
- `Vampir: MPI:` `% export TAU_TRACE=1; export TAU_TRACE_FORMAT=otf2`
  `% mpirun -np 64 tau_exec ./a.out; vampir traces.otf2 &`
- `Chrome:` `% export TAU_TRACE=1; mpirun -np 64 tau_exec ./a.out; tau_treemerge.pl;`
  `% tau_trace2json tau.trc tau.edf -chrome -ignoreatomic -o app.json`

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

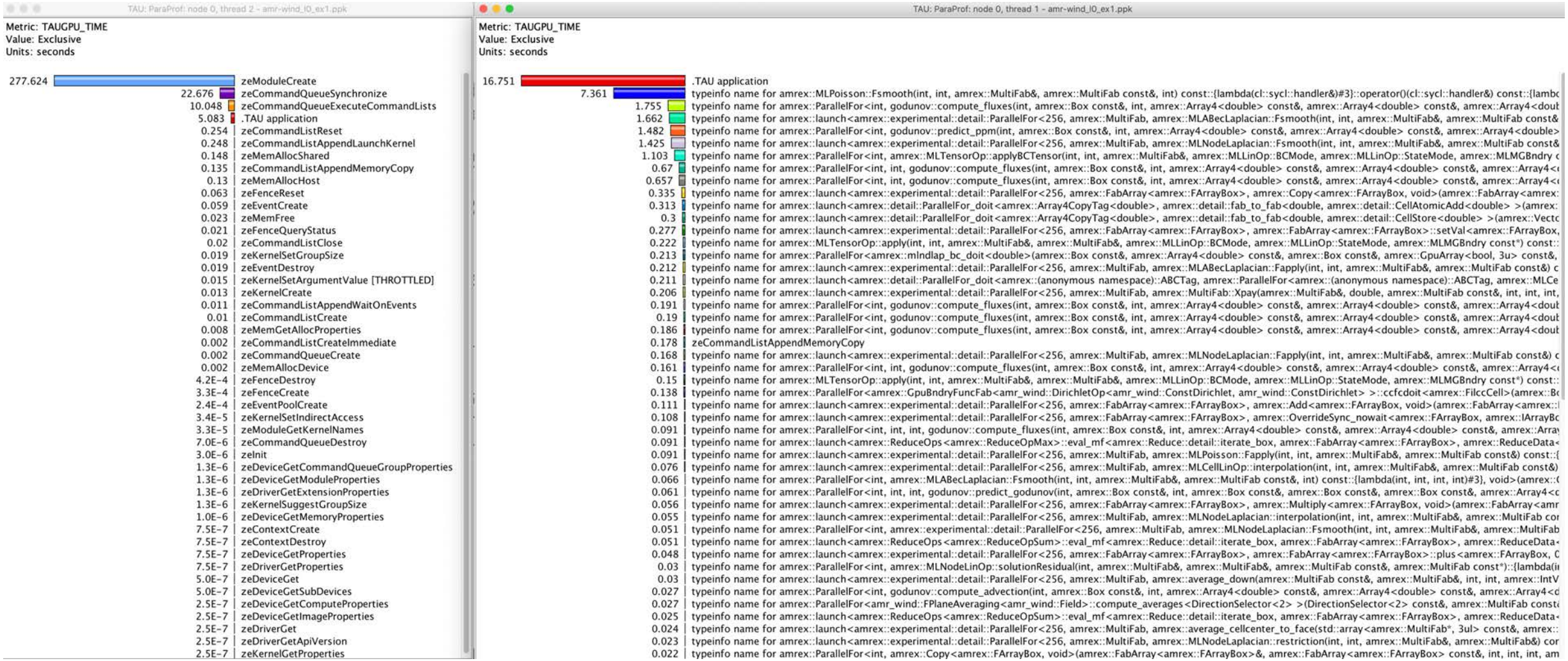
Inclusive Measurements



Exclusive Time

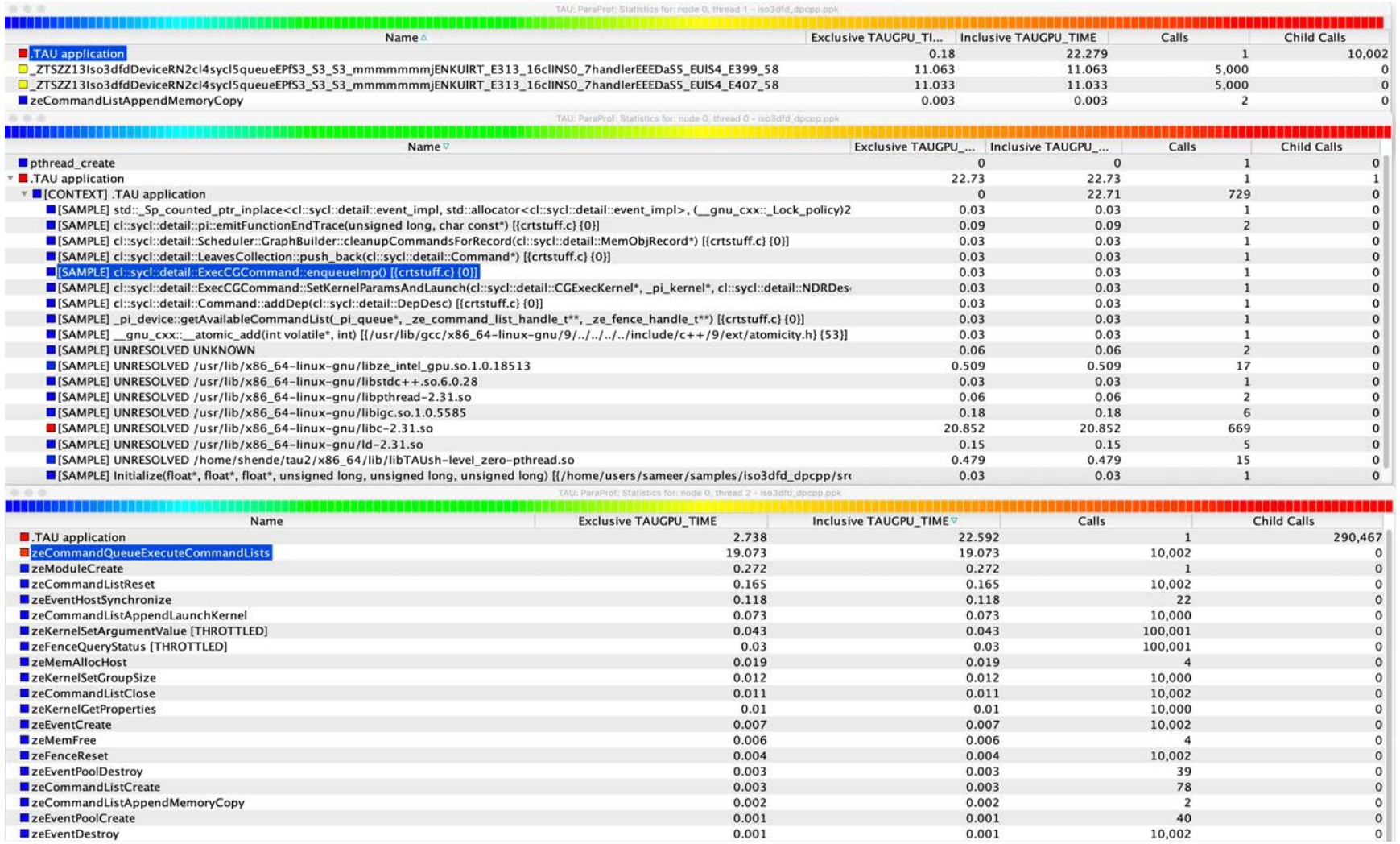


TAU: Intel oneAPI DPC++ on an Intel Gen12LP or DG1 GPU



% 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_dpcpp.ppk

Name	Exclusive TAUGPU_TI...	Inclusive TAUGPU_TIME	Calls	Child Calls
.TAU application	0.18	22.279	1	10,002
_ZTSZZ13Iso3dfdDeviceRN2cl4sycl5queueEPfS3_S3_S3_mmmmmmmjENKUlRT_E313_16clINS0_7handlerEEEDaS5_EUlS4_E399_58	11.063	11.063	5,000	0
_ZTSZZ13Iso3dfdDeviceRN2cl4sycl5queueEPfS3_S3_S3_mmmmmmmjENKUlRT_E313_16clINS0_7handlerEEEDaS5_EUlS4_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_dpcpp.ppk

Name	Exclusive TAUGPU_...	Inclusive TAUGPU_...	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*) [{crtstuff.c} {0}]	0.09	0.09	2	0
[SAMPLE] cl::sycl::detail::Scheduler::GraphBuilder::cleanupCommandsForRecord(cl::sycl::detail::MemObjRecord*) [{crtstuff.c} {0}]	0.03	0.03	1	0
[SAMPLE] cl::sycl::detail::LeavesCollection::push_back(cl::sycl::detail::Command*) [{crtstuff.c} {0}]	0.03	0.03	1	0
[SAMPLE] cl::sycl::detail::ExecCGCommand::enqueueImp() [{crtstuff.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) [{crtstuff.c} {0}]	0.03	0.03	1	0
[SAMPLE] _pi_device::getAvailableCommandList(_pi_queue*, _ze_command_list_handle_t**, _ze_fence_handle_t**) [{crtstuff.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/libigc.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_dpcpp/sr	0.03	0.03	1	0

TAU: ParaProf: Statistics for: node 0, thread 2 - iso3dfd_dpcpp.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-z	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

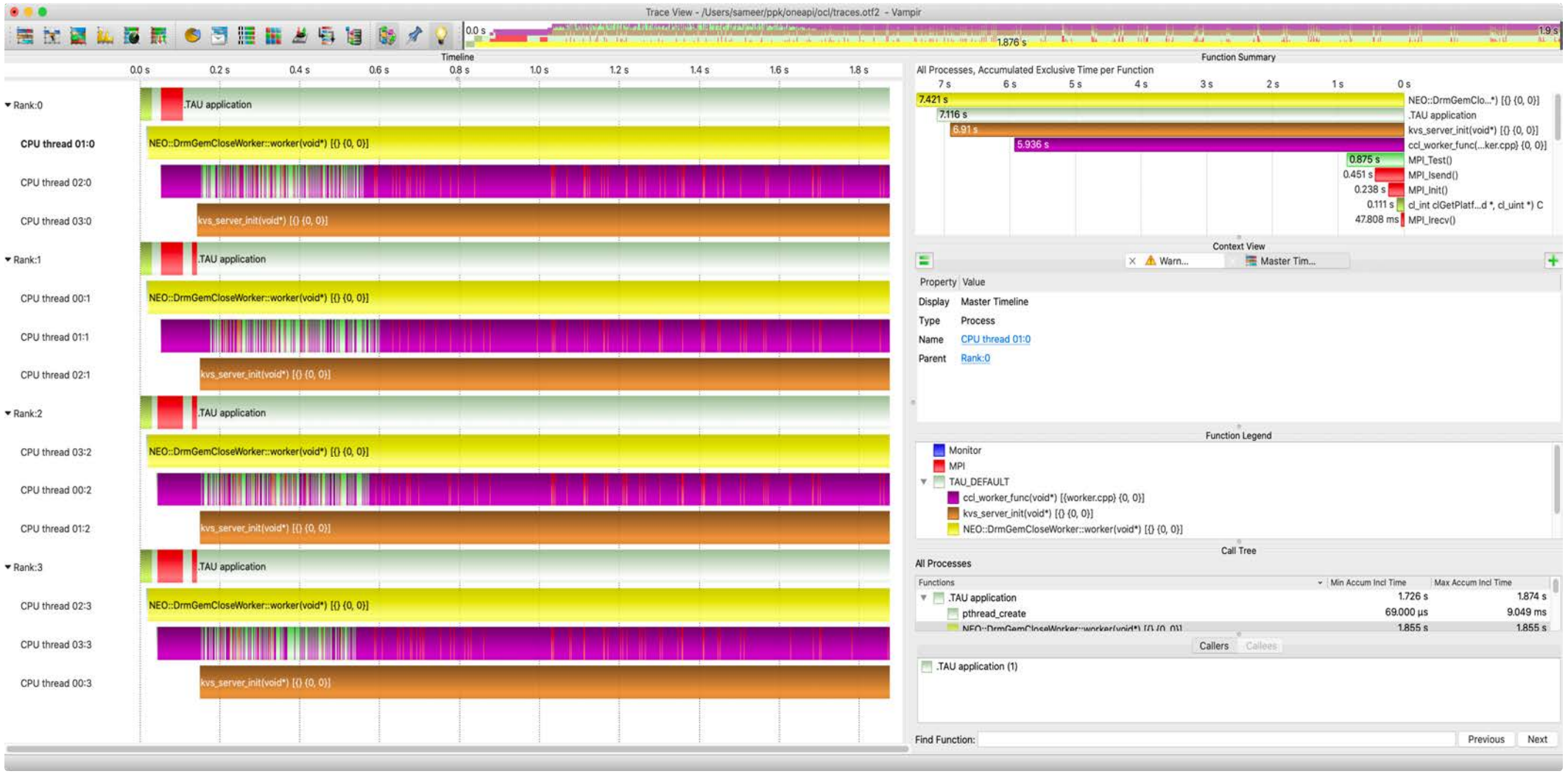
Name	Exclusive TAU...	Inclusive TAUG...	Calls	Child Calls
.TAU application	0.131	29.88	1	24
<Barrier>	0	0	8	0
<MemoryCopy>	0.049	0.049	12	0
GEMM	29.7	29.7	4	0

Units: seconds

Time spent in GEMM kernel

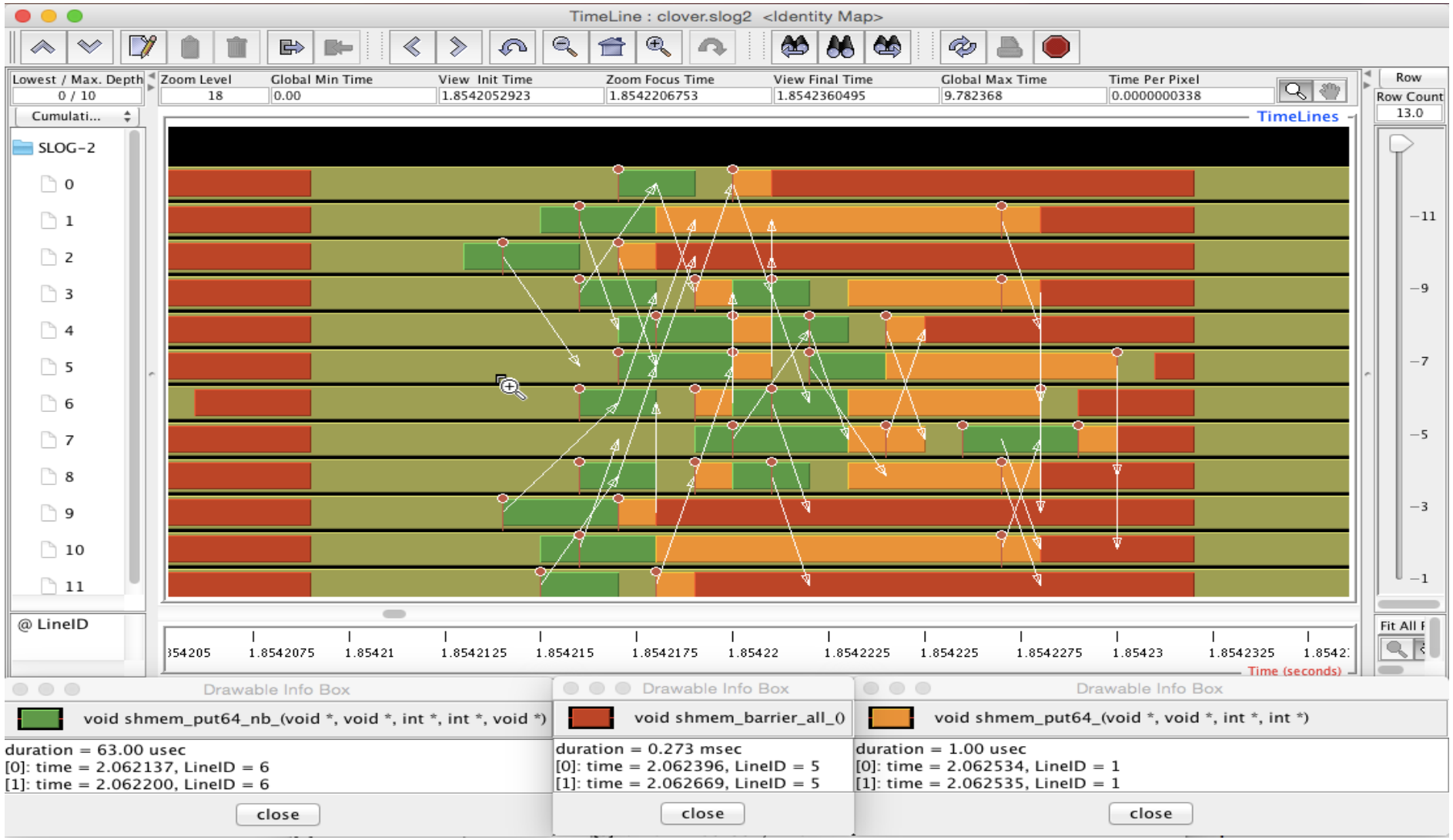
% mpirun –np 64 tau_exec –l0 ./a.out

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

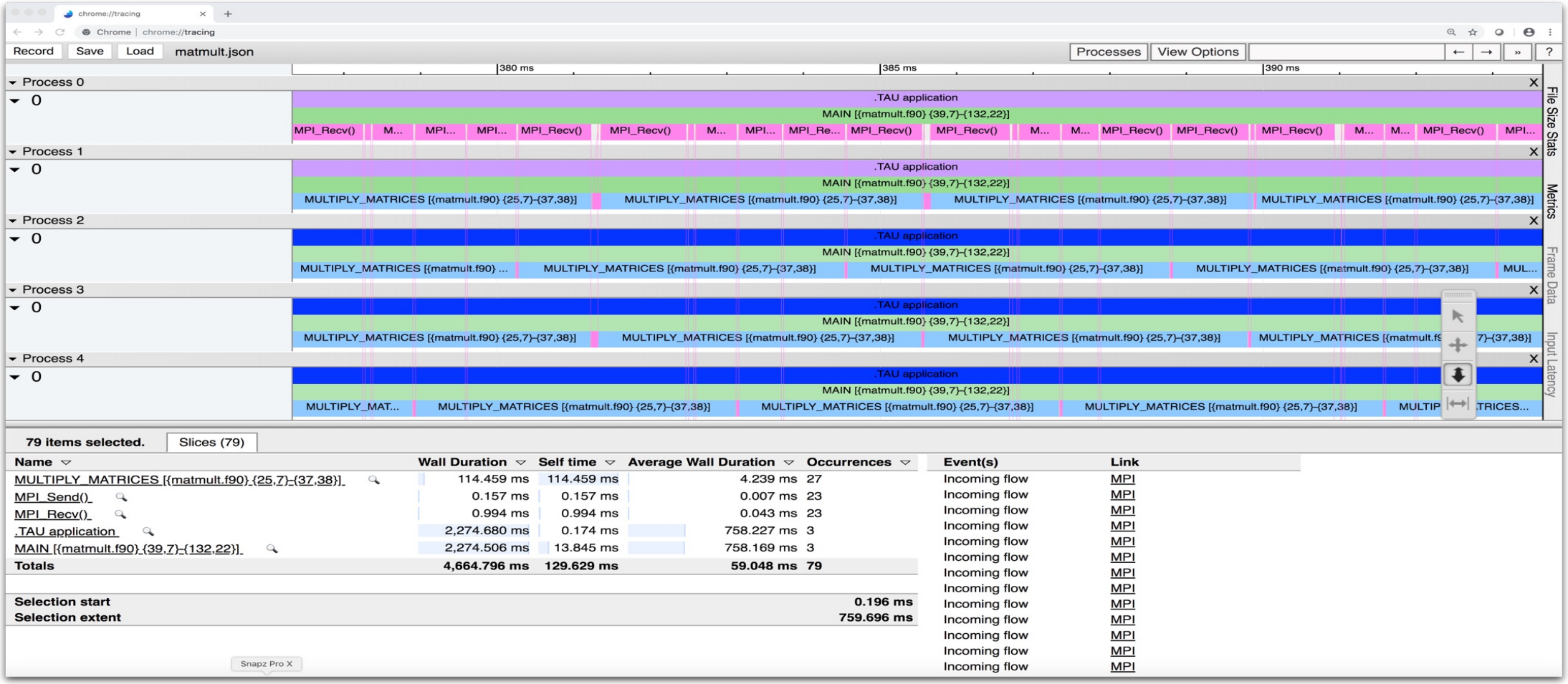



```
% export TAU_TRACE=1; export TAU_TRACE_FORMAT=otf2
% mpirun –np 4  tau_exec –T level_zero –opencl ./a.out
```

Tracing: Jumpshot (ships with TAU)



Tracing: Chrome Browser



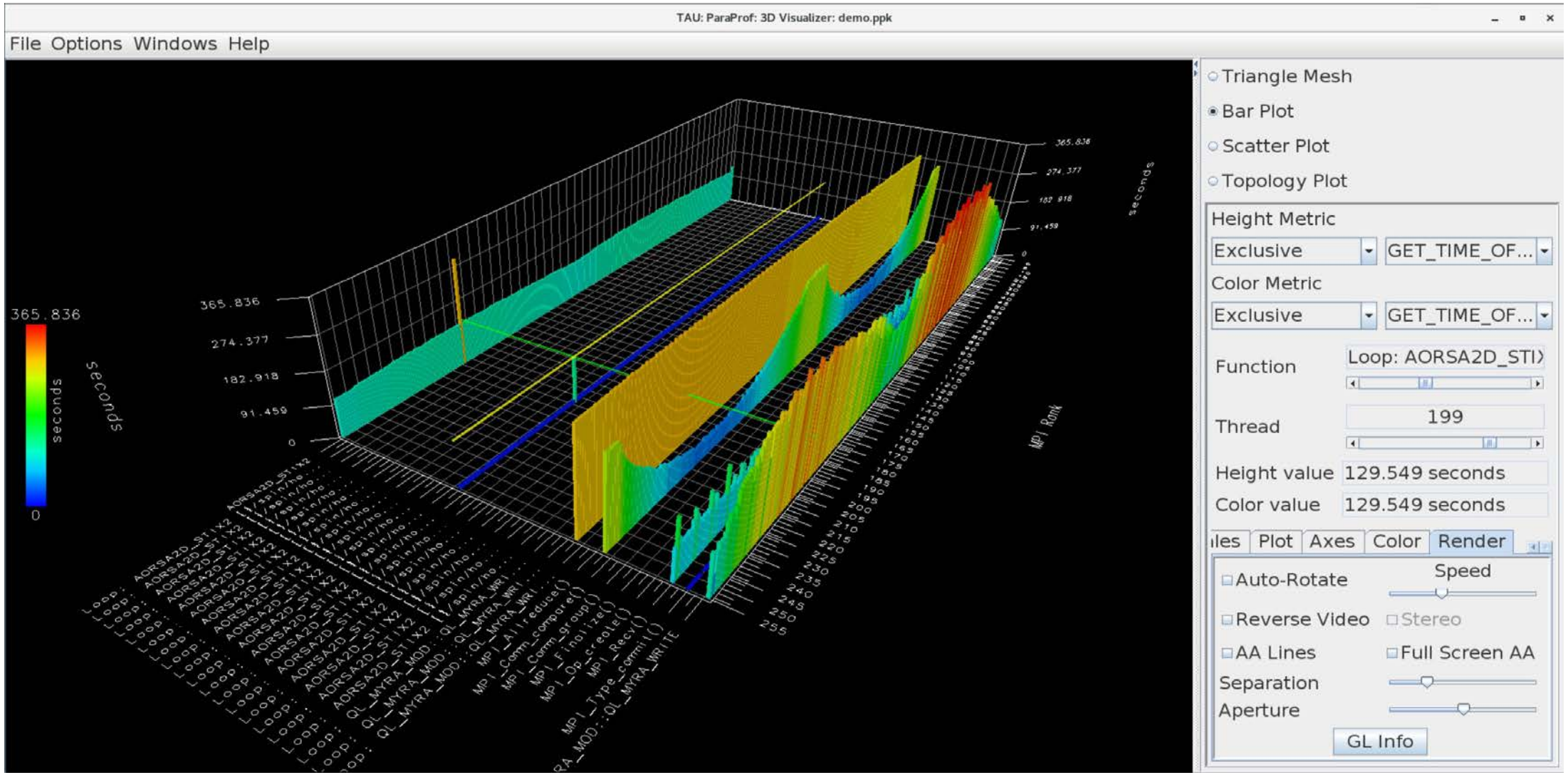
% export TAU_TRACE=1
% mpirun –np 256 tau_exec ./a.out
% tau_treemerge.pl; tau_trace2json tau.trc tau.edf –chrome –ignoreatomic –o app.json

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

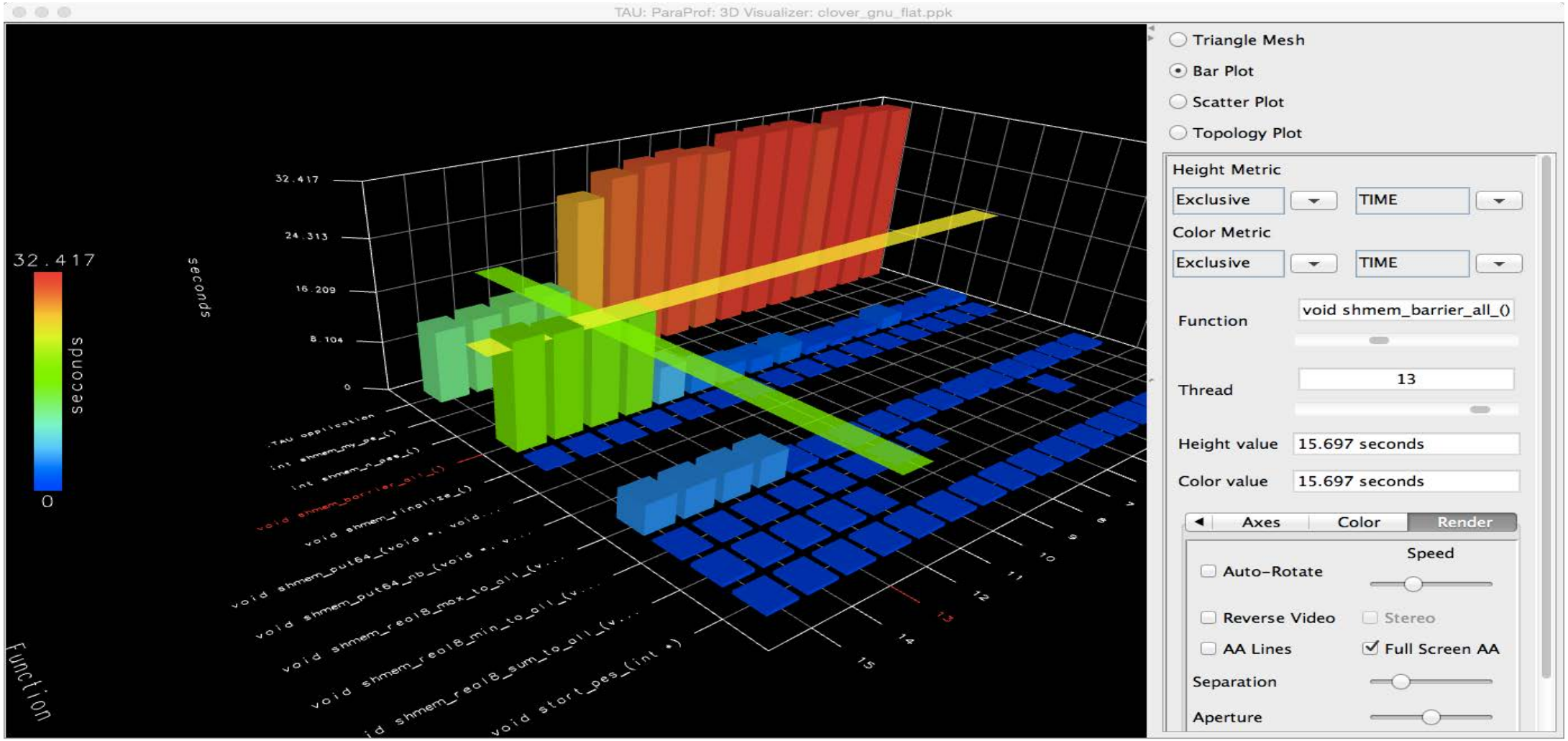
ParaProf Profile Browser

```
% paraprof
```

ParaProf 3D Profile Browser

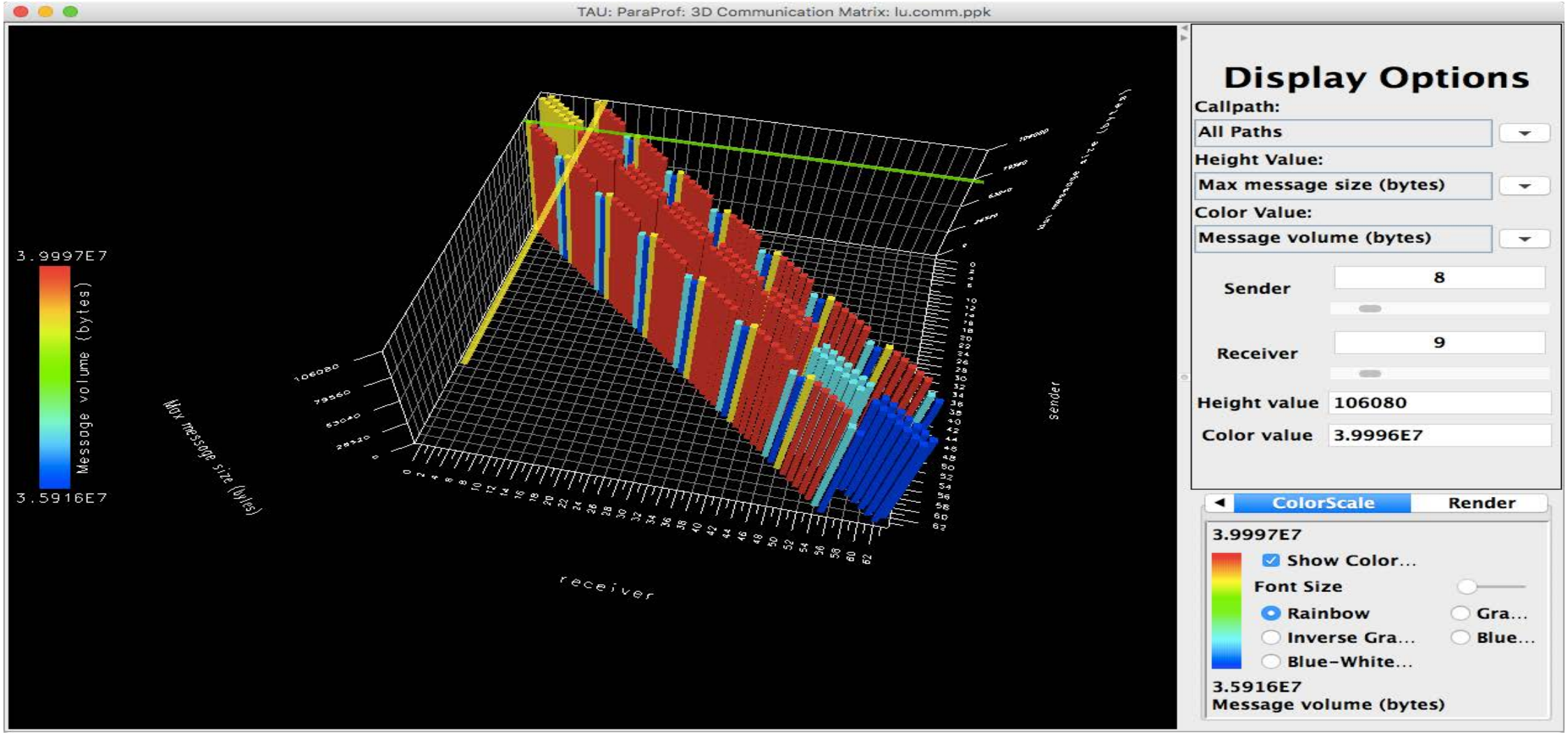


TAU – ParaProf 3D Visualization



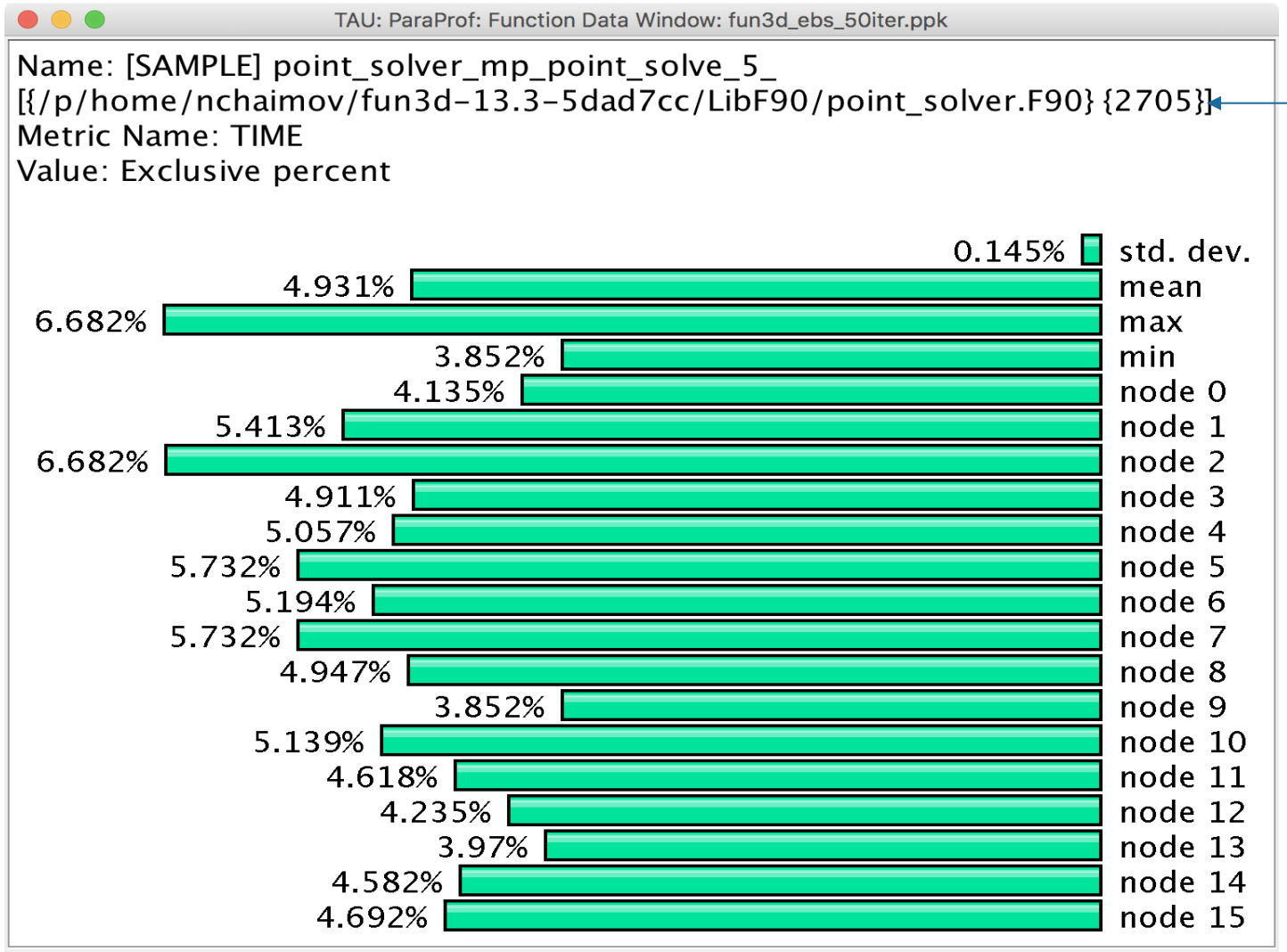
% paraprof app.ppk
Windows -> 3D Visualization -> Bar Plot (right pane)

TAU – 3D Communication Window



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

Event Based Sampling (EBS)



File: point_solver.F90
Line: 2705

Uninstrumented!

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

TAU's Runtime Environment Variables

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

Runtime Environment Variables

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

Runtime Environment Variables

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

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 &

TAU: Quickstart Guide

Setup:

- `% module load tau`

Profiling with an un-instrumented application:

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

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

Tracing:

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

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

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 comp_perf_workshop -q comp_perf_workshop -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.

```
% module load cobalt/cobalt-gpu; qsub -I -n 1 -A comp_perf_workshop -t 50
% module use ~sameer/modulefiles; module load tau;
% tar zxf ~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)

```
% module load cobalt/cobalt-gpu; qsub -I -n 1 -A comp_perf_workshop -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)

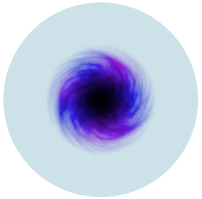
```
% module load cobalt/cobalt-gpu; qsub -I -n 1 -A comp_perf_workshop -t 50
% module use ~sameer/modulefiles; module load tau;
% tar zxf /soft/perftools/tau/workshop.tgz
% cd workshop/CloverLeaf/CloverLeaf_CUDA;
% make clean
% make -j
% mpirun -np 3 ./clover_leaf
% mpirun -np 3 tau_exec -T cupti,mpi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

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 22.02 – February

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

https://e4s.io

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
- 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

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

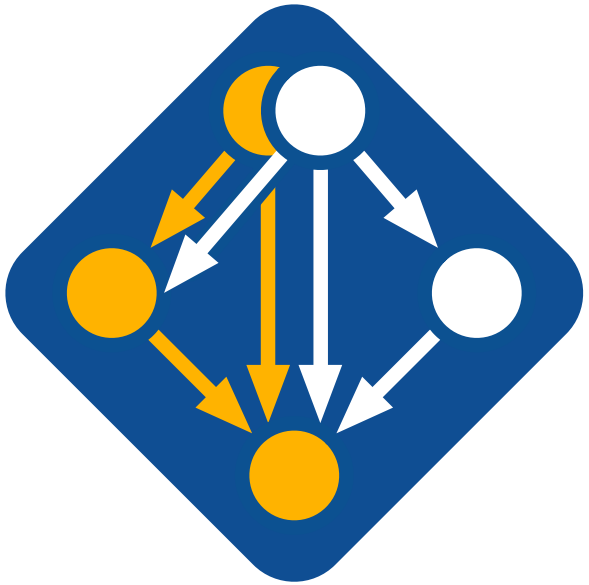
- How to install Spack (works out of the box):

```
$ 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

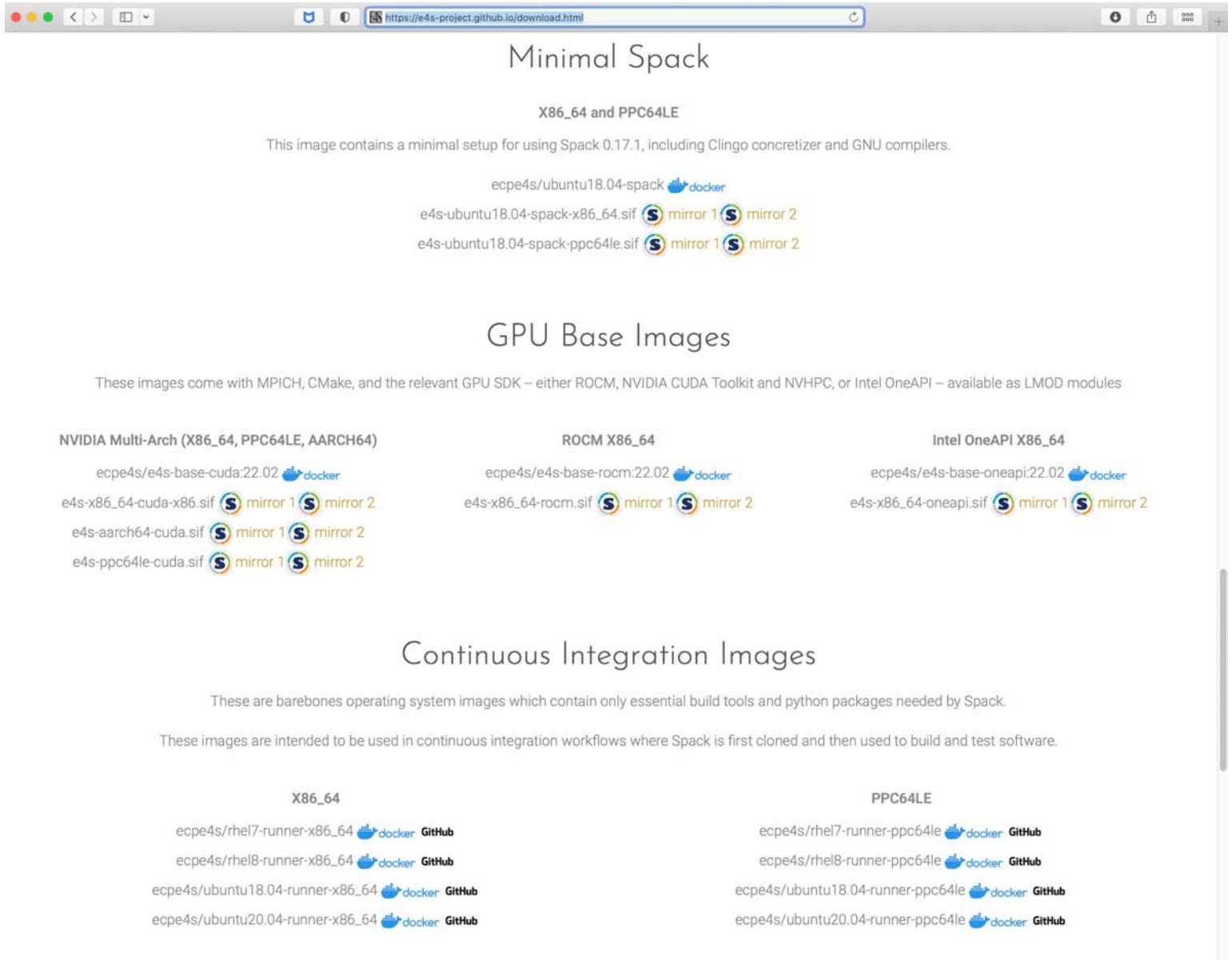
Spack provides the *spec* syntax to describe custom configurations

```
$ 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
```

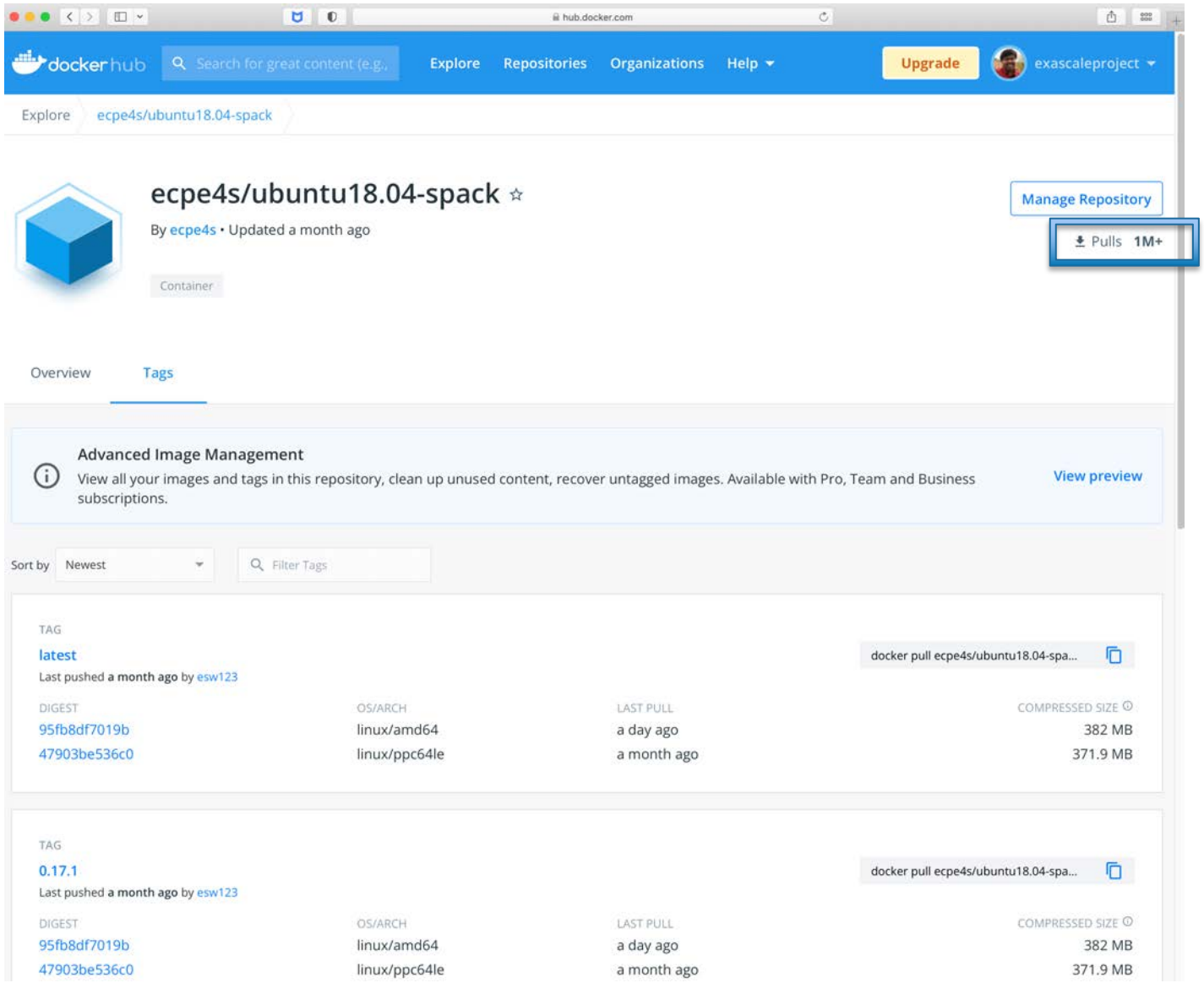
- Each expression is a ***spec*** for a particular configuration
  - Each clause adds a constraint to the spec
  - Constraints are optional – specify only what you need.
  - Customize install on the command line!
- Spec syntax is recursive
  - Full control over the combinatorial build space

E4S base container images for x86_64, ppc64le, and aarch64



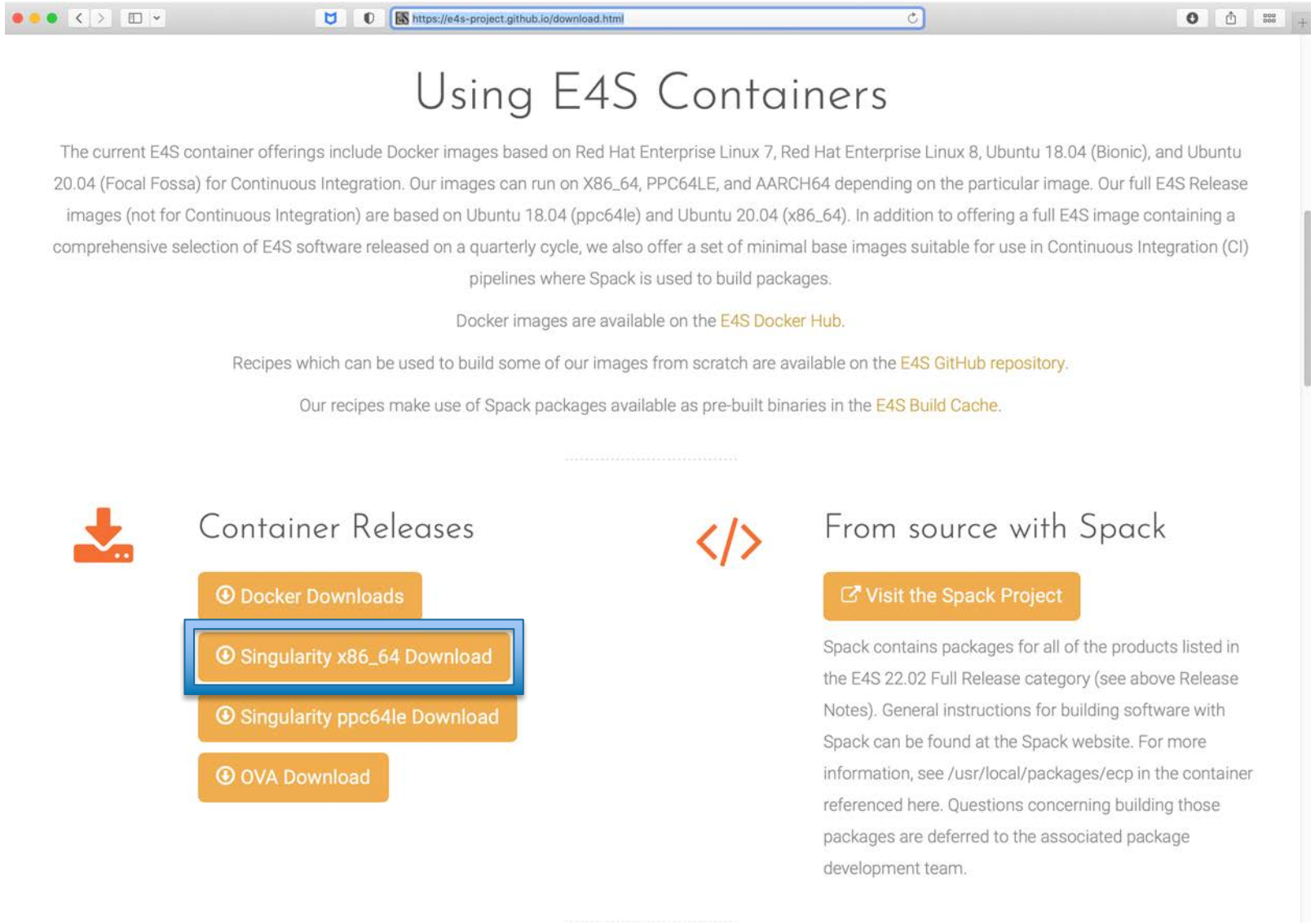
- Hub.docker.com
- ecpe4s
- Platforms:
  - x86_64
  - ppc64le
  - aarch64
- GPU runtimes:
  - Cuda
  - ROCm
  - oneAPI
- Singularity images
- Miminal Spack image

Minimal Spack base image on Dockerhub



- Create custom container images
- 1M+ downloads!

Download E4S 22.02 GPU Container Image: NVIDIA, AMD, Intel



- Full featured Singularity image
- GPU base images for
  - x86_64 (Intel, AMD, NVIDIA)
  - ppc64le
  - aarch64
- Packages with support for all three GPU runtimes:
  - Kokkos
  - TAU

https://e4s.io

22.02 Release: 100 Official Products + dependencies (gcc, x86_64)

```
  1: adios2                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/adios2-2.7.1-vrqqwksvvumpvuvi2f3zvhrudbhrgvr7
  2: alquimia              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/alquimia-1.0.9-5pxq2rf35knkrbdjz2hdqifjpsvsj2ay
  3: aml                   spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/aml-0.1.0-52bcp4rwi6xzklr2qpl3a3huqle6sszh
  4: amrex                 spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/amrex-22.02-xjb77ajgucyfcyswmioly672gck3s2fy
  5: arborx                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/arborx-1.1-x54ta6aq3vgvzhqaznybw63nbpwgp2c7
  6: archer                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/archer-2.0.0-wkdybteqjoqfupcjcnr3syh4kgjza4mv
  7: argobots              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/argobots-1.1-6vbx4fbx3ert23po2fzeuddnyal2wniy
  8: ascent                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/ascent-0.7.1-y6ozlrcntdjrten3eel7di6fuuoe6f7x
  9: axom                  spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/axom-0.6.1-vbde3r3uveb6n37vzqq6xuobett2y7l2
 10: bolt                  spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/bolt-2.0-fh7dq6fzfeie5fl3nzgindyzvgggges6v
 11: butterflypack         spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/butterflypack-2.1.0-vwr7qf256rg2n63auewcyuko3wy3gzzt
 12: cabana                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/cabana-0.4.0-ubam723mz433hemjuepsvmq553v3geln
 13: caliper               spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/caliper-2.7.0-xvpd7krs6gxtyqekpaulssn4efm72zlj
 14: catalyst              spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/catalyst-5.6.0-5ao2vfmbfis3na5p4a5j7uvykihdgxaf
 15: chai                  spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/chai-2.4.0-nkjjn2do7p747ysc2ywxa4n7nqhnmh2v
 16: charliecloud          spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/charliecloud-0.26-imxvh6utmc4icpeieodkonunb7zn4eez
 17: conduit               spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/conduit-0.8.2-nhruflxgas6lzwjy5scaucveyncwox44
 18: darshan-runtime       spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/darshan-runtime-3.3.1-ws6gpwomoa7nmgzcc4ztga6lwx55oeg2
 19: datatransferkit       spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/datatransferkit-3.1-rc3-euqumxqzcu7f3c4hvsvhbc3mtpvi2jpu
 20: dyninst               spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/dyninst-12.0.1-dslp7foewbfnxe2pn2z3mbiqwztmf57c
 21: faodel                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/faodel-1.2108.1-rdn5dmxtyf2rpiz5cimijutrqr7p2zwk
 22: flecsi                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/flecsi-2.1.0-gcqxn654rmz4vxndkmup62o3wmoebtiu
 23: flit                  spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/flit-2.1.0-qfegiopjkolncxhhraopx6s3nr4g23xi
 24: flux-sched            spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/flux-sched-0.20.0-eaf5kwa3r46vxwnyuljl7zhpitjthp3k
 25: fortrilinos           spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/fortrilinos-2.0.0-nh7wozfevbp3rdy3iu3wei5f7u2kzzl2
 26: gasnet                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/gasnet-2021.9.0-37bcasne2t26z4f7rju7fy52eeqooolx
 27: geopm                 spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/geopm-1.1.0-o2b57hvdpzkd7as754onu5cdzhg6boc6
 28: ginkgo                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/ginkgo-1.4.0-tlueryyabtnd6yg7sen6iknpyyzkpfbt
 29: globalarrays          spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/globalarrays-5.8-auttuj4uxg5s45agb2pr4oih7rhjchbv
 30: gotcha                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/gotcha-1.0.3-u6ttykuc7w75fpckuy4piy72uhdxvdxy
 31: gptune                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/gptune-2.1.0-yocmmqkzvmaqewybyn2o4i7qu6x73f7i
 32: hdf5                  spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hdf5-1.10.7-ydvek2t5h4kz2bc7qxrnborep7ljkye6
 33: heffte                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/heffte-2.2.0-gt4xlhl6oe2abi5tc6psrdqdnz2hs2gj
 34: hpctoolkit            spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hpctoolkit-2022.01.15-5bpxdxxdkagebetg4c2vqa3ca36elwvs
 35: hpx                   spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hpx-1.7.1-udoriqk2dx6vactf3gl6746r2ykw7s5j
 36: hypre                 spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/hypre-2.24.0-rubtvtyzb7i6fk52vryghtcr62bgnlvt
 37: kokkos                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/kokkos-3.5.00-jcqkaxownuoufxxbsiw5tm2s7p763rkc
 38: kokkos-kernels        spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/kokkos-kernels-3.5.00-w6r3jgo7i5qzb5crtr3wqlo7l3a2gskn
 39: lammps                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/lammps-20220107-dxuaklopsx4q3t4gtwx274l7ear3d6v5
 40: legion                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/legion-21.03.0-ewj6mv6kyslktjgj5reeyoasegc5insn
 41: libnrm                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/libnrm-0.1.0-zt2trrdexkcjkcxsag4hvlry7q7x2aqv
 42: libquo                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/libquo-1.3.1-ot45gb6c3cbjddanrmoy4yxpqfdapoey
 43: loki                  spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/loki-0.1.7-2zpo6dh6bdrko47n4gziacm6xteojflm
 44: magma                 spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/magma-2.6.1-hjnxgt33n2nwmg6jsolrilai6dnycxc3
 45: mercury               spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mercury-2.1.0-5by37sm7nto6t7tz6rfnq6355vu6fbnw
 46: metall                spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/metall-0.17-a3qixbbz5hpkkvmocpiqbp4e5lehf2j2
 47: mfem                  spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mfem-4.3.0-7b7vcw33k4brllinosrhvii2oj63bwzs
 48: mpich                 spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mpich-3.4.2-b2hsqqqnsiodzp3kw63u425osorilfty
 49: mpifileutils          spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/mpifileutils-0.11.1-x6mkbu3osheeiba7rqb3xjsu4fequ7tu
 50: netlib-scalapack      spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/netlib-scalapack-2.1.0-mu7sj7fu3nmrtzknsrkvquuoud2eupvf
```

```
Singularity> which dpcpp
/opt/intel/oneapi/compiler/2022.0.2/linux/bin/dpcpp
Singularity> which hipcc
/opt/rocm-4.5.2/bin/hipcc
Singularity> spack find cuda
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / gcc@9.3.0 ------------------------
cuda@11.4.2
Singularity> spack find nvhpc
==> 1 installed package
-- linux-ubuntu20.04-x86_64 / gcc@9.3.0 ------------------------
nvhpc@22.1
Singularity>
```

GPU runtimes

- AMD (ROCm)
  - 4.5.2
- Intel (oneAPI)
  - 2022.0.2
- NVIDIA (CUDA)
  - 11.4.2
- NVHPC
  - 22.1

22.02 Release: 100 Official Products + dependencies (gcc, x86_64)

```
  51: nccmp           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/nccmp-1.9.0.1-2hkqbcchaexl22f3lnkkozvznjr6h3g4
  52: nco             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/nco-5.0.1-nzqjzuwz3pvkslc32fnshotwr7nwlcgu
  53: ninja           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/ninja-1.10.2-2gpjomjrzlvinikx2qrm3rsasypnptvl
  54: nrm             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/nrm-0.1.0-omwezy5dwi7qshkr5v2eo64lj37scwhw
  55: omega-h         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/omega-h-9.34.1-syd6ahkexymz5ik24msxcki4fnatgvta
  56: openpmd-api     /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/openpmd-api-0.14.4-k6wknbemtkoujp5fh3lxum5x5lklmf7u
  57: openmpi         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/openmpi-4.1.2-5yqclfs7ipo3u6ap4aeffacgvxqt5674
  58: papi            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/papi-6.0.0.1-mjwlkr6yrsrcnufl7nv47435mjmiifij
  59: papyrus         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/papyrus-1.0.1-oawas4327vvwwy7cpgkuftqnberp4dbj
  60: parallel-netcdf /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/parallel-netcdf-1.12.2-ojopqbmuz6rhdtxq3xl4icd7euvmhwoj
  61: paraview        /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/paraview-5.10.0-ai6ih3nx3rhwtepdlojfx57oupjlht7j
  62: parsec          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/parsec-3.0.2012-mmut76y5frfk22qlraeihmyb6noruw3c
  63: pdt             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/pdt-3.25.1-c57l5pqsnjyt7f3tfa256lkotm3mwaow
  64: petsc           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/petsc-3.16.4-o3kxlwykh3lflqg3unx2vwykitgodpjh
  65: phist           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/phist-1.9.5-ejcz3wgujbcpi4wkoxcr63w4hkyb5yyp
  66: plasma          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/plasma-21.8.29-447maohfkz3idurx33gxypl5jc54cblq
  67: plumed          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/plumed-2.6.3-3d6ibkubuzle3a4pd3duhi56y6ajaclt
  68: precice         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/precice-2.3.0-rjrp7whhwk7x3ztvq6p4pfbxigpbkso5
  69: pumi            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/pumi-2.2.6-z26nhhtfcbhv62ceukc4hhy77wzkavut
  70: py-cinemasci    /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-cinemasci-1.3-6ah5lcb5kno2owdxils677ngylt5asfv
  71: py-jupyterhub   /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-jupyterhub-1.4.1-wdouha5jog55a6u2mnq34yw5hguohc2l
  72: py-libensemble  /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-libensemble-0.8.0-6upb3t7cbizf2bzg2mkaufm52ki7n5zx
  73: py-parsl        /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-parsl-1.1.0-qi4ema4wexehbxwiy4yfatdx4ltkqhdy
  74: py-radical-saga /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/py-radical-saga-1.11.1-yroolargjs4w3wid4copj6qqn7li4ji4
  75: qthreads        /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/qthreads-1.16-oqsr5vtyypuqmjowxy7cf7l4c7o35hao
  76: raja            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/raja-0.14.0-wug2hk4iuvwdiqaylipykempp227o6ek
  77: rempi           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/rempi-1.1.0-7szviepug5lw2khdoxcwvs6d7pg2u2nt
  78: scr             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/scr-3.0rc2-wmnhwtvh7uzfwth7q6l3shphnunvqeoe
  79: slate           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/slate-2021.05.02-7ck5664dxjjhdn63dp7xrkxgr7b3zqzf
  80: slepc           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/slepc-3.16.2-tk2zp7s5kqqjbbw3unvqqebf2infp4us
  81: strumpack       /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/strumpack-6.3.0-mdvvav6jov5rq2qk6gubl6xr7u7xeafz
  82: sundials        /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/sundials-6.1.1-nin5qvr6nywydyqfoitwdmnueifvowhi
  83: superlu-dist    /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/superlu-dist-develop-jbyhfjjr2s24yhiqhb2fop3o4qe72ugc
  84: stc             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/stc-0.9.0-4ldizggme2pk22wvbmxstlmdljz7daft
  85: swig            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/swig-4.0.2-fortran-hdwur55hnamozikupngwlygilofxgact
  86: sz              /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/sz-2.1.12-ncwe7eipqstaikf6w5yuisut7ohu7cfo
  87: tasmanian       /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/tasmanian-7.7-ntlsb3dbnklrlyqb44c7td7tln7y4ji4
  88: tau             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/tau-2.31-pbccumbikldui ftms63x2jqtviwvk764
  89: trilinos        /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/trilinos-develop-d5semjk4u4axs7mlep2yj4aarwfgxttw
  90: turbine         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/turbine-1.3.0-lpu56cphuxnmonv5dpojvcbsecfxewo2
  91: umap            /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/umap-2.1.0-qwldcv45isedxa2xiq2lui6eorvsknvd
  92: umpire          /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/umpire-6.0.0-kfzrcgjnnisrevs422hgg622djvshvdp
  93: unifyfs         /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/unifyfs-0.9.1-xfqgf74ejwrfo4y3ue45phglzh6hidmz
  94: upcxx           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/upcxx-2021.9.0-x7yedv4bmia4dsupr3x2elvngjw2e6ep
  95: variorum        /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/variorum-0.4.1-iucjprimf7tpjo6jz7w2hyrouvfwflwe
  96: veloc           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/veloc-1.5-xnjowfax7ysawyyygo46mikk7ss36uw3
  97: vtk-m           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/vtk-m-1.7.1-iqkpaoty4ot66d5w6urgdpowyncgpoq2
  98: wannier90       /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/wannier90-3.1.0-fz3t3zaslhan5fbgghjmzvo5xvaucub3
  99: warpx           /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/warpx-22.02-yq75dzo7ycj6y5kpcuvc74mt6wvbeq7l
 100: zfp             /spack/linux-ubuntu20.04-x86_64/gcc-9.3.0/zfp-0.5.5-glocwgycmhef4w4pnqemrcct6xpac3t5
```

Languages:
- Julia
- Python

AI products with GPU support
- Tensorflow
- Pytorch

3D Visualization
- Paraview
- VisIt
- TAU's paraprof …

22.02 Release: 100 Official Products + dependencies (gcc, ppc64le)

1:	adios2	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/adios2-2.7.1-4jqdeeg24ievjsmidstktyiwlv2kws55
2:	alquimia	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/alquimia-1.0.9-kl2uuwk4ihcda7fhyxkedopuqhultaqf
3:	aml	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/aml-0.1.0-dvzmjcuzox3ubd7lnxdgoggoksk5v43k
4:	amrex	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/amrex-22.02-zc7mv3makq5c2qpw7jjlmwrb4k66rvvl
5:	arborx	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/arborx-1.1-szs54gusdjuwibxshd27xq5pmds5por3
6:	archer	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/archer-2.0.0-vcvzy6okrw4mjxtqgmuo3725ulboietr
7:	argobots	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/argobots-1.1-trhfaqcmt2ib5tsw4axzqzls4tbxxt45
8:	ascent	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ascent-0.7.1-6nzrbj2mgi7fqfrseyuhjm5rencldn3c
9:	axom	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/axom-0.6.1-ymb5ju6djdwurkxjbwo6yzpkgkybagan
10:	bolt	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/bolt-2.0-lfkm2qifo3qdvdgdgckeq2b7rgv3yesq
11:	butterflypack	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/butterflypack-2.1.0-eusmk3wvyju7wm4uekimknyl7ftz77j5
12:	cabana	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/cabana-0.4.0-bv6y5ek6w42tufhkgzztxnhz4nyzdmcy
13:	caliper	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/caliper-2.7.0-yt7las4hzzmk75a4mehej4c5klt62dnk
14:	chai	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/chai-2.4.0-k3mrmb3ywq6ixwrn6mn7jl4gcxmqxkmy
15:	charliecloud	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/charliecloud-0.26-2byo4we7isxo5m77ixm6hjb2wbevymrr
16:	conduit	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/conduit-0.8.2-lnpv6hggqcap5v4q4wkacna3id53wosr
17:	darshan-runtime	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/darshan-runtime-3.3.1-fig7a4dxy56f5xbibb6fbi5wbawyv6b4
18:	datatransferkit	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/datatransferkit-3.1-rc3-wa4d7h6s2ui3r375rirnsxs6mduiynu7
19:	dyninst	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/dyninst-12.0.1-h3kpxhzv7iqylpjvqbneegatif7qs67t
20:	exaworks	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/exaworks-0.1.0-vlseszxfohskd3t2wujfabjkqspdxhaa
21:	faodel	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/faodel-1.2108.1-7cbwmf5olgoff34nrf6aciayewwh5ol5
22:	flecsi	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flecsi-1.4.2-2ny3vyzvo3kfe7oi37awx3im4pzuenem
23:	flit	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flit-2.1.0-tiazm5zdjun5fpgbilqwuyv75sdng4yn
24:	flux-sched	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/flux-sched-0.20.0-ntaytdbybyy3d2vvr4yw3o6sqlmdautz
25:	fortrilinos	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/fortrilinos-2.0.0-5lwnkjhu2pfqa7i53r5dmjwrtdlfmchj
26:	gasnet	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gasnet-2021.9.0-vov6viwltjtgd2xdcjebkcuysd22yk4f
27:	ginkgo	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ginkgo-1.4.0-43puh65asdbyuppjvnkclvlhbcbypdxi
28:	globalarrays	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/globalarrays-5.8-u3ksyg4nk4q6hyzq2m7uhil5obsaej4s
29:	gotcha	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gotcha-1.0.3-nyelkzzoqqa4ca4lug5wjl2jkhibrvpq
30:	gptune	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/gptune-2.1.0-ejaasogpqkkirlslnr4fa3xpjlkniuut
31:	hdf5	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hdf5-1.10.7-55dzf6dfzrzfygclkniva73v3am77j7y
32:	heffte	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/heffte-2.2.0-zs4yjubwwqoplaxiyzeabe6ol4ytratl
33:	hpctoolkit	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpctoolkit-2022.01.15-qljk5ibsjxsvxbwbom5z7qj4hmhhzvwu
34:	hpx	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hpx-1.7.1-usg36dncwef4p4ekynejmyaqv54rlqay
35:	hypre	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/hypre-2.24.0-35mmfx5qlvsjklkqblmbtxabp446f76h
36:	kokkos	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-3.5.00-ooeb3ky7vlwbhwbatfdbqtgyxpwwa4ow
37:	kokkos-kernels	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/kokkos-kernels-3.5.00-elayrtzesapufvrxqqdeiwqjvplytpb4
38:	lammps	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/lammps-20220107-qfojnjyzxoyfzvtnxrswy4d22h5qm6vy
39:	legion	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/legion-21.03.0-mmgybyncfgefmdaj3v5nhztxtsjbjd2x
40:	libnrm	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libnrm-0.1.0-icb2b2szd3gxcrmw5gewvdvoxxriyzar
41:	libquo	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/libquo-1.3.1-bqqr2ucgacsvbkdob2sjamurqjyqdcc4
42:	loki	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/loki-0.1.7-ggwkzpwhjztzezp5x2fnimeesnu5i6un
43:	magma	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/magma-2.6.1-cgwcbhobvdoxdbmz7laf6cvwusfq3pp4
44:	mercury	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mercury-2.1.0-rw3fop4oagnr7kn3pkv76u5fmahpv3ii
45:	metall	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/metall-0.17-m2umsb6xkpybnjb2ggd54bhk2d72yikf
46:	mfem	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mfem-4.3.0-cy43egzrzhl6qqsfo32iqyymkxqei6x6
47:	mpark-variant	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpark-variant-1.4.0-xyf5xrvdszmtlswk35ayonajo2falqg5
48:	mpich	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpich-3.4.2-ylw3nuwbq2kvtrmmtkohrqttkggksr4g
49:	mpifileutils	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/mpifileutils-0.11.1-qdsthysxq4h5hievlaeiwhumdbc4pslt
50:	netlib-scalapack	spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/netlib-scalapack-2.1.0-bdwubudmyuuvk4ddcqb46hmn4qnlk2bx

GPU runtimes for IBM Power
- CUDA 11
- NVHPC 22.1

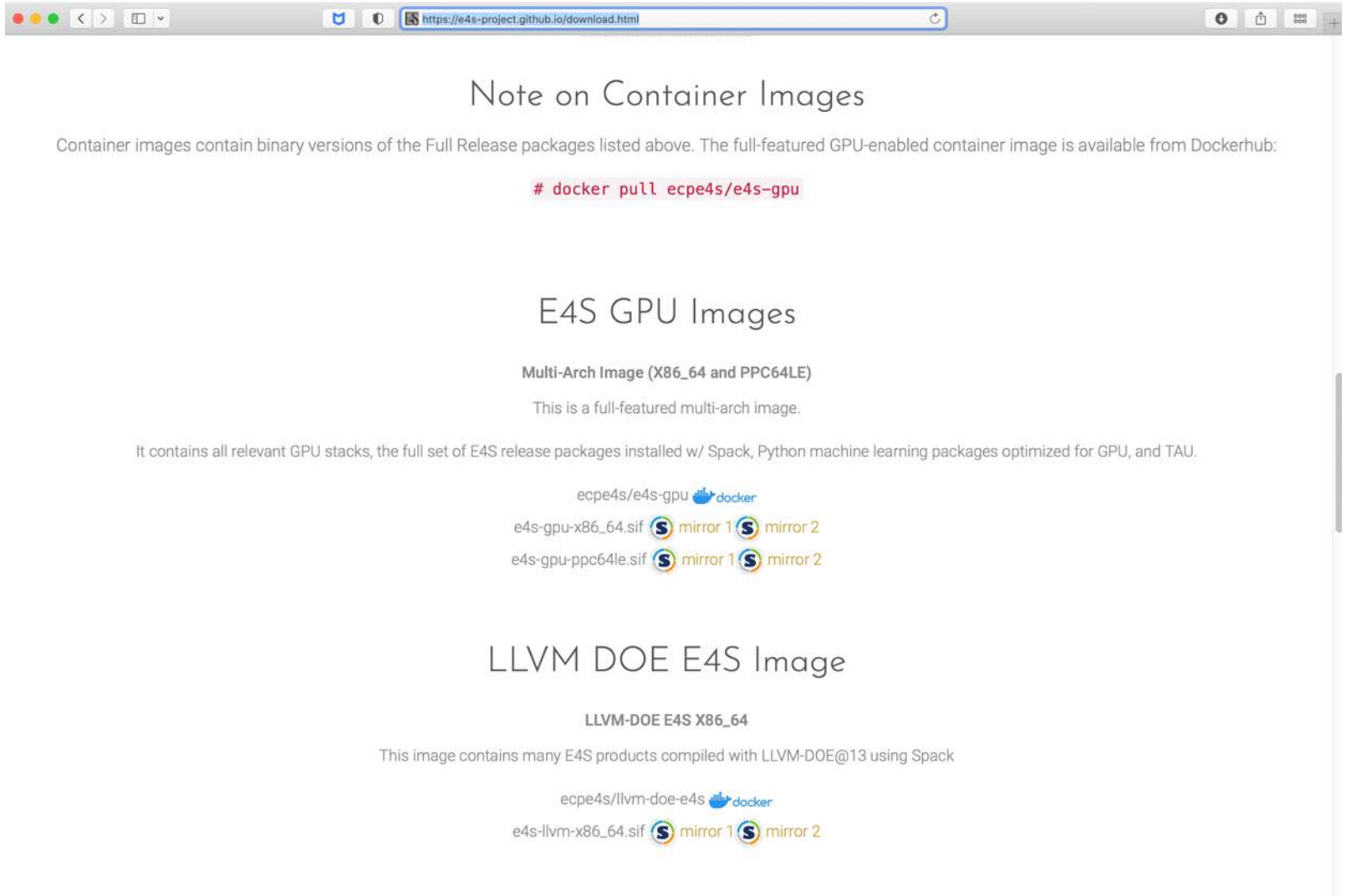
Languages
- Julia
- Python

AI packages for NVIDIA GPU
- TensorFlow
- PyTorch

22.02 Release: 100 Official Products + dependencies (gcc, ppc64le)

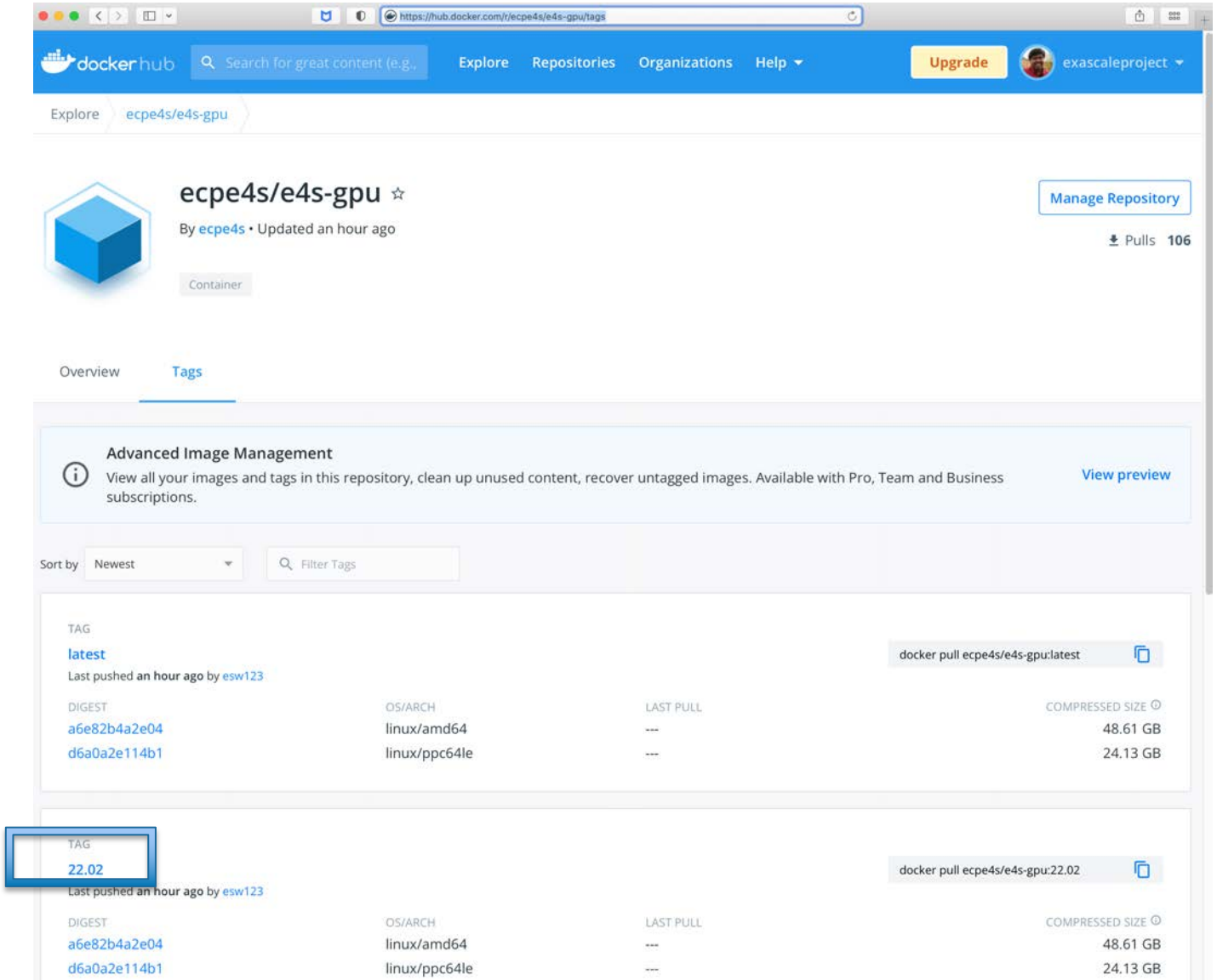
```
  51: nccmp          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nccmp-1.9.0.1-pq554jkehwzda5aeebmj36h6maclzykk
  52: nco            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nco-5.0.1-sdtngoaodihhafblfplykjwgegmelvvj
  53: ninja          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/ninja-1.10.2-txpvjbtkrg7ovnuluobagoqgn5gabg3d
  54: nrm            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/nrm-0.1.0-wr7vo4mitz3ig42i7vaezwebxiep4ky7
  55: omega-h        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/omega-h-9.34.1-6urugkbhaolrzpl4i5ligoelkyrmqqrq
  56: openpmd-api    /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openpmd-api-0.14.4-7gfvhisxtj5o37obnqgoh5r5oashdfyk
  57: openmpi        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/openmpi-4.1.2-wlurs7nh53mkbcff5xmm7cyzpfmhdahz
  58: papi           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papi-6.0.0.1-j35bykhaeufp5heiaqly6q25qotqmttj
  59: papyrus        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/papyrus-1.0.1-str3rilmozozbsutftr5djq4cfkavoxv
  60: parallel-netcdf /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parallel-netcdf-1.12.2-33rzdxxg65zqr3cwezvjmb4jp547fs3t
  61: paraview       /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/paraview-5.10.0-fo23tjskoerryh2j44d7dw6tfambrqv7
  62: parsec         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/parsec-3.0.2012-44e7355zpzsitd3umlxw33d5omdlowok
  63: pdt            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pdt-3.25.1-dfzobkfuiqczpxae5hnfezqm6gpqi3wk
  64: petsc          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/petsc-3.16.4-4gppqwtlxqjcdlvxixgdifiu4qyfhfzk
  65: plasma         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plasma-21.8.29-ym55wql2kluudjfmsnguxa5524urx6k5
  66: plumed         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/plumed-2.6.3-co5f5mocjw4tshji7qnskscjoeutnsay
  67: precice        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/precice-2.3.0-3lntwf73n3sxiiszhdmth3u7fgzdy6ab
  68: pumi           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/pumi-2.2.6-sognwzwhnjfhx4yjj43bvzy3k4fogzcj
  69: py-cinemasci   /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-cinemasci-1.3-awg5ln4mavzhqtsj47zeq7yl3uf4f7ya
  70: py-jupyterhub  /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-jupyterhub-1.4.1-tmqhrglytercluboxu7gsbnhrfkuwlep
  71: py-libensemble /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-libensemble-0.8.0-cnr27aysatnm6k54qpbcjhxvmjptw6ut
  72: py-parsl       /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-parsl-1.1.0-qtfq7fr22pjynprxyhpaxjbemdqmvx5m
  73: py-radical-pilot /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-pilot-1.11.2-4yopypwcrqywxwg4tpzz4xi5uos3k4hy
  74: py-radical-saga /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/py-radical-saga-1.11.1-e4vdj67jjokqimcrabtuqnrdb3kklmqd
  75: qthreads       /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/qthreads-1.16-z2esuoqorzcr4tcuqyeh4zgx7kh2gy4j
  76: raja           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/raja-0.14.0-ow63lt5olwwomoxwfqbz7464df4ek2bl
  77: rempi          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/rempi-1.1.0-2tpsr2ppdahbbplqtur45vyvt6tdwlpb
  78: scr            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/scr-3.0rc2-wzvfcuxwbcwqx3rjg27wbwcpo53kjsc5
  79: slate          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slate-2021.05.02-mnnpn3ezdopcraqjo5expxcyh7pa7zfo
  80: slepc          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/slepc-3.16.2-sklcgra3kvyrzfqanwuefezqrrinsllz
  81: spot           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/spot-2.9.4-y5pxssx23mkdiygis2jraucj3d6kdarp
  82: strumpack      /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/strumpack-6.3.0-gjauyvljjlh6gew4egajp7x4i7q6xudu
  83: sundials       /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sundials-6.1.1-ycocpnjvrmncp7ttoxqno7p4kgr64aet
  84: superlu-dist   /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/superlu-dist-7.2.0-o5sqg2lsaklwsqmbvct72epkivllsono
  85: stc            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/stc-0.9.0-id3urr2mljdhry2pu7bbkqhwt3o2a3as
  86: swig           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/swig-4.0.2-fortran-exxngdij3rqd7rgcnkn5go4vc7dugrxw
  87: sz             /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/sz-2.1.12-n5wgbtryijanb6p6qh27p36daq4y2mce
  88: tasmanian      /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tasmanian-7.7-veo5oikqc5ajmubpa6f5jehy4xc7d2ev
  89: tau            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/tau-2.31-4bounoz2d6rchlf4h4lut5dn7r3tkkaq
  90: trilinos       /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/trilinos-13.2.0-crlw734mrosiph5og5ashcz64df23qbi
  91: turbine        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/turbine-1.3.0-cldrv363ejpzhi3zpexxboapsbkyi6mr
  92: umap           /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umap-2.1.0-7sqkyikt6qkgfbgnxgwbjwy2ia47cc5d
  93: umpire         /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/umpire-6.0.0-fje4b6sdckggwney53z2rnwdhrfswmja
  94: unifyfs        /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/unifyfs-0.9.1-3sgocddzc3xyvog7vti54qr7owlnu5o5
  95: upcxx          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/upcxx-2021.9.0-ypki2vvo2isqf3xrtww55ww5arwbjudm
  96: veloc          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/veloc-1.5-new5o35pn6y7w4wn465xna6znfumwqzw
  97: vtk-m          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/vtk-m-1.7.1-nj4wujmfy5gos57ntvwc7m24raslrkoe
  98: wannier90      /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/wannier90-3.1.0-cjmkyyxukbvoxg56ugmpqmcnlp6x7ebr
  99: warpx          /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/warpx-22.02-6cv6qr45lyyg3z2ym625wx2i7okqwe3l
 100: zfp            /spack/linux-ubuntu18.04-ppc64le/gcc-7.5.0/zfp-0.5.5-cmhh4bkpgptkbhyg6g4s4csjuamh6525
```

E4S 22.02 Release: full featured GPU image, LLVM DOE image



- Full featured images
  - ppc64le and x86_64
  - Docker and Singularity
- LLVM DOE E4S image

E4S 22.02 Release: GPU, ppc64le for Docker Containers

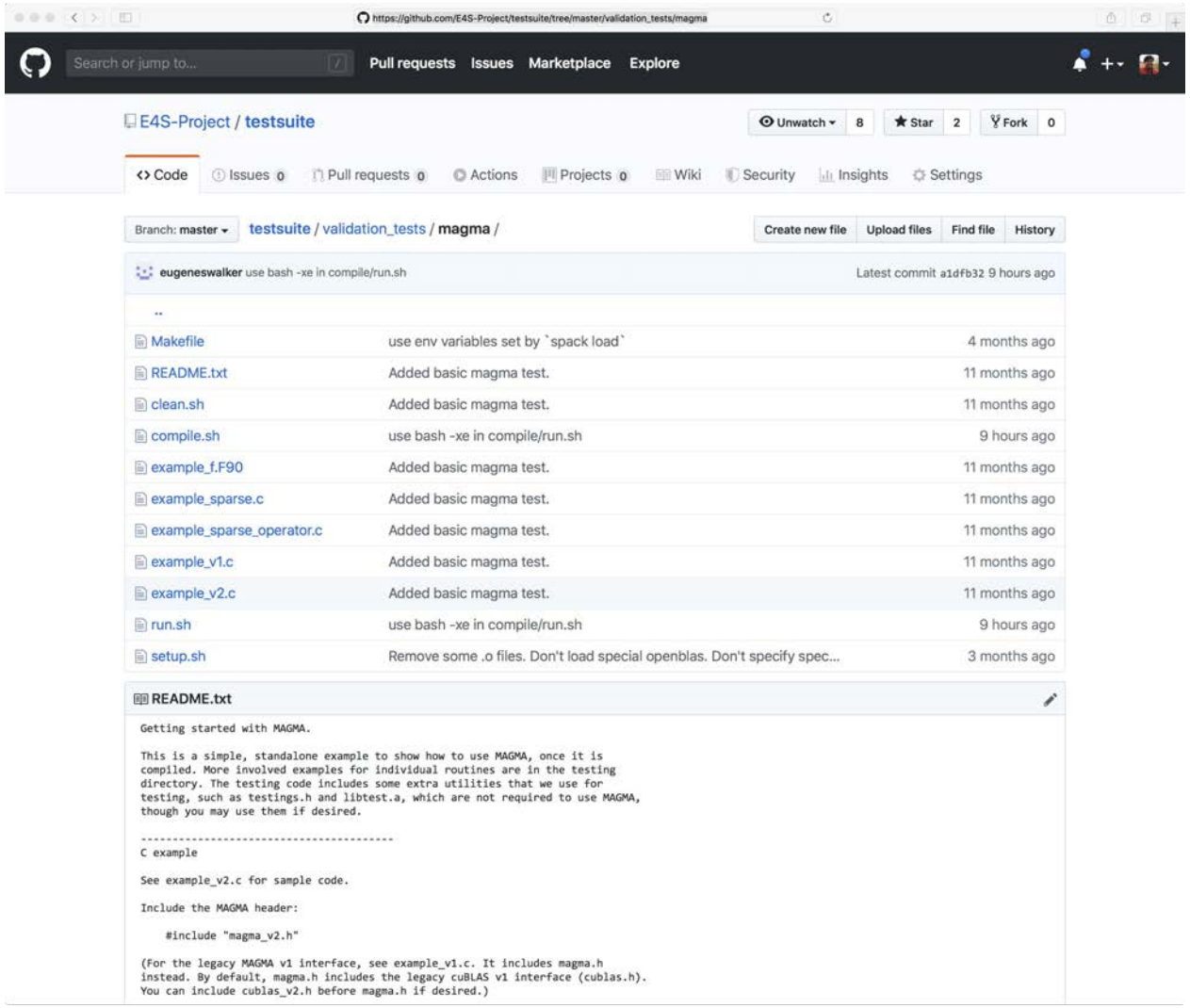


- 100 E4S Products
- Support for GPUs
  - ppc64le and x86_64

% docker pull ecpe4s/e4s-gpu

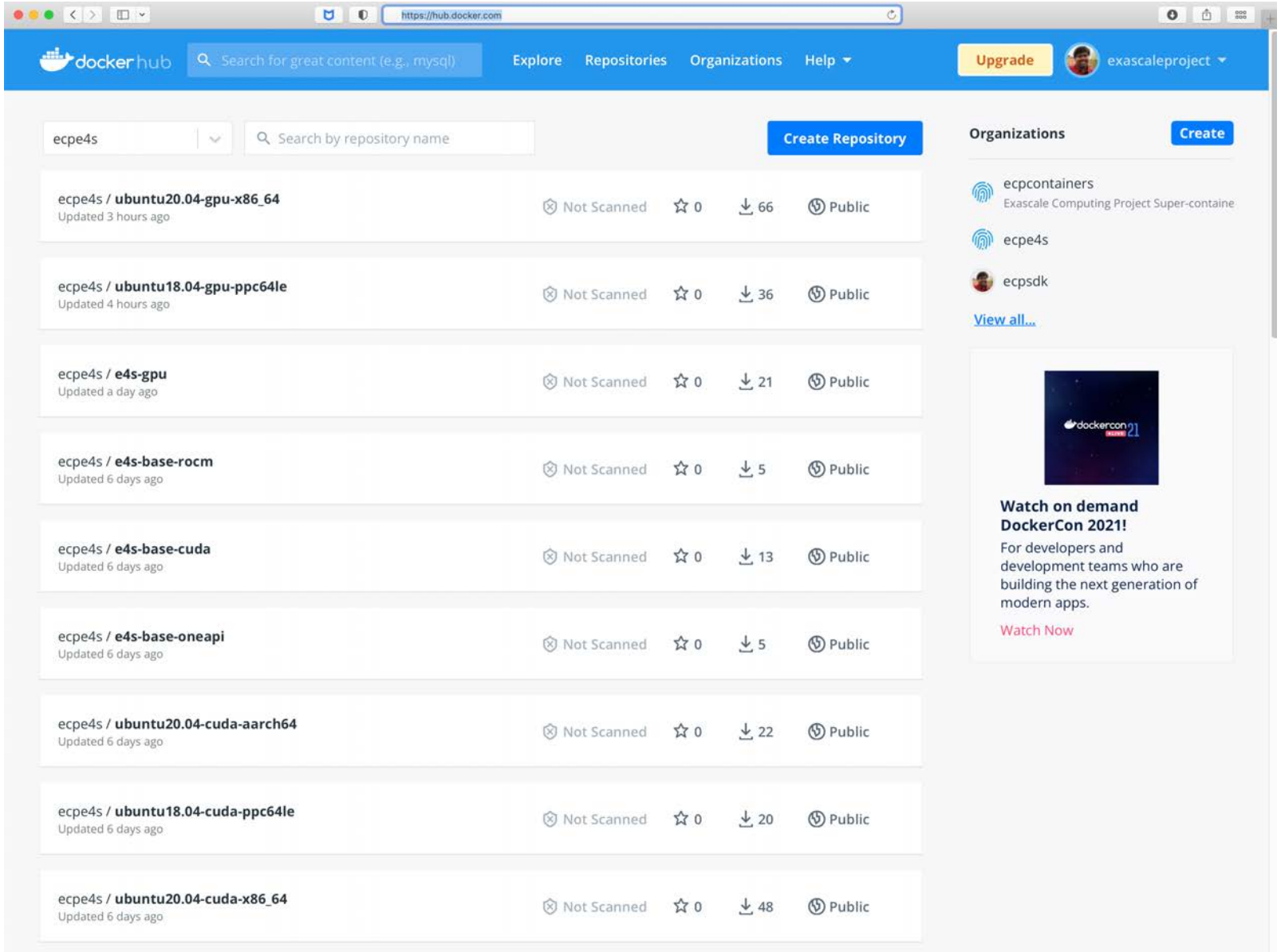
E4S Validation Test Suite

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



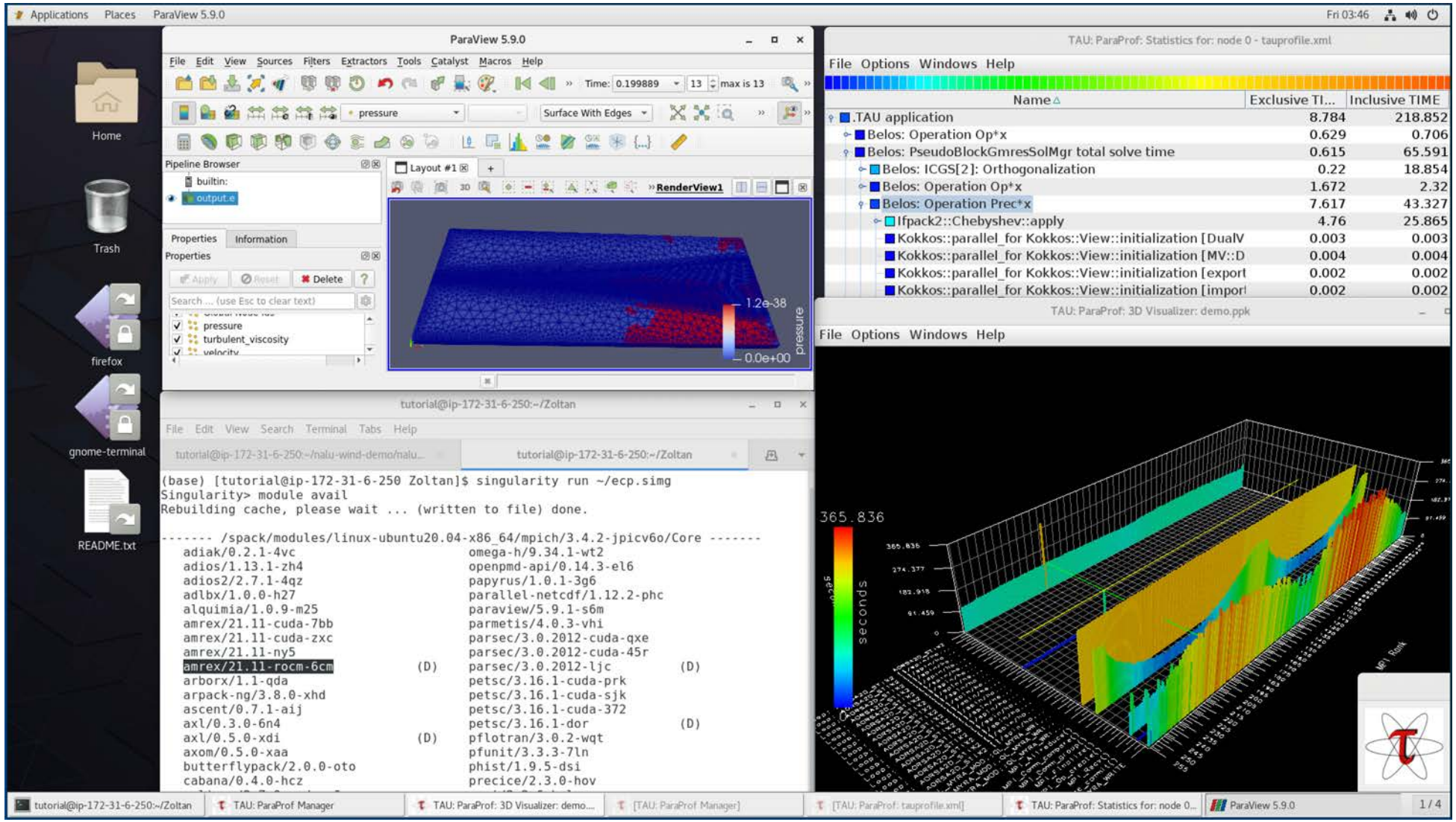
- git clone https://github.com/E4S-Project/testsuite.git

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 21.11 AWS image: US-West2 (OR)



E4S 22.02 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

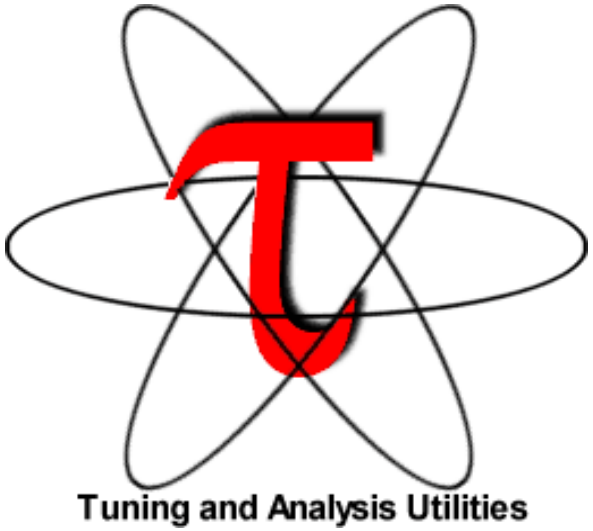
https://github.com/E4S-Project/e4s-cl

Using E4S on ThetaGPU

Setup preferred program environment compilers (check instructions)

```
% module load cobalt/cobalt-gpu; qsub -I -n 1 -A comp_perf_workshop -t 50
% singularity run --nv -e ~sameer/scr/e4s/ecp.simg
Singularity> conda activate cuda
Singularity> cd /opt/demo/python_tests; python ./f2.py
Singularity> spack find
Singularity> module avail
Singularity> ls $TAU/Makefile*
/opt/tau/tau_latest/x86_64/lib/Makefile.tau
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-level_zero-intel-icpc-mpi-pthread-pdt
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-level_zero-pthread-pdt
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-mpi-pdt
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-mpi-python-cupti-pdt
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-papi-mpi-pthread-pdt
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-python-cupti-pdt
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-rocprofiler-rocm-clang-pthread-python-pdt
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-rocprofiler-rocm-mpi-pthread-python-pdt
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-roctracer-rocm-clang-pthread-python-pdt
/opt/tau/tau_latest/x86_64/lib/Makefile.tau-roctracer-rocm-mpi-pthread-python-pdt
```

Download TAU from U. Oregon



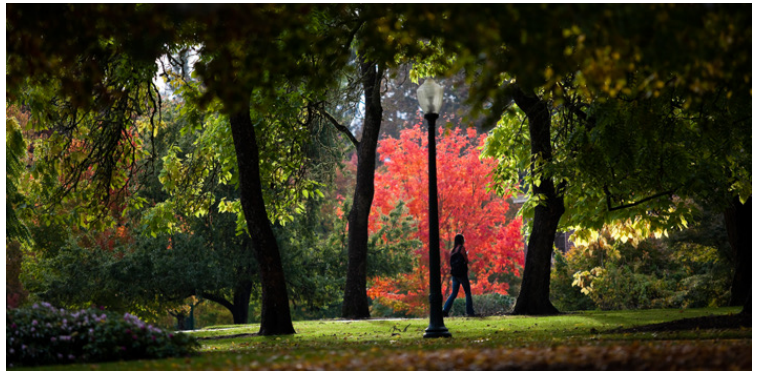
http://tau.uoregon.edu

https://e4s.io [TAU in Docker/Singularity containers]

for more information

Free download, open source, BSD license

Performance Research Laboratory, University of Oregon, Eugene



www.uoregon.edu

Support Acknowledgements

- US Department of Energy (DOE)
  - ANL
  - Office of Science contracts, ECP
  - SciDAC, LBL contracts
  - LLNL-LANL-SNL ASC/NNSA contract
  - Battelle, PNNL and ORNL contract
- Department of Defense (DoD)
  - PETTT, HPCMP
- National Science Foundation (NSF)
  - SI2-SSI, Glassbox, E4S Workshop
- NASA
- Intel
- CEA, France
- Partners:
  - University of Oregon
  - The Ohio State University
  - ParaTools, Inc.
  - University of Tennessee, Knoxville
  - T.U. Dresden, GWT
  - Jülich Supercomputing Center

Thank you

https://www.exascaleproject.org

This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative.

Thank you to all collaborators in the ECP and broader computational science communities. The work discussed in this presentation represents creative contributions of many people who are passionately working toward next-generation computational science.