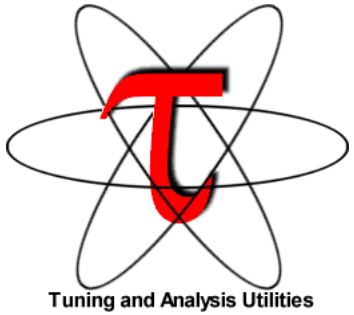
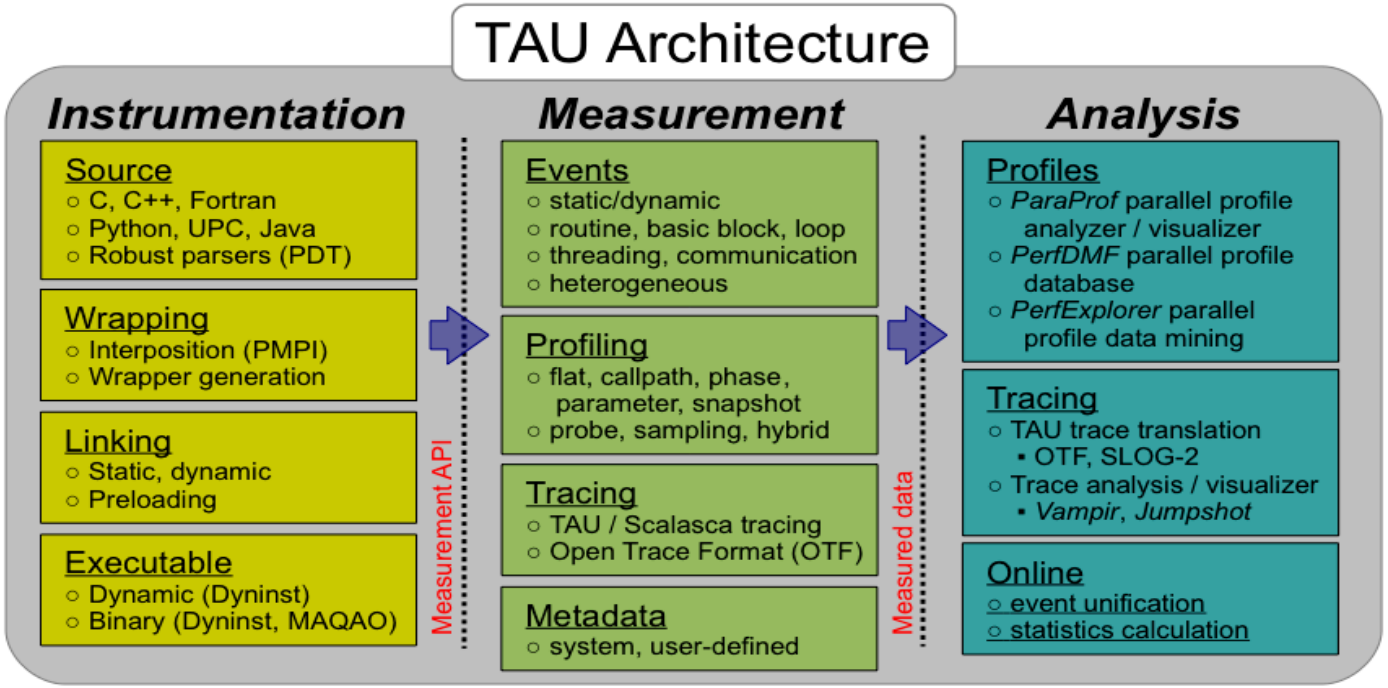
TAU Performance System®



Sameer Shende
sameer@cs.uoregon.edu
University of Oregon
http://tau.uoregon.edu

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
  - Automatic instrumentation
- Measurement and analysis support
  - MPI, OpenSHMEM, ARMCI, PGAS, DMAPP
  - pthreads, OpenMP, OMPT interface, hybrid, other thread models
  - GPU, CUDA, OpenCL, OpenACC, ROCm, HIP
  - Parallel profiling and tracing
  - Use of Score-P for native OTF2 and CUBEX generation
  - Efficient callpath proflles and trace generation using Score-P
- Analysis
  - Parallel profile analysis (ParaProf), data mining (PerfExplorer)
  - Performance database technology (TAUdb)
  - 3D profile browser

TAU Performance System

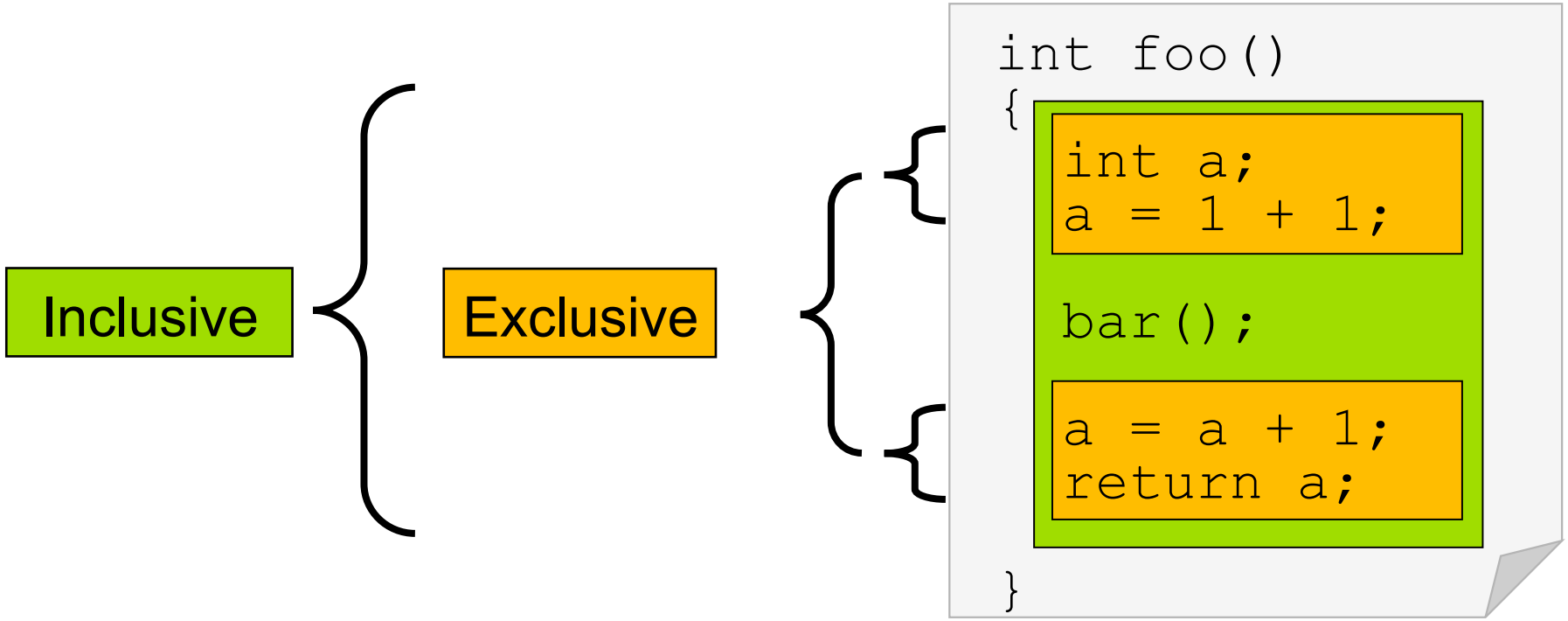
- TAU supports both sampling and direct instrumentation
- Memory debugging as well as I/O performance evaluation
- Profiling as well as tracing
- Interfaces with Score-P for more efficient measurements
- TAU's instrumentation covers:
  - Runtime library interposition (tau_exec)
  - Compiler-based instrumentation
  - Native generation of OTF2 traces (TAU_TRACE=1, TAU_TRACE_FORMAT=otf2)
  - Callsite instrumentation with profiles and traces (TAU_CALLSITE=1)
  - PDT based Source level instrumentation: routine & loop
  - Event based sampling (TAU_SAMPLING=1 or tau_exec -ebs)
  - Callstack unwinding with sampling (TAU_EBS_UNWIND=1)
  - OpenMP Tools Interface TR6 (OMPT, tau_exec –T ompt,tr6)
  - CUDA CUPTI, OpenCL (tau_exec -T cupti -cupti)

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?
- 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 on Intel MIC?
- 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?
- What is the contribution of each *phase* of the program? What is the time wasted/spent waiting for collectives, and I/O operations in Initialization, Computation, I/O phases?
- How does the application *scale*? What is the efficiency, runtime breakdown of performance across different core counts?

Inclusive vs. Exclusive values

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



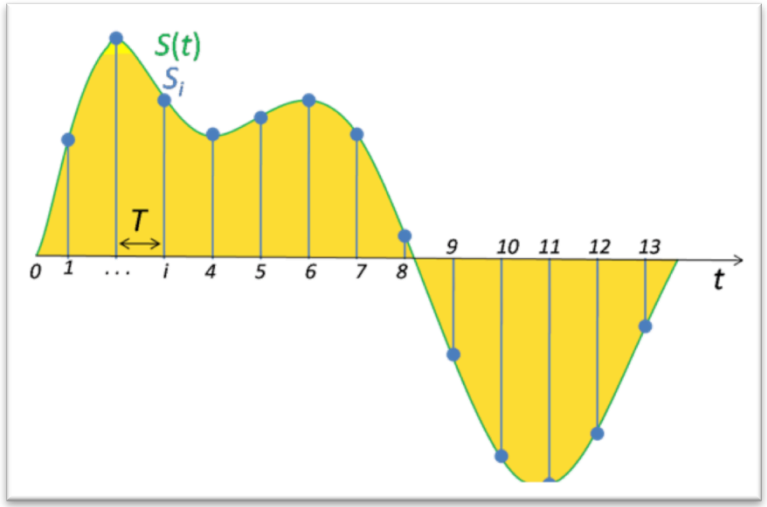
Performance Data Measurement

Direct via Probes

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

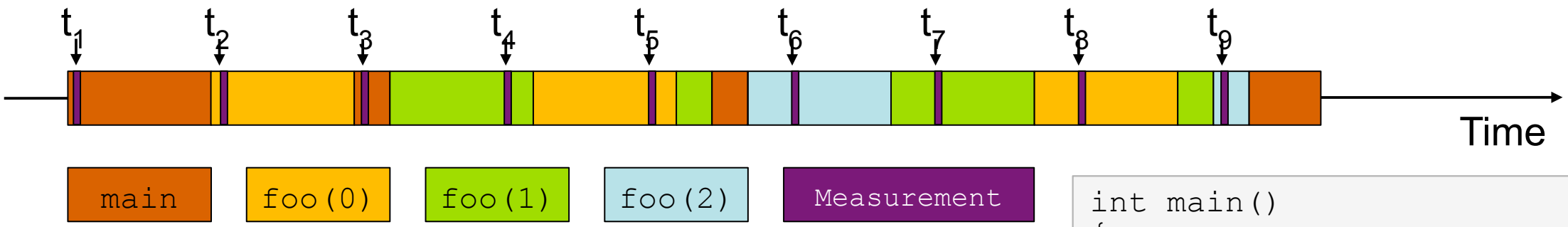
- Exact measurement
- Fine-grain control
- Calls inserted into code

Indirect via Sampling



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

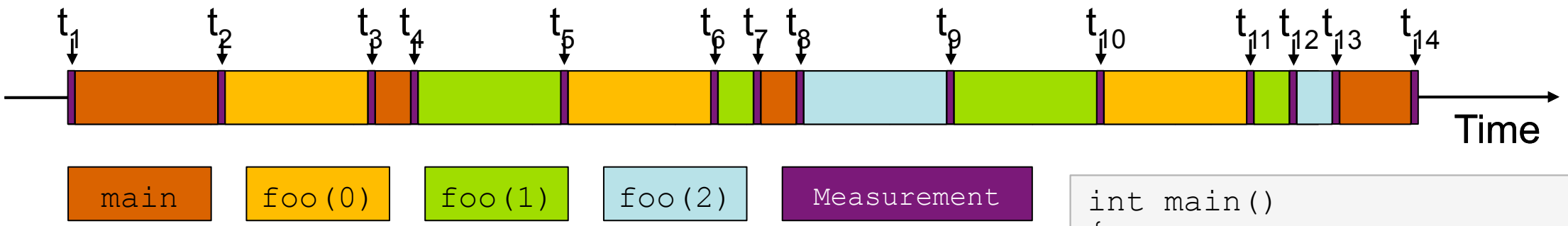
Event-Based Sampling (EBS)



- 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);

}
```

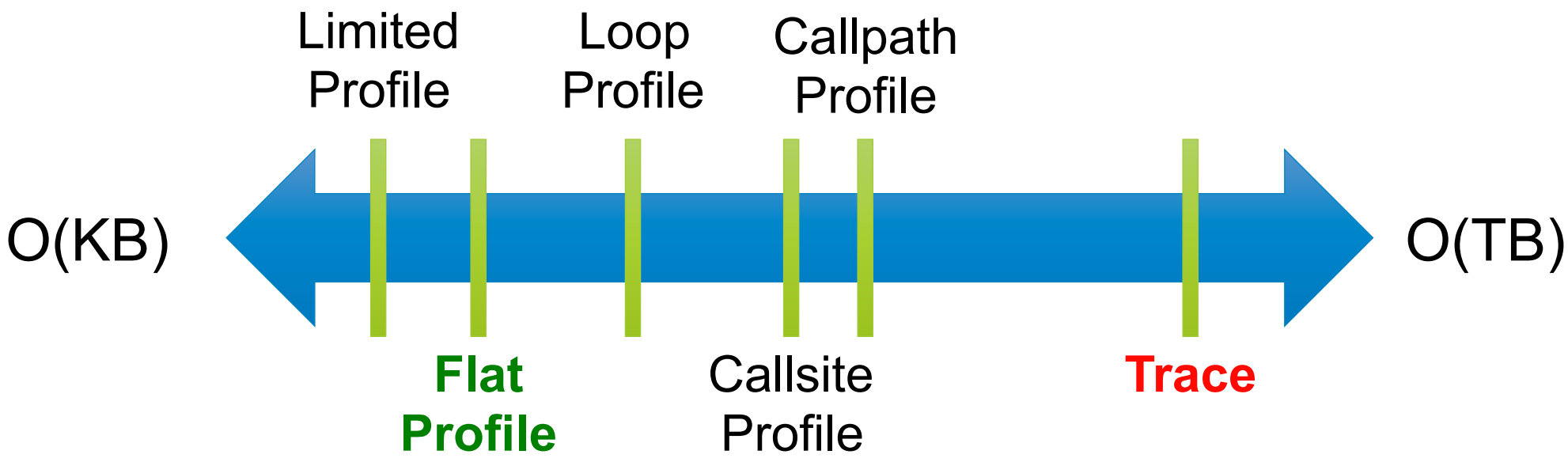
Instrumentation



- 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?



Types of Performance Profiles

- *Flat* profiles
  - Metric (e.g., time) spent in an event
  - Exclusive/inclusive, # of calls, child calls, …
- *Callpath* profiles
  - Time spent along a calling path (edges in callgraph)
  - "*main=> f1 => f2 => MPI_Send*"
  - Set the TAU_CALLPATH and TAU_CALLPATH_DEPTH environment variables
- *Callsite* profiles
  - Time spent along in an event at a given source location
  - Set the TAU_CALLSITE environment variable
- *Phase* profiles
  - Flat profiles under a phase (nested phases allowed)
  - Default "main" phase
  - Supports static or dynamic (e.g. per-iteration) phases

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)
- Add tau_exec before the name of the binary
  - srun tau_exec ./a.out
  - srun tau_exec −T ompt,tr6,mpi,papi -ompt ./a.out

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!

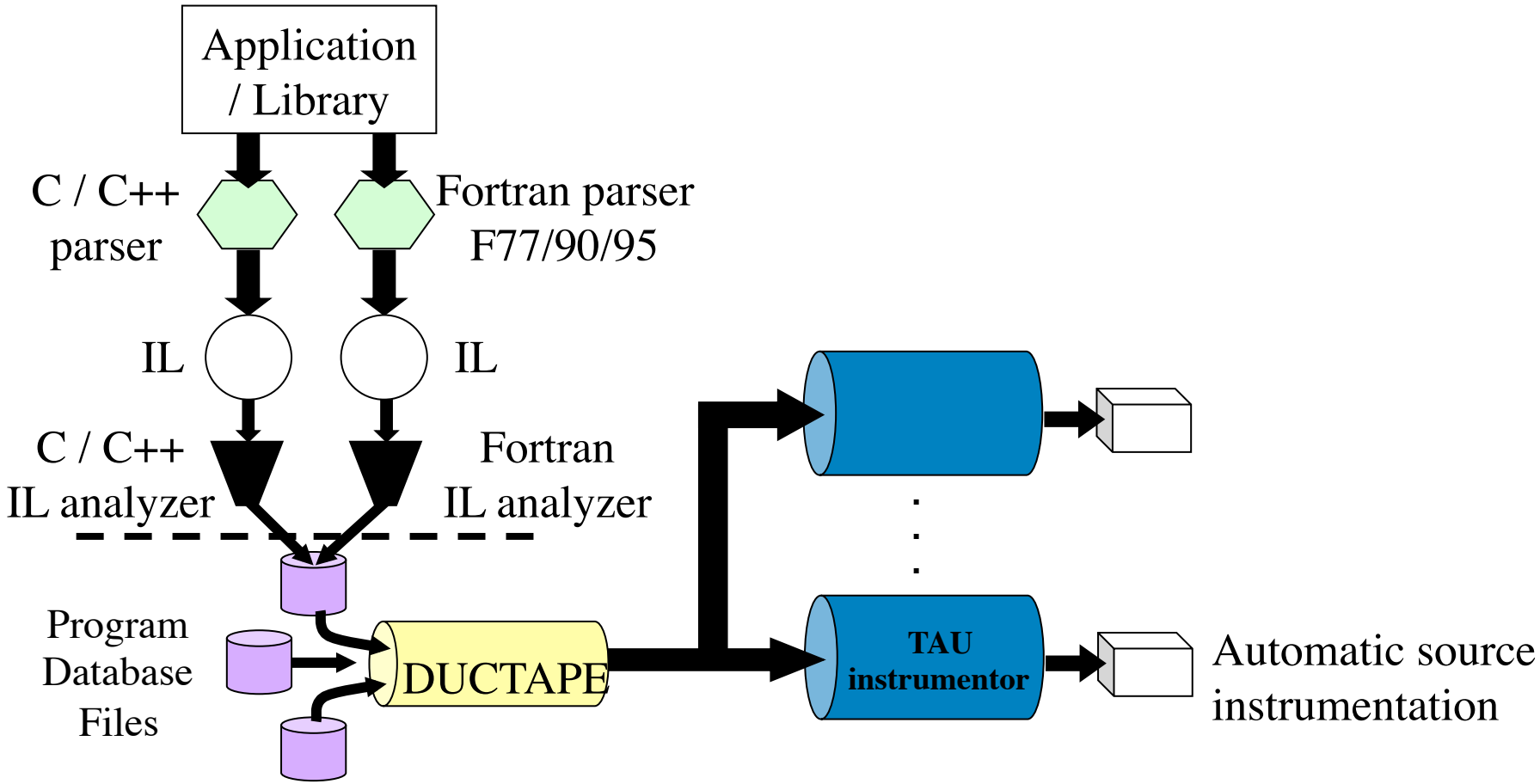
tau_exec Example (continued)

```
Example:
    mpirun –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)
    mpirun –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
```

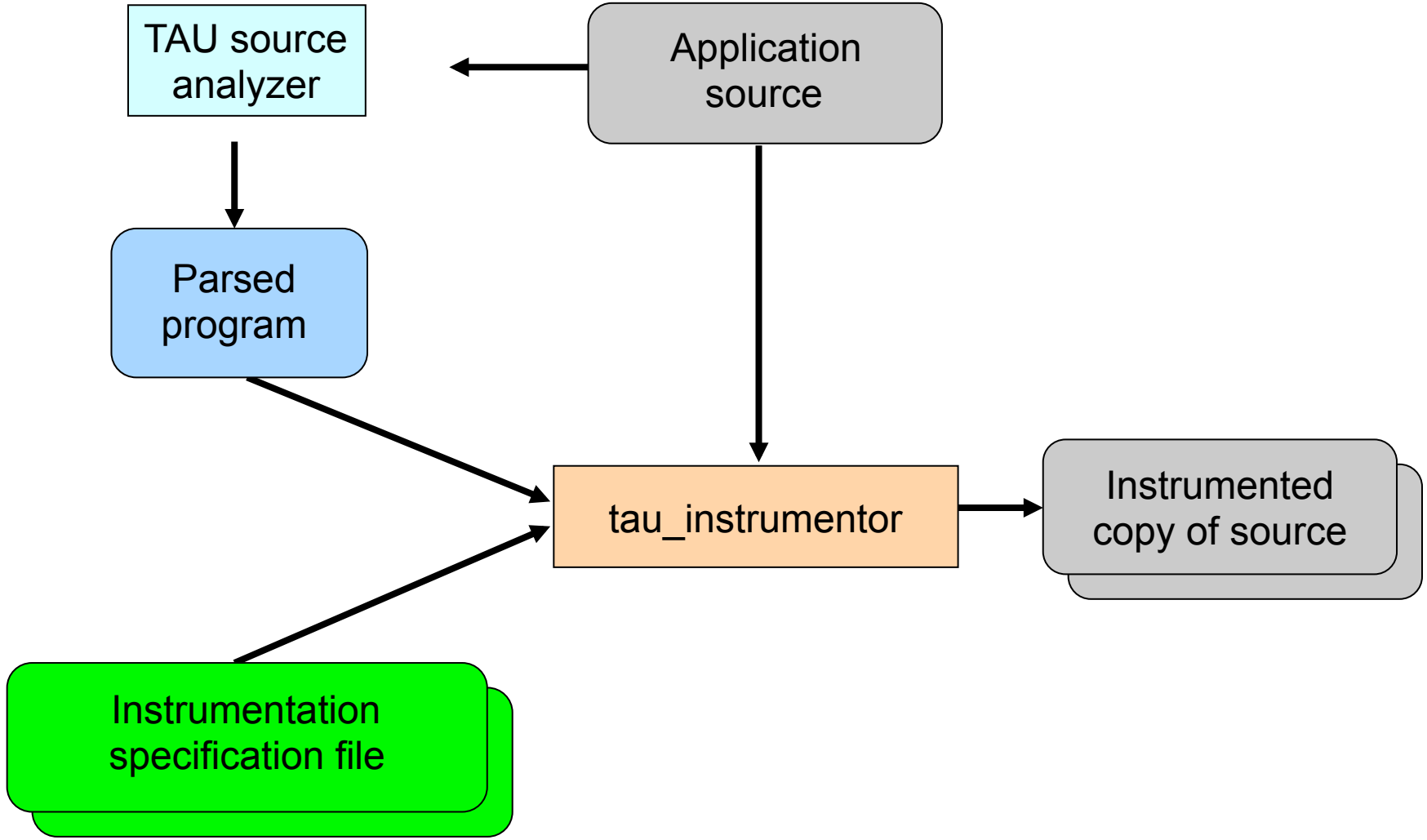
- tau_exec can enable event based sampling while launching the executable using the –ebs flag!

TAU's Source Instrumentation

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



Automatic Source Instrumentation using PDT



Installing and Configuring TAU

- Installing PDT:
  - wget http://tau.uoregon.edu/pdt.tgz
  - ./configure; make ; make install
- Installing TAU:
  - wget http://tau.uoregon.edu/tau.tgz
  - ./configure –ompt=download-tr6 –c++=mpiicpc –cc=mpiicc –fortran=mpiifort -mpi -bfd=download -pdt=<dir> -papi=<dir> ...
  - make install; export PATH=<taudir>/x86_64/bin:$PATH
- Using TAU for source instrumentation:
  - export TAU_MAKEFILE=<taudir>/x86_64/lib/Makefile.tau-<TAGS>
  - make CC=tau_cc.sh CXX=tau_cxx.sh F90=tau_f90.sh

Using TAU's Source Code Instrumentation

- TAU supports several compilers, measurement, and thread options
  - Intel compilers, profiling with hardware counters using PAPI, MPI library, CUDA…
  - Each measurement configuration of TAU 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:

```
% source /home/ri-sshende/tau.bashrc
% export TAU_MAKEFILE=$TAU/Makefile.tau-gnu-mpi-pdt-openmp-opari
% export TAU_OPTIONS='-optVerbose …' (see tau_compiler.sh )
```

  - Use tau_f90.sh, tau_cxx.sh, tau_upc.sh, or tau_cc.sh as F90, C++, UPC, or C compilers respectively:

```
% mpif90 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)
```

Makefiles for TAU Compiler and Runtime Options (Isambard)

```
% source /home/ri-sshende/tau.bashrc
% echo $TAU
/home/ri-sshende/pkgs/tau_latest/craycnl/lib
% ls $TAU/Makefile.*
```

tau_latest/craycnl/lib/Makefile.tau-gnu-mpi-pdt
tau_latest/craycnl/lib/Makefile.tau-gnu-mpi-pdt-openmp-opari
tau_latest/craycnl/lib/Makefile.tau-gnu-mpi-pthread-pdt
tau_latest/craycnl/lib/Makefile.tau-gnu-ompt-tr6-mpi-pdt-openmp
tau_latest/craycnl/lib/Makefile.tau-gnu-papi-ompt-tr6-mpi-pdt-openmp
tau_latest/craycnl/lib/Makefile.tau-allinea-ompt-tr6-mpi-pdt-openmp

For an MPI+OpenMP+F90 application with Cray MPI, you may choose

Makefile.tau-gnu-mpi-pdt-openmp-opari

- Supports MPI instrumentation & PDT for automatic source instrumentation

```
% export TAU_MAKEFILE=$TAU/Makefile.tau-gnu-mpi-pdt-openmp-opari
% tau_f90.sh matmult.f90 -o matmult
% aprun -n 16 ./matmult
% paraprof
```

Makefiles for TAU Compiler and Runtime Options (Archer)

```
% source /home/y14/y14/shende/tau.bashrc
% echo $TAU
/home/y14/y14/shende/pkgs/tau_latest/craycnl/lib
% ls $TAU/Makefile.*
/home/y14/y14/shende/pkgs/tau_latest/craycnl/lib/Makefile.tau-gnu-mpi
/home/y14/y14/shende/pkgs/tau_latest/craycnl/lib/Makefile.tau-gnu-papi-mpi
/home/y14/y14/shende/pkgs/tau_latest/craycnl/lib/Makefile.tau-gnu-papi-mpi-openmp-opari
/home/y14/y14/shende/pkgs/tau_latest/craycnl/lib/Makefile.tau-gnu-papi-mpi-pdt-openmp-opari
/home/y14/y14/shende/pkgs/tau_latest/craycnl/lib/Makefile.tau-gnu-papi-mpi-pthread
/home/y14/y14/shende/pkgs/tau_latest/craycnl/lib/Makefile.tau-gnu-papi-ompt-tr6-mpi-pdt-openmp
```

For an MPI+OpenMP+F90 application with Cray MPI, you may choose

Makefile.tau-gnu-mpi-pdt-openmp-opari

- Supports MPI instrumentation & PDT for automatic source instrumentation

```
% export TAU_MAKEFILE=$TAU/Makefile.tau-gnu-papi-mpi-pdt-openmp-opari
% tau_f90.sh matmult.f90 -o matmult
% aprun -n 16 ./matmult
% paraprof
```

Configuration tags for tau_exec

```
% ./configure -pdt=<dir> -mpi -papi=<dir>; make install
```
Creates in $TAU:
```
Makefile.tau-papi-mpi-pdt (Configuration parameters in stub makefile)
shared-papi-mpi-pdt/libTAU.so

% ./configure -pdt=<dir> -mpi; make install
```
creates
```
Makefile.tau-mpi-pdt
shared-mpi-pdt/libTAU.so
```
To explicitly choose preloading of shared-<options>/libTAU.so change:
```
% aprun -n 256 ./a.out      to
% aprun -n 256  tau_exec -T <comma_separated_options> ./a.out

% aprun -n 256  tau_exec -T papi,mpi,pdt ./a.out
```
Preloads `$TAU/shared-papi-mpi-pdt/libTAU.so`
```
% aprun -n 256  tau_exec -T papi ./a.out
```
Preloads `$TAU/shared-papi-mpi-pdt/libTAU.so by matching.`
```
% aprun -n 256 tau_exec -T papi,mpi,pdt -s ./a.out
```
Does not execute the program. Just displays the library that it will preload if executed without the –s option.
NOTE: -mpi configuration is selected by default. Use –T serial for
Sequential programs.

Simplifying TAU's usage (tau_exec)

- Uninstrumented execution
  - % aprun -n 16 ./a.out
- Track MPI performance
  - % aprun -n 16 tau_exec ./a.out
- Track OpenMP, and MPI performance (MPI enabled by default)
  - % export TAU_OMPT_SUPPORT_LEVEL=full; export TAU_OMPT_RESOLVE_ADDRESS_EAGERLY=1
  - % aprun -n 16 tau_exec –T mpi,pdt,ompt,papi –ompt ./a.out
- Track memory operations
  - % export TAU_TRACK_MEMORY_LEAKS=1
  - % mpirun –np 16 tau_exec –memory_debug ./a.out (bounds check)
- Use event based sampling (compile with –g)
  - % mpirun –np 16 tau_exec –ebs ./a.out
  - Also –ebs_source=<PAPI_COUNTER> -ebs_period=<overflow_count>
- Load wrapper interposition library
  - % mpirun –np 16 tau_exec –loadlib=<path/libwrapper.so> ./a.out
- Track GPGPU operations (-rocm, -opencl, -cupti, -cupti −um, -openacc):
  - % mpirun –np 16 tau_exec –cupti ./a.out

TAU hands-on exercises

TAU tutorial exercise objectives

- Familiarise with usage of TAU tools
  - complementary tools' capabilities & interoperability
- Prepare to apply tools productively to *your* applications(s)
- Exercise is based on a small portable benchmark code
  - unlikely to have significant optimisation opportunities

- Optional (recommended) exercise extensions
  - analyse performance of alternative configurations
  - investigate effectiveness of system-specific compiler/MPI optimisations and/or placement/binding/affinity capabilities
  - investigate scalability and analyse scalability limiters
  - compare performance on different HPC platforms
  - …

Local Installation (*Isambard*)

- Setup preferred program environment compilers

```
% source /home/ri-sshende/tau.bashrc

# If you have previous performance data from Score-P, you may view it with TAU's paraprof
% paraprof profile.cubex &
```

Local Installation (*Archer*)

- Setup preferred program environment compilers

```
% source /home/y14/y14/shende/tau.bashrc

# If you have previous performance data from Score-P, you may view it with TAU's paraprof
% paraprof profile.cubex &
```

NPB-MZ-MPI Suite

- The NAS Parallel Benchmark suite (MPI+OpenMP version)
  - Available from:

    http://www.nas.nasa.gov/Software/NPB
  - 3 benchmarks in Fortran77
  - Configurable for various sizes & classes
- Move into the NPB3.3-MZ-MPI root directory

```
% ls
bin/     common/  jobscript/  Makefile  README.install   SP-MZ/
BT-MZ/   config/  LU-MZ/      README    README.tutorial  sys/
```

- Subdirectories contain source code for each benchmark
  - plus additional configuration and common code
- The provided distribution has already been configured for the tutorial, such that it's ready to “make” one or more of the benchmarks and install them into a (tool-specific) “bin” subdirectory

NPB-MZ-MPI / BT (Block Tridiagonal Solver)

- What does it do?
  - Solves a discretized version of the unsteady, compressible Navier-Stokes equations in three spatial dimensions
  - Performs 200 time-steps on a regular 3-dimensional grid
- Implemented in 20 or so Fortran77 source modules

- Uses MPI & OpenMP in combination
  - Proposed hands-on setup on Stampede2:
    - 2 compute nodes with 1 Intel Xeon Phi 7250 CPU (Knights Landing, KNL) each
    - 32 MPI processes with 4 OpenMP threads each
  - bt-mz_C.16 should run in less than 30 seconds

- Use tau_exec with dynamic executables

NPB-MZ-MPI / BT: config/make.def : Use default compiler!

```
#                SITE- AND/OR PLATFORM-SPECIFIC DEFINITIONS.
#
#-----------------------------------------------------------------------

#-----------------------------------------------------------------------
# Configured for generic MPI with GCC compiler
#-----------------------------------------------------------------------
#COMPILER = -homp            # Cray/CCE compiler
COMPILER = -fopenmp          # GNU/GCC compiler
#COMPILER = -qopenmp         # Intel compiler

...
#---------------------------------------------------------------------
# The Fortran compiler used for MPI programs
#---------------------------------------------------------------------
# ftn = ftn # OpenMPI with Intel compiler
ftn = ftn
# Alternative variant to perform instrumentation
# ftn = tau_f90.sh
# PREP is a generic preposition macro for instrumentation preparation
#ftn = $(PREP) ftn -f77=ifort
#ftn = scorep …

FLINKFLAGS = $(FFLAGS) -dynamic
...
```

Default (no instrumentation)

Uncomment ftn and comment Score-P's compiler wrapper to generate uninstrumented binary! Add -dynamic flag to link line.

Building an NPB-MZ-MPI Benchmark

```
% make
  ========================================
  =      NAS PARALLEL BENCHMARKS 3.3     =
  =      MPI+OpenMP Multi-Zone Versions  =
  =      F77                             =
  ========================================

  To make a NAS multi-zone benchmark type

        make <benchmark-name> CLASS=<class> NPROCS=<nprocs>

  where <benchmark-name> is "bt-mz", "lu-mz", or "sp-mz"
        <class>          is "S", "W", "A" through "F"
        <nprocs>         is number of processes

  [...]

 ***********************************************************
 * Custom build configuration is specified in config/make.def  *
 * Suggested tutorial exercise configuration for HPC systems:  *
 *       make bt-mz CLASS=C NPROCS=16                          *
 ***********************************************************
```

- Type "make" for instructions

Building an NPB-MZ-MPI Benchmark

```
% make bt-mz CLASS=C NPROCS=16
make[1]: Entering directory `BT-MZ'
make[2]: Entering directory `sys'
cc  -o setparams setparams.c -lm
make[2]: Leaving directory `sys'
../sys/setparams bt-mz 16 C
make[2]: Entering directory `../BT-MZ'
ftn -c  -O3 -fopenmp       bt.f
[…]
Ftn -c  -O3 -fopenmp       mpi_setup.f
cd ../common;  ftn  -c  -O3 -fopenmp        print_results.f
cd ../common;  ftn  -c  -O3 -fopenmp        timers.f
ftn -O3 -fopenmp   -o -dynamic ../bin/bt-mz_C.16 bt.o
 initialize.o exact_solution.o exact_rhs.o set_constants.o adi.o
 rhs.o zone_setup.o x_solve.o y_solve.o  exch_qbc.o solve_subs.o
 z_solve.o add.o error.o verify.o mpi_setup.o ../common/print_results.o
 ../common/timers.o
make[2]: Leaving directory `BT-MZ'
Built executable ../bin/bt-mz_C.16
make[1]: Leaving directory `BT-MZ'
```

- Specify the benchmark configuration
  - benchmark name: **bt-mz**, lu-mz, sp-mz
  - the number of MPI processes: NPROCS=**16**
  - the benchmark class (S, W, A, B, C, D, E): CLASS=**C**

Shortcut: `% make suite`

NPB-MZ-MPI / BT reference execution on Isambard

```
% cd bin
% cp ../jobscript/isambard/run.pbs .
% cat run.pbs
% qsub run.pbs
% less mzmpibt.o<job_id>
 NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:  16 x  16
 Iterations:  200   dt:   0.000100
 Number of active processes:    32
 Total number of threads:      128   (  4.0 threads/process)

 Time step    1
 Time step   20
  [...]
 Time step  180
 Time step  200
 Verification Successful

 BT-MZ Benchmark Completed.
 Time in seconds = 22.34
```

- Copy jobscript and launch as a hybrid MPI+OpenMP application

Hint: save the benchmark output (or note the run time) to be able to refer to it later

NPB-MZ-MPI / BT reference execution on Archer

```
% cd bin
% cp ../jobscript/archer/run.pbs .
% cat run.pbs
% qsub run.pbs
% less mzmpibt.o<job_id>
 NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:  16 x  16
 Iterations:  200   dt:   0.000100
 Number of active processes:    32
 Total number of threads:      128   (  4.0 threads/process)

 Time step    1
 Time step   20
  [...]
 Time step  180
 Time step  200
 Verification Successful

 BT-MZ Benchmark Completed.
 Time in seconds = 22.34
```

- Copy jobscript and launch as a hybrid MPI+OpenMP application

Hint: save the benchmark output (or note the run time) to be able to refer to it later

NPB-MZ-MPI / BT with TAU's Event-Based Sampling on Isambard (tau_exec –T openmp,gnu –ebs)

```
% cd bin
% cp /home/ri-sshende/isambard/tau.pbs .
% qsub tau.pbs
% cat mzmpibt.o<job_id>
NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:  16 x  16
 Iterations:  200   dt:   0.000100
 Number of active processes:    32
 Total number of threads:      128   (  4.0 threads/process)

 Time step    1
 Time step   20
  [...]
 Time step  180
 Time step  200
 Verification Successful

 BT-MZ Benchmark Completed.
 Time in seconds = 23
% pprof –a –m | more
% paraprof &
% paraprof --pack bt_ebs.ppk
<Copy file over to desktop using scp>
% paraprof bt_ebs &
```

- Copy jobscript and launch as a hybrid MPI+OpenMP application

tau_exec launches un-instrumented binaries!

NPB-MZ-MPI / BT with TAU's Event-Based Sampling on Archer (tau_exec –T openmp,gnu –ebs)

```
% cd bin
% cp /home/ri-sshende/isambard/tau.pbs .
% qsub tau.pbs
% cat mzmpibt.o<job_id>
NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:  16 x  16
 Iterations:  200   dt:   0.000100
 Number of active processes:    32
 Total number of threads:      128   (  4.0 threads/process)

 Time step    1
 Time step   20
  [...]
 Time step  180
 Time step  200
 Verification Successful

 BT-MZ Benchmark Completed.
 Time in seconds = 23
% pprof –a –m | more
% paraprof &
% paraprof --pack bt_ebs.ppk
<Copy file over to desktop using scp>
% paraprof bt_ebs &
```

- Copy jobscript and launch as a hybrid MPI+OpenMP application

tau_exec launches un-instrumented binaries!

Source Instrumentation: Compiler and MPI modules on Isambard

- Select appropriate compiler / MPI combination (if not done automatically)

```
source /home/ri-sshende/tau.bashrc
```

- Copy tutorial sources to your scratch directory

```
% tar zxvf /projects/bristol/vi-hps/tutorial/NPB3.3-MZ-MPI.tar.gz
% cd NPB3.3-MZ-MPI; make clean;
echo $TAU_MAKEFILE
/home/ri-sshende/pkgs/tau_latest/craycnl/lib/Makefile.tau-gnu-mpi-pdt-openmp-opari
% make suite MPIF77=tau_f77.sh
% cd bin.tau
% cp ../jobscript/archer/run.pbs  .
% qsub run.pbs
% pprof -a -m | more
% paraprof --pack bt.ppk
<SCP to your laptop/desktop>
% paraprof bt.ppk &
```

Compiler and MPI modules on Archer

- Select appropriate compiler / MPI combination (if not done automatically)

```
source /home/y14/y14/shende/tau.bashrc
```

- Copy tutorial sources to your scratch directory

```
% tar zxvf /work/y14/shared/tutorial/NPB3.3-MZ-MPI.tar.gz
% cd NPB3.3-MZ-MPI; make clean
% echo $TAU_MAKEFILE
/home/y14/y14/shende/pkgs/tau_latest/craycnl/lib/Makefile.tau-gnu-papi-mpi-pdt-openmp-opari

% make suite MPIF77=tau_f77.sh
% cd bin.tau
% cp ../jobscript/archer/run.pbs  .
% qsub run.pbs
% pprof -a -m | more
% paraprof --pack bt.ppk
<SCP to your laptop/desktop>
% paraprof bt.ppk &
```

Compile-Time Options for TAU's compiler scripts (e.g., tau_f90.sh)

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

-optMICOffload	Links code for Intel MIC offloading, requires both host and MIC TAU libraries
-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.

…

Compiling Fortran Codes with TAU

- If your Fortran code uses free format in .f files (fixed is default for .f), you may use:
  % export TAU_OPTIONS= '-optPdtF95Opts="-R free" -optVerbose '

- To use the compiler based instrumentation instead of PDT (source-based):
  % export TAU_OPTIONS= '-optCompInst -optVerbose'

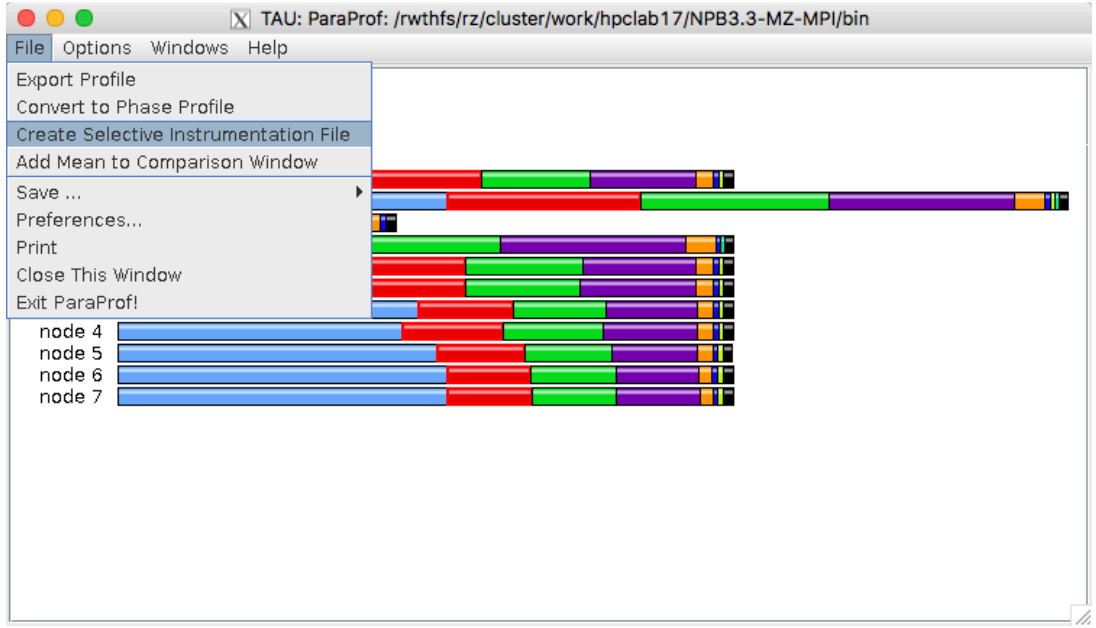
- If your Fortran code uses C preprocessor directives (#include, #ifdef, #endif):
  % export TAU_OPTIONS= '-optPreProcess -optVerbose -optDetectMemoryLeaks'

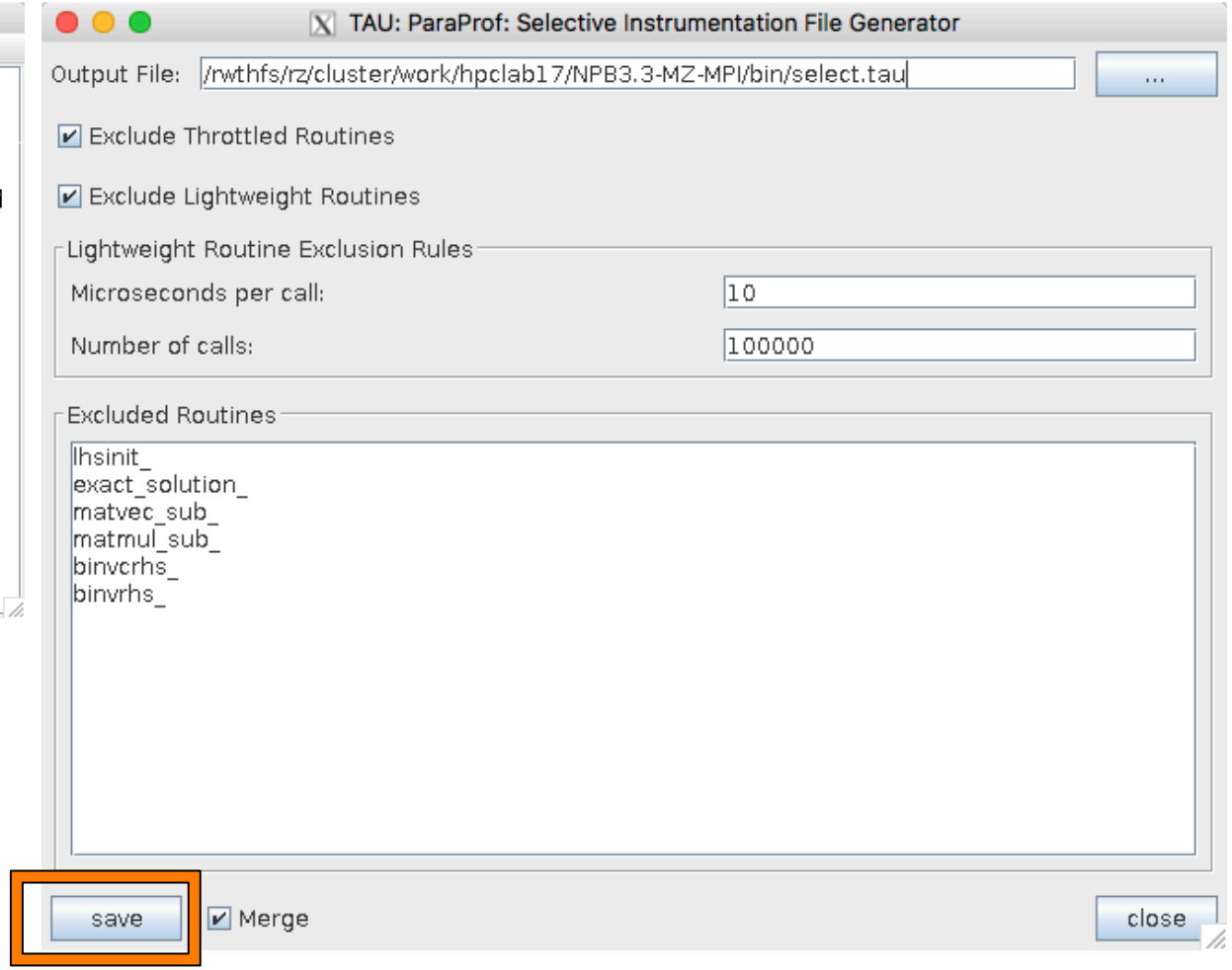
- To use an instrumentation specification file:
  % export TAU_OPTIONS= '-optTauSelectFile=select.tau -optVerbose -optPreProcess'
  % cat select.tau
  BEGIN_INSTRUMENT_SECTION
  loops routine="#"
  # this statement instruments all outer loops in all routines. # is wildcard as well as comment in first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

TAU's Selective Instrumentation (Filter) File Format

```
% export TAU_OPTIONS='-optTauSelectFile=/path/to/select.tau …'
% cat select.tau
BEGIN_INCLUDE_LIST
int main#
int dgemm#
END_INCLUDE_LIST
BEGIN_FILE_INCLUDE_LIST
Main.c
Blas/*.f77
END_FILE_INCLUDE_LIST
# replace INCLUDE with EXCLUDE list for excluding routines/files

BEGIN_INSTRUMENT_SECTION
loops routine="foo"
loops routine="int main#"
END_INSTRUMENT_SECTION
% export TAU_SELECT_FILE=select.tau    (to use at runtime)
```

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





% paraprof

Re-instrument with TAU

- Select appropriate compiler / MPI combination (if not done automatically)

```
source /home/ri-sshende/tau.bashrc (Isambard)
source /home/y14/y14/shende/tau.bashrc  (Archer)
```

- Choose path to selective instrumentation file saved by paraprof (copy if necessary):

```
% export TAU_OPTIONS='-optTauSelectFile=/path/to/select.tau -optVerbose'
% echo $TAU_MAKEFILE
…/pkgs/tau_latest/craycnl/lib/Makefile.tau-gnu-papi-mpi-pdt-openmp-opari
% make clean
% make suite MPIF77=tau_f77.sh
% cd bin.tau
% cp ../jobscript/archer/run.pbs  .
% qsub run.pbs
% pprof -a -m | more
% paraprof --pack bt.ppk
<SCP to your laptop/desktop>
% paraprof bt.ppk &
```

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

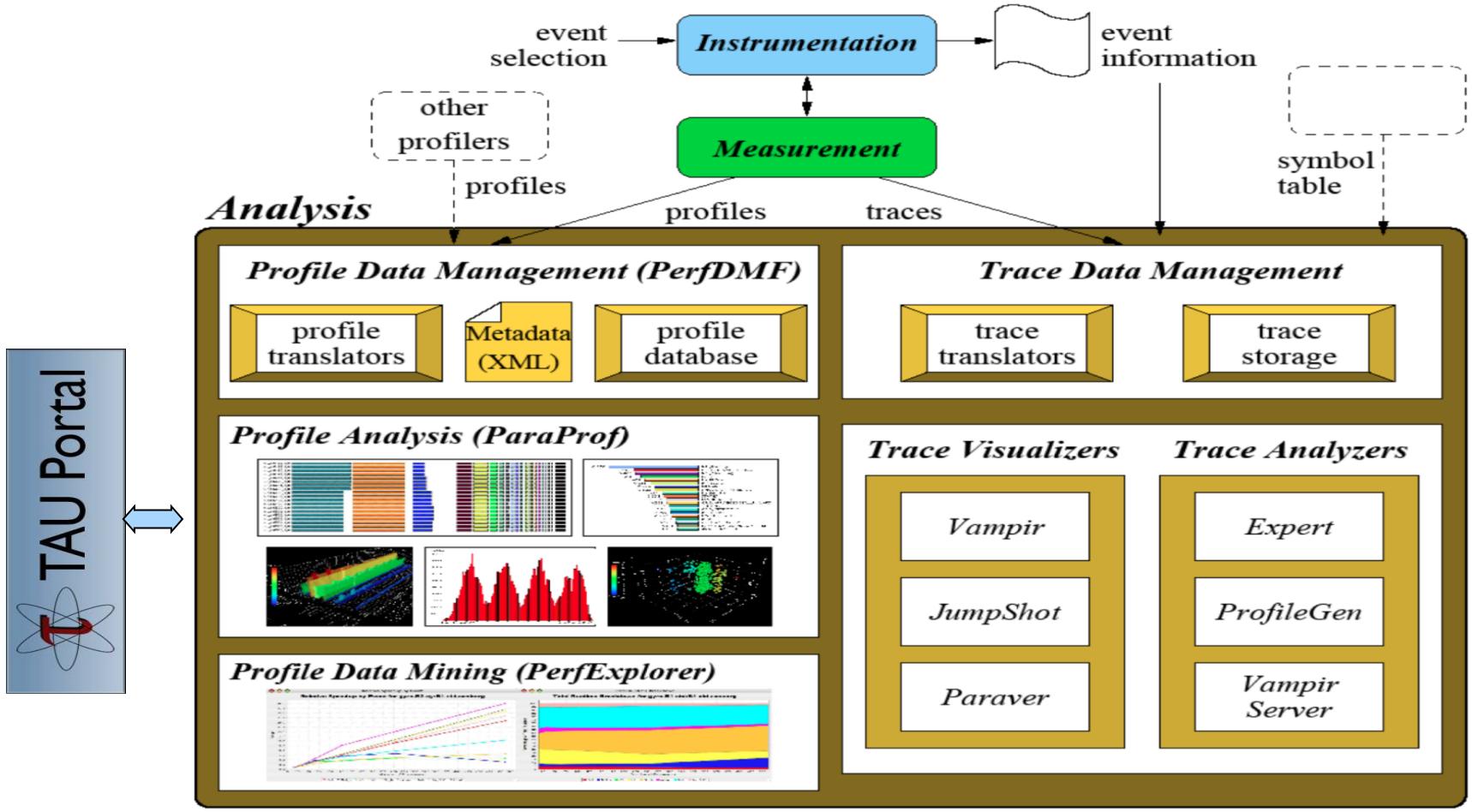
Environment Variable	Default	Description
TAU_TRACE	0	Setting to 1 turns on tracing
TAU_TRACE_FORMAT	Default	Setting to “otf2” turns on TAU’s native OTF2 trace generation (configure with –otf=download)
TAU_EBS_UNWIND	0	Setting to 1 turns on unwinding the callstack during sampling (use with tau_exec –ebs 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	0	Setting to 1 is necessary for event based sampling to resolve addresses with OMPT TR6 (-ompt=download-tr6)

Runtime Environment Variables

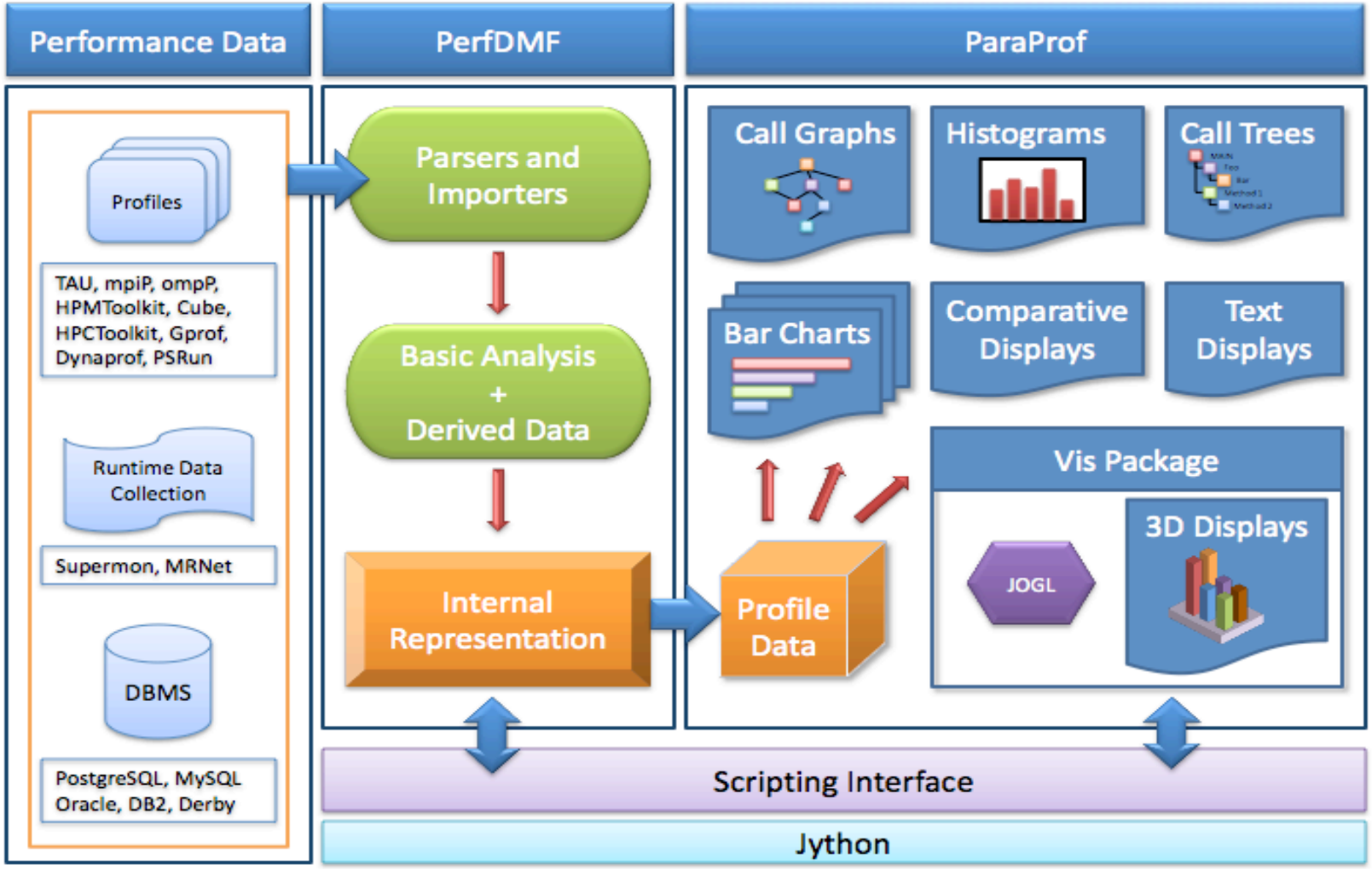
Environment Variable	Default	Description
TAU_TRACK_MEMORY_LEAKS	0	Tracks allocates that were not de-allocated (needs –optMemDbg or tau_exec –memory)
TAU_EBS_SOURCE	TIME	Allows using PAPI hardware counters for periodic interrupts for EBS (e.g., TAU_EBS_SOURCE=PAPI_TOT_INS when TAU_SAMPLING=1)
TAU_EBS_PERIOD	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

TAU's Analysis Tools: ParaProf

TAU Analysis



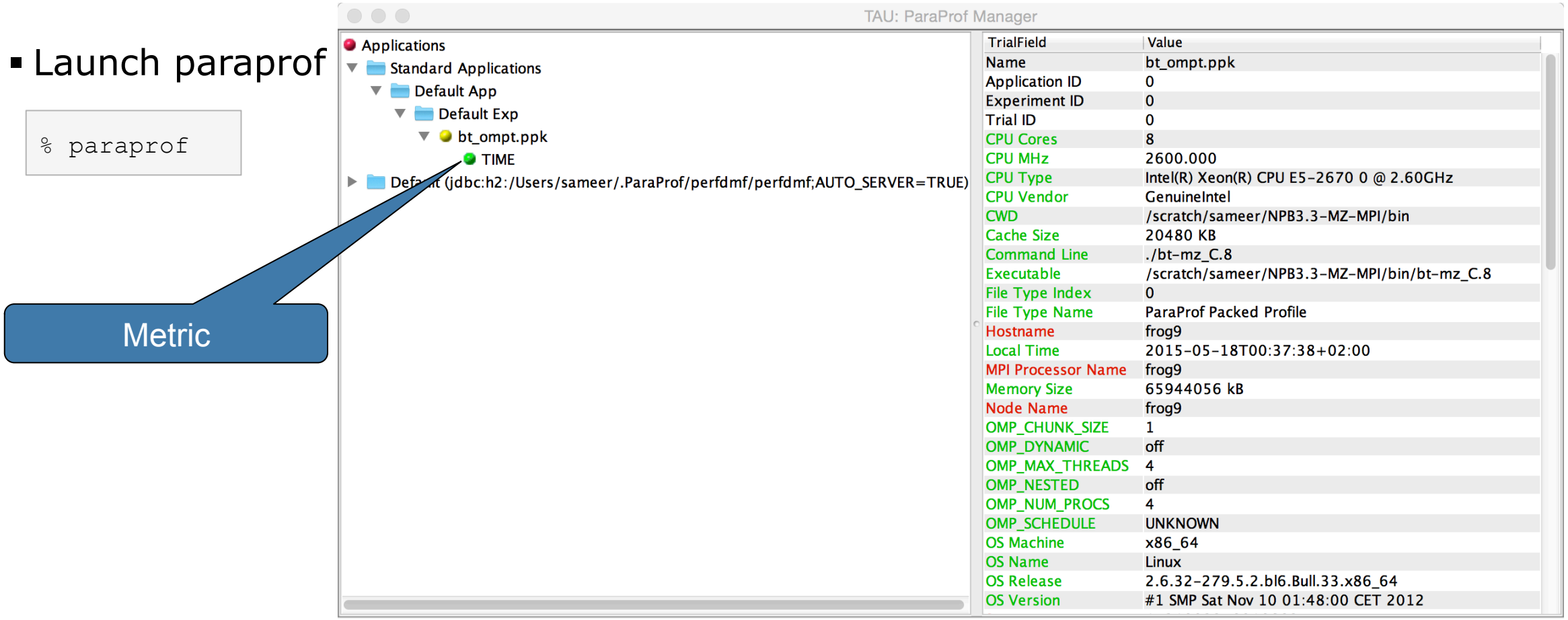
ParaProf Profile Analysis Framework



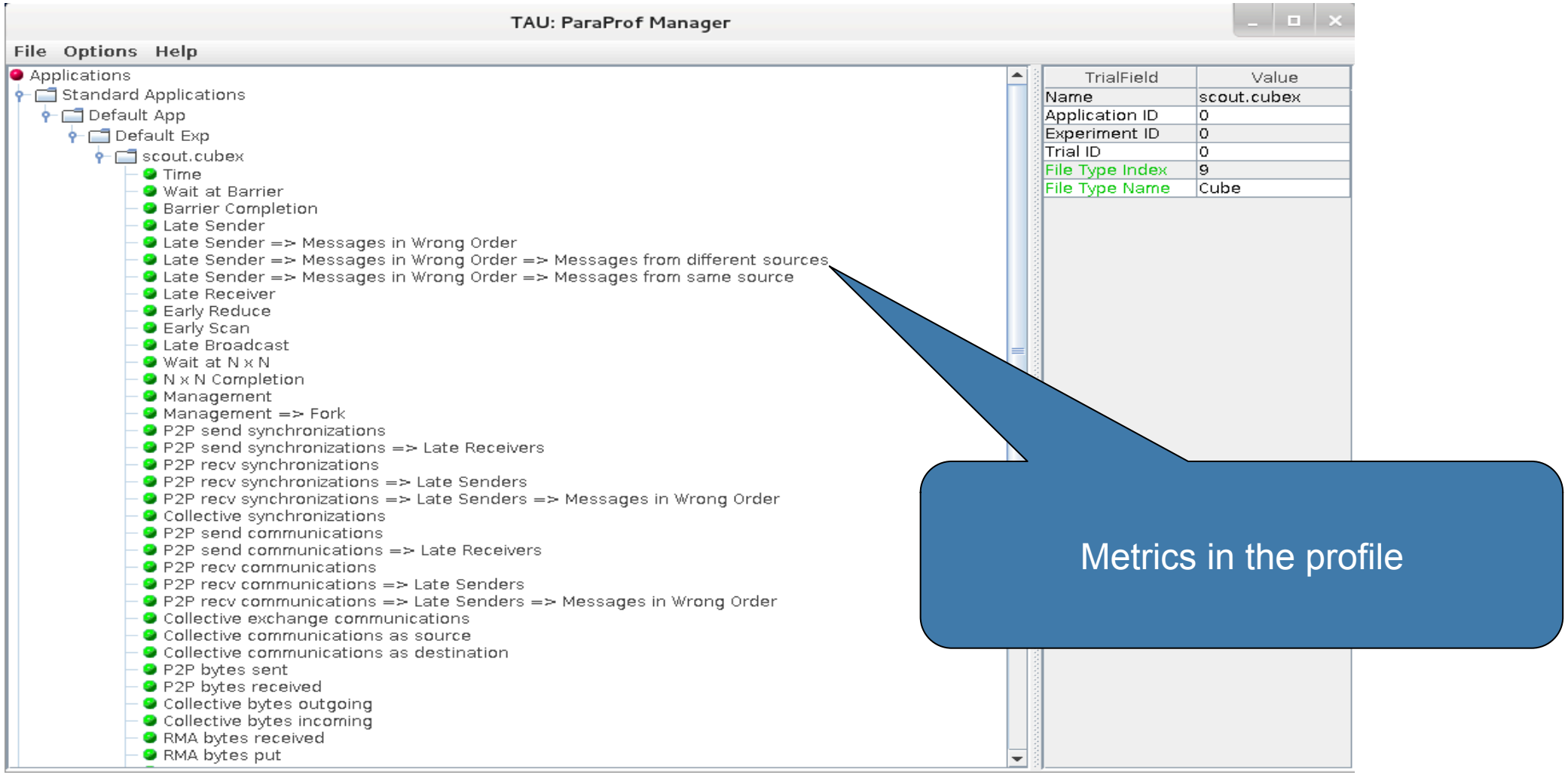
TAU Analysis Tools: paraprof

- Launch paraprof

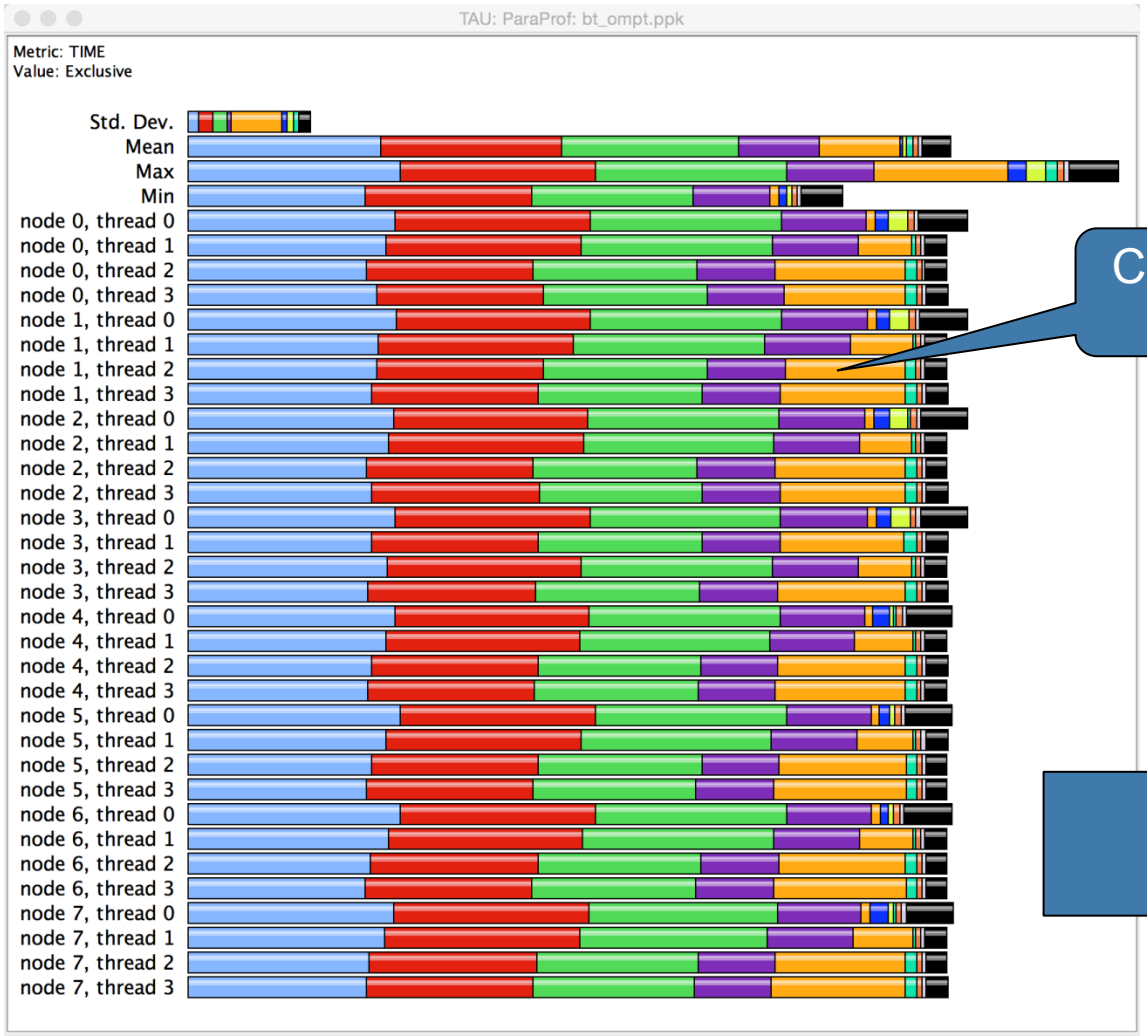
```
% paraprof
```



ParaProf Manager Widow: scout.cubex



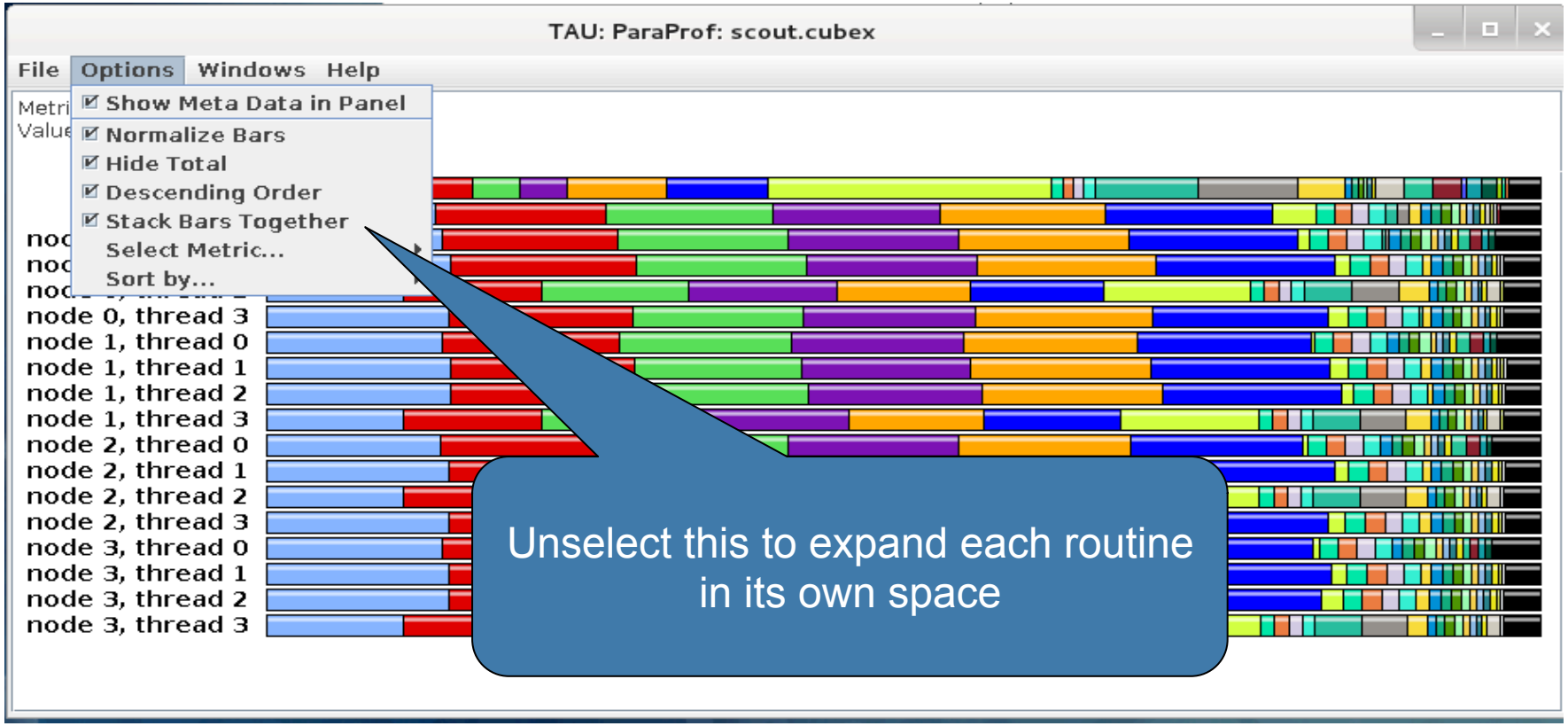
Paraprof main window



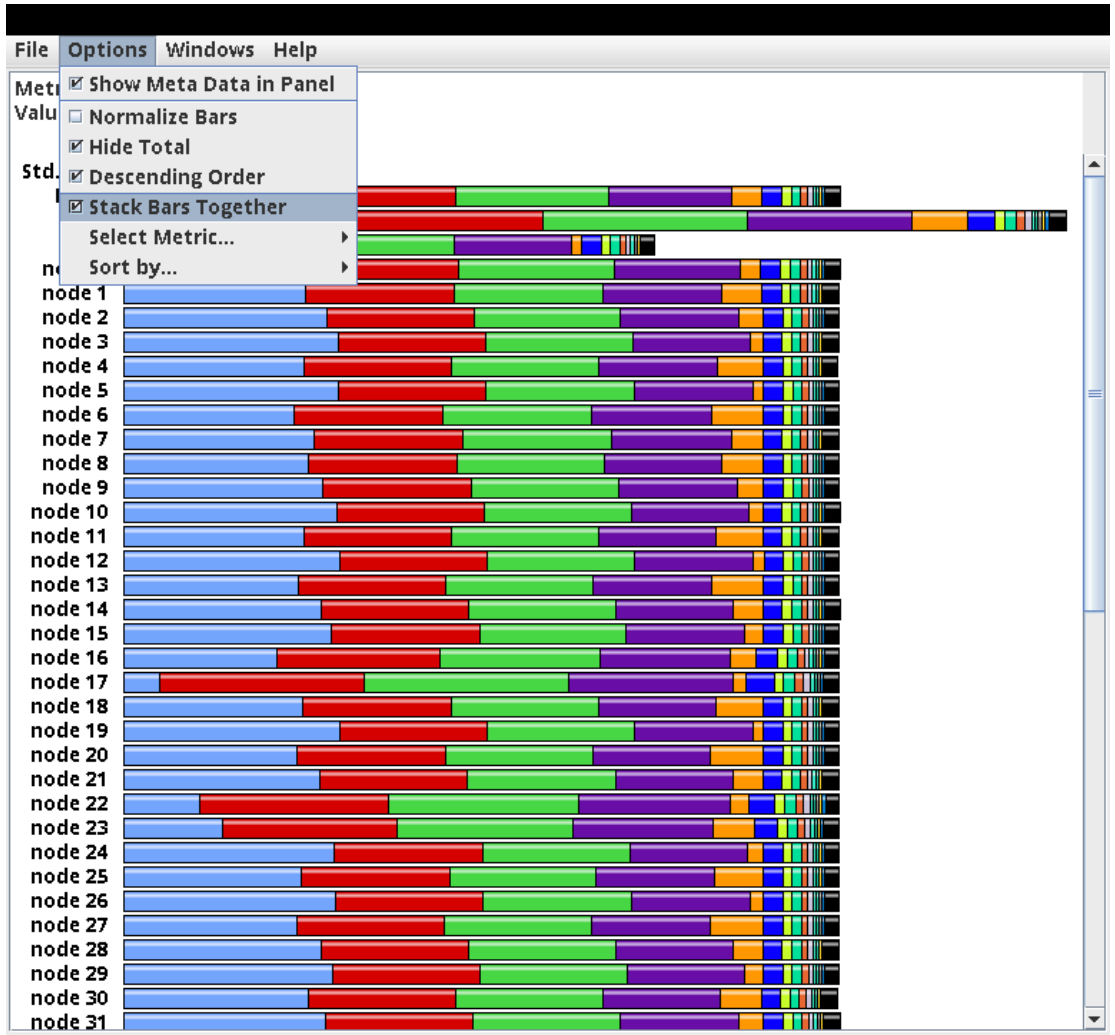
Colors represent code regions

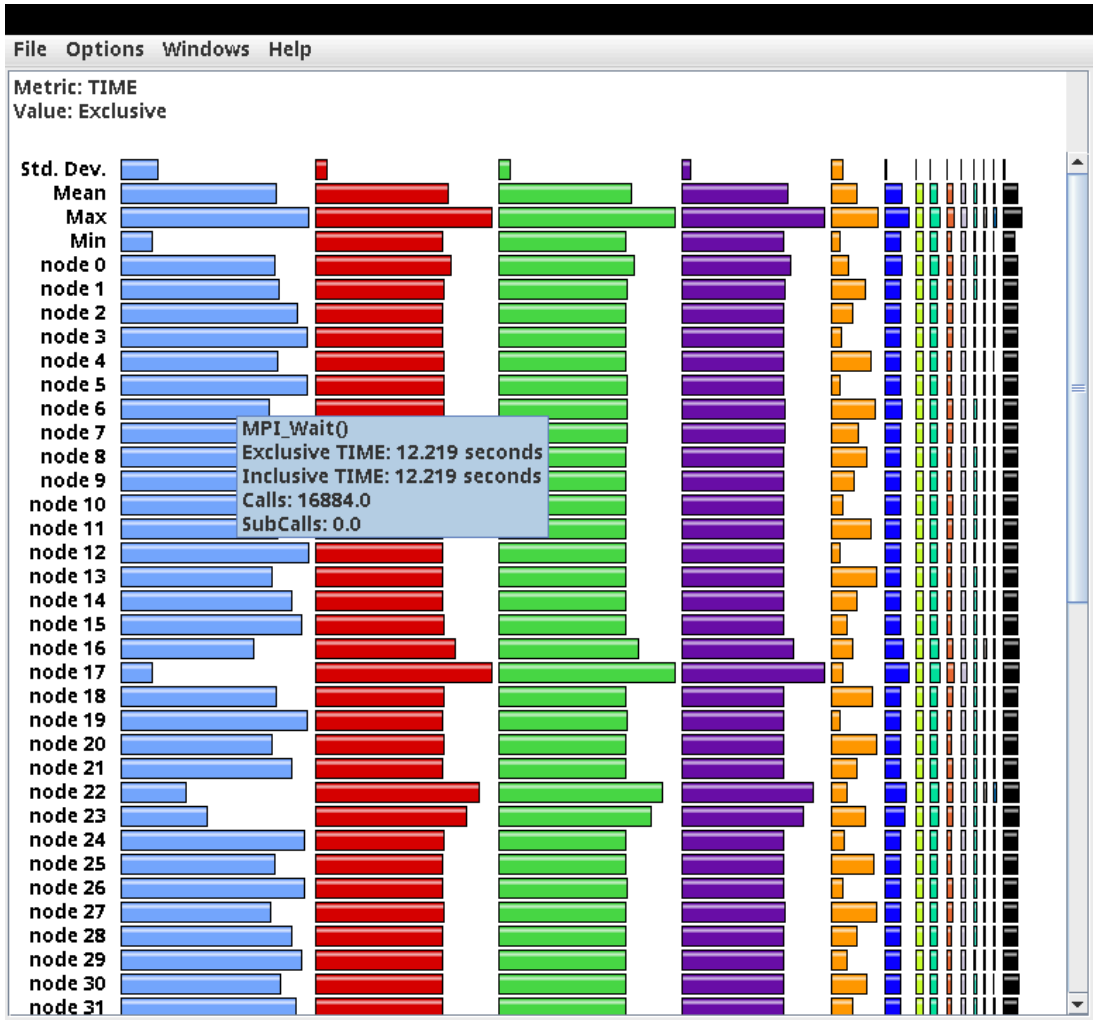
Options -> uncheck Stack Bars Together

Paraprof main window



ParaProf Profile Browser





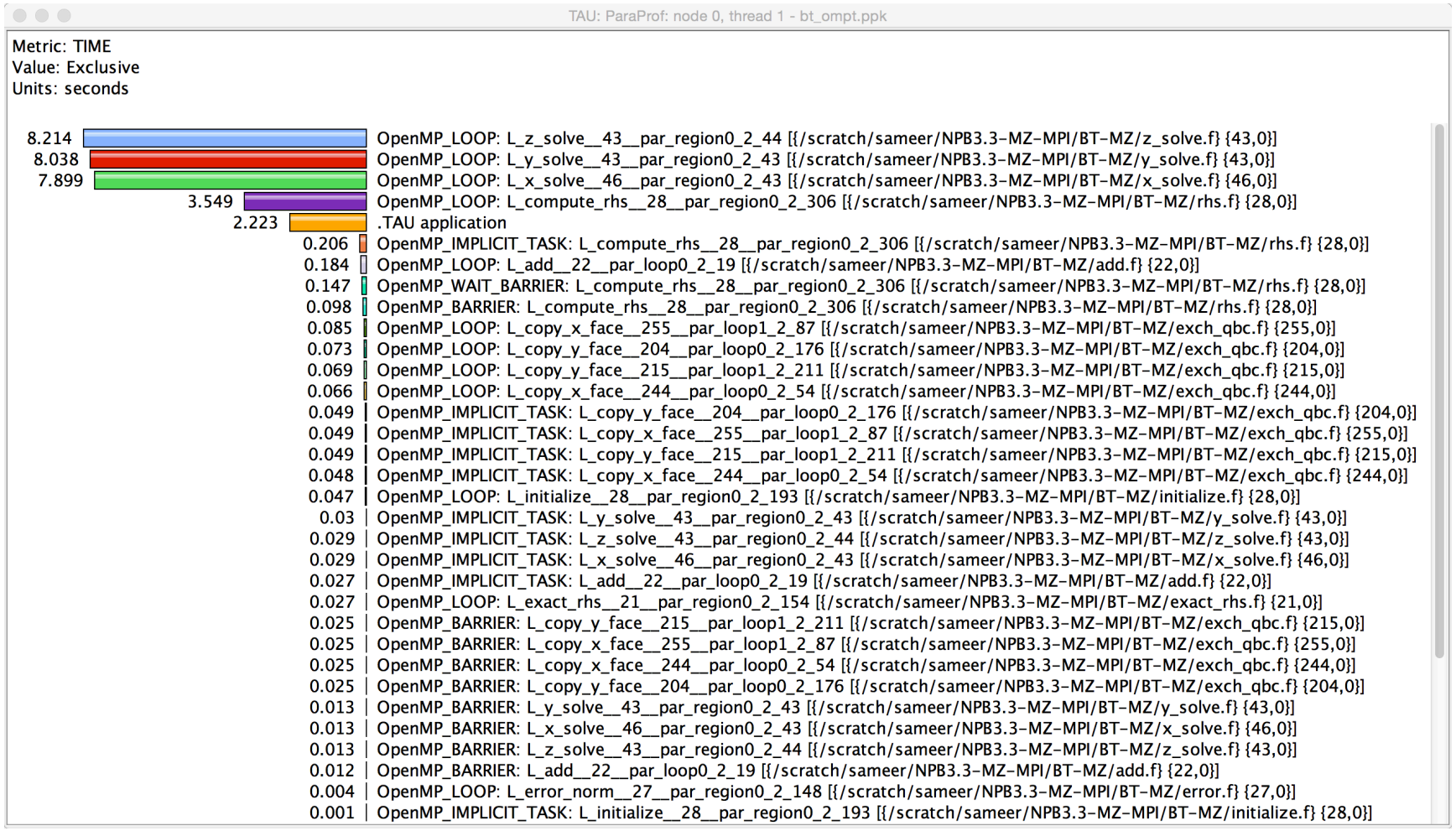
Paraprof main window

Left/right click here

Each routine occupies its own space. Can see the extent of imbalance across all threads.

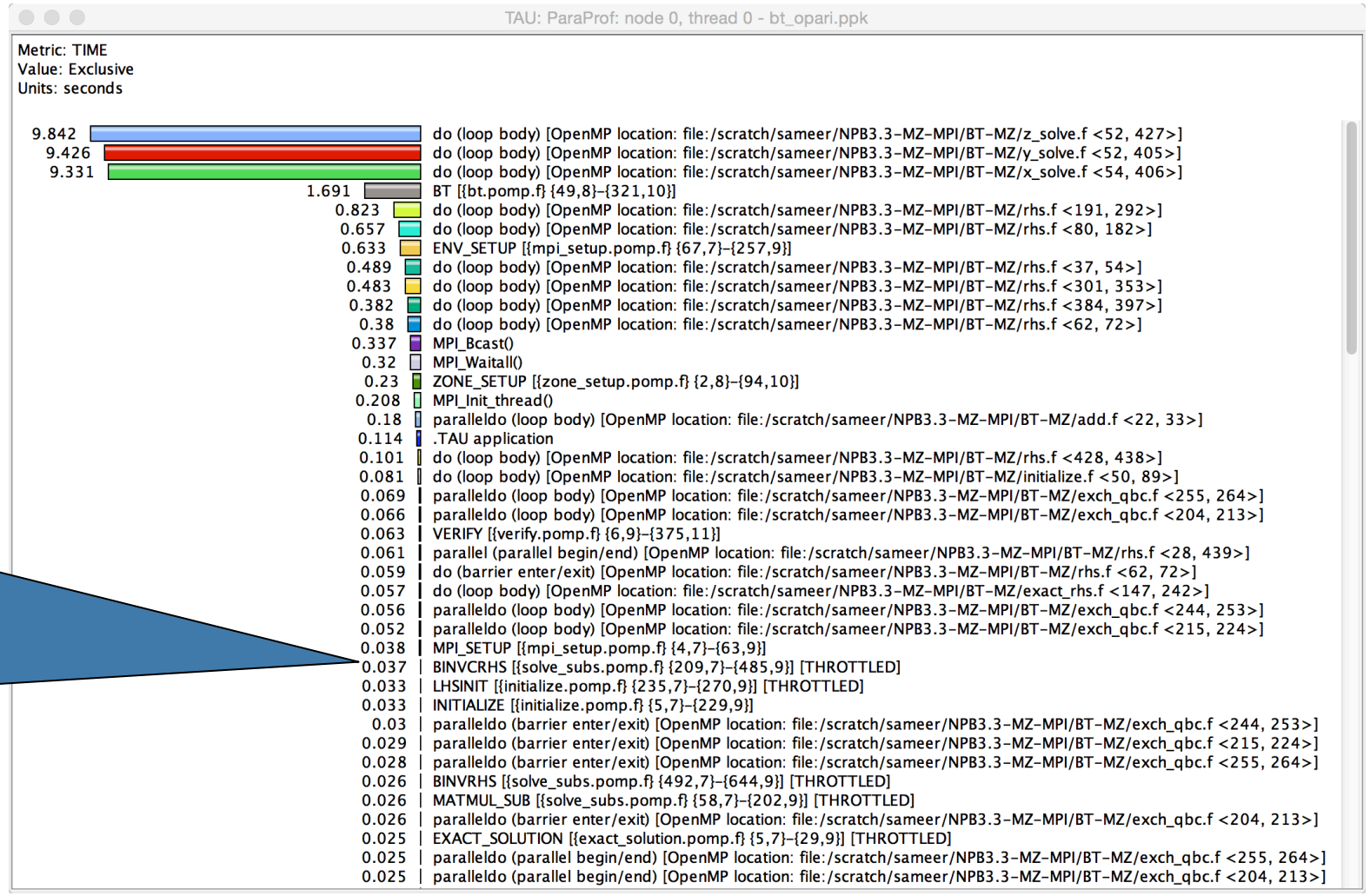
Paraprof node window (function barchart window)

Exclusive time spent in each code region (OpenMP loop) is shown here for MPI rank 0 thread 1

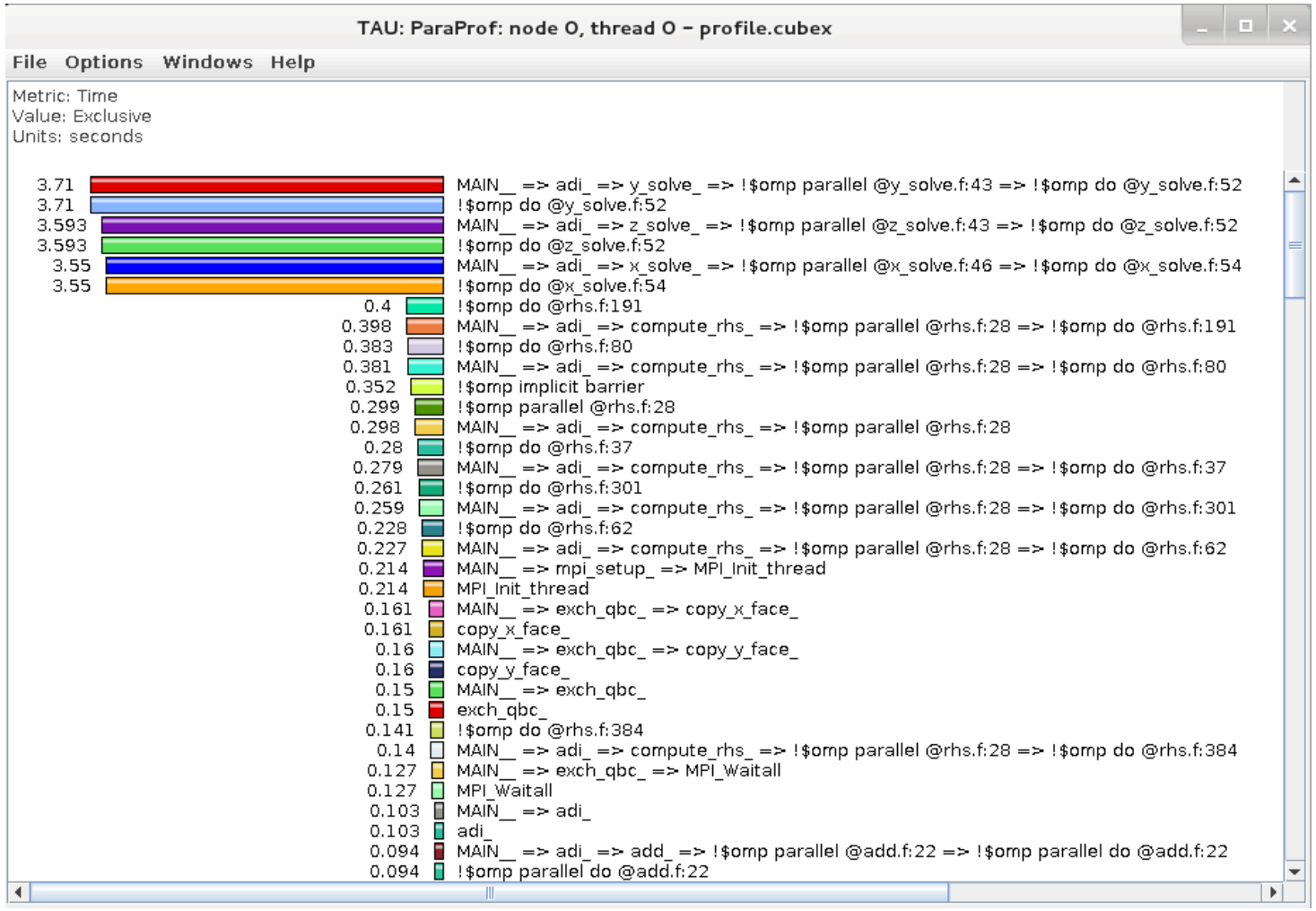


Instrumenting Source Code with PDT and Opari

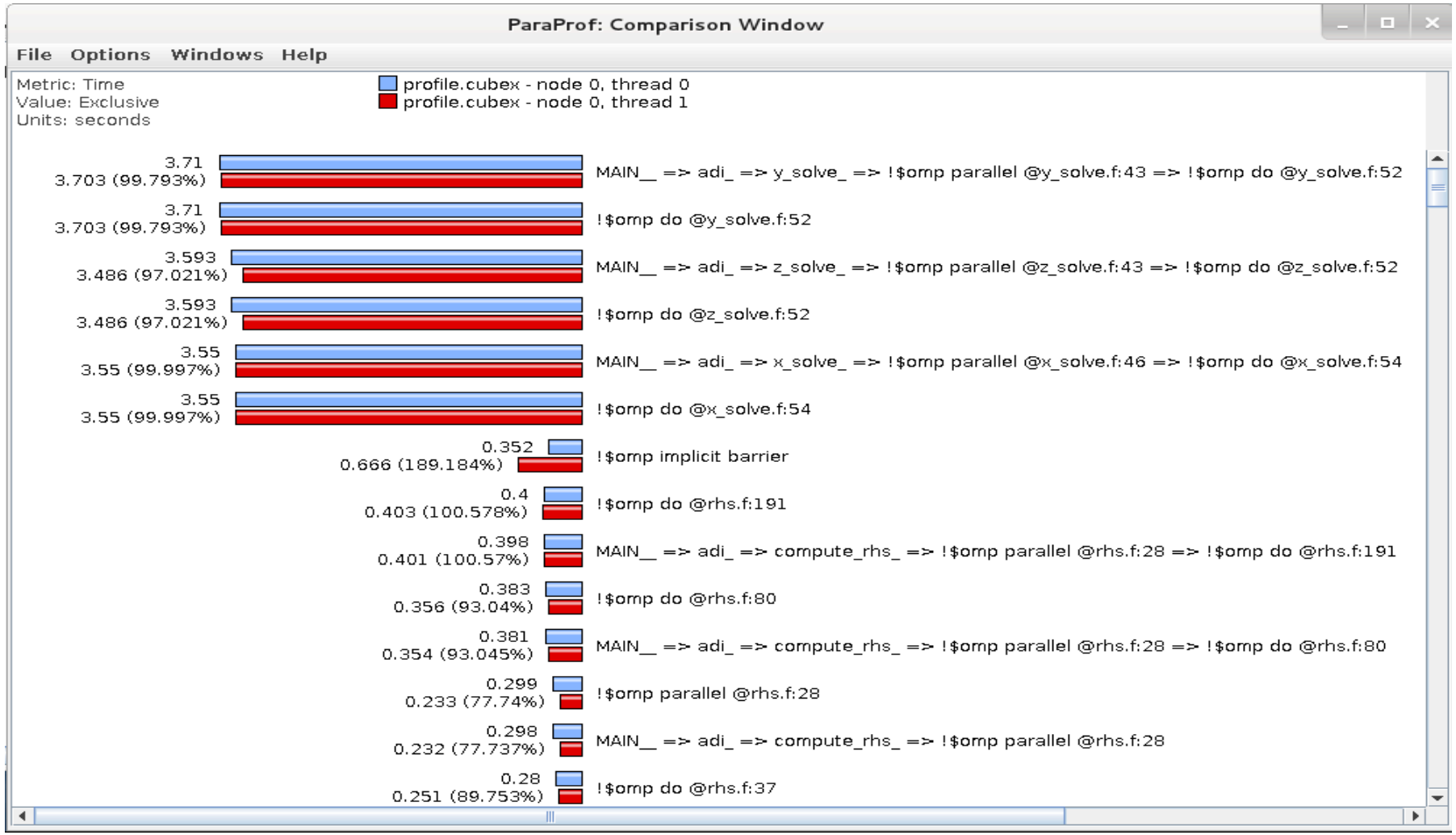
Frequently executing lightweight routines are automatically throttled at runtime. Reduces runtime dilation.



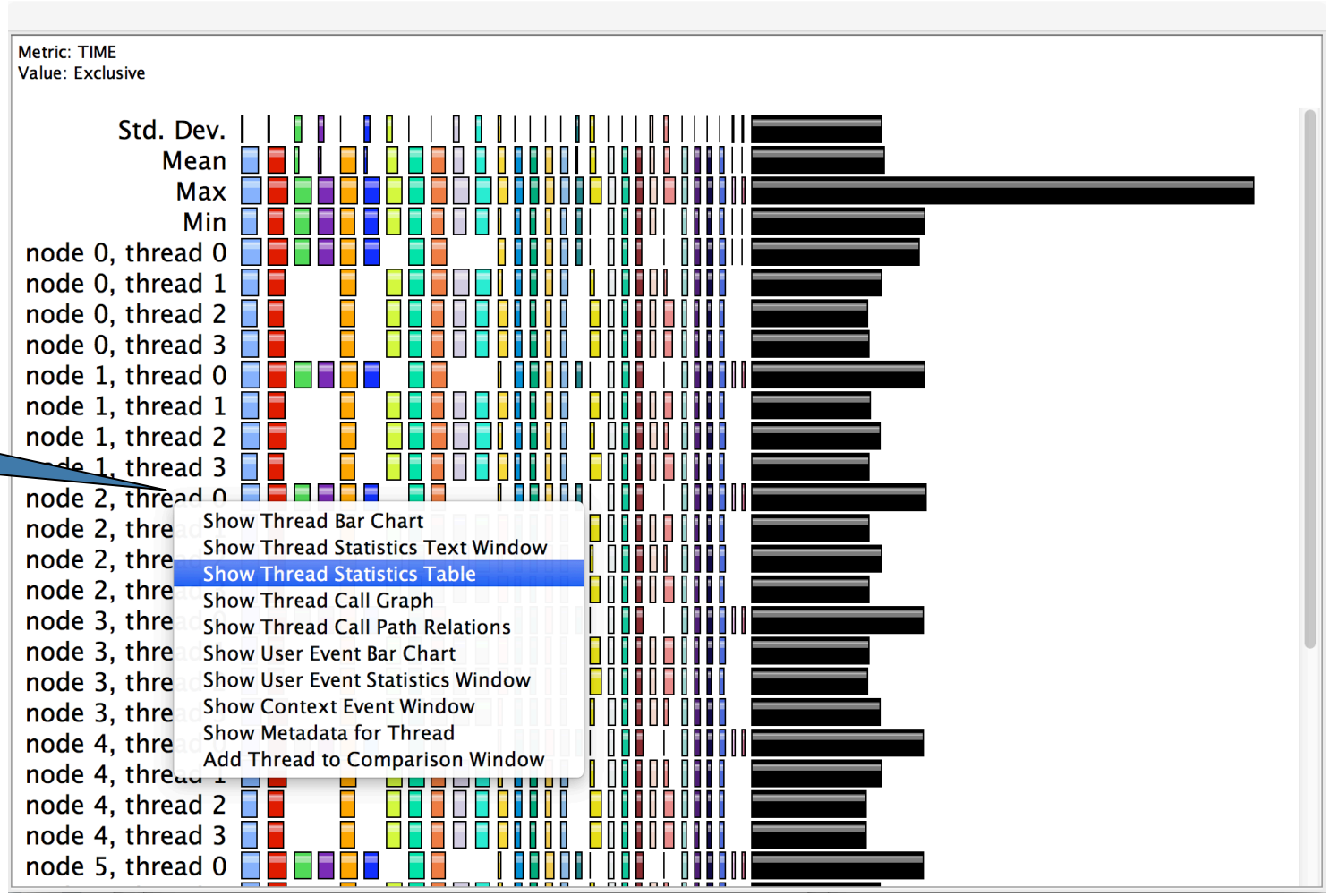
ParaProf: Node view in a callpath profile



ParaProf: Add thread to comparison window

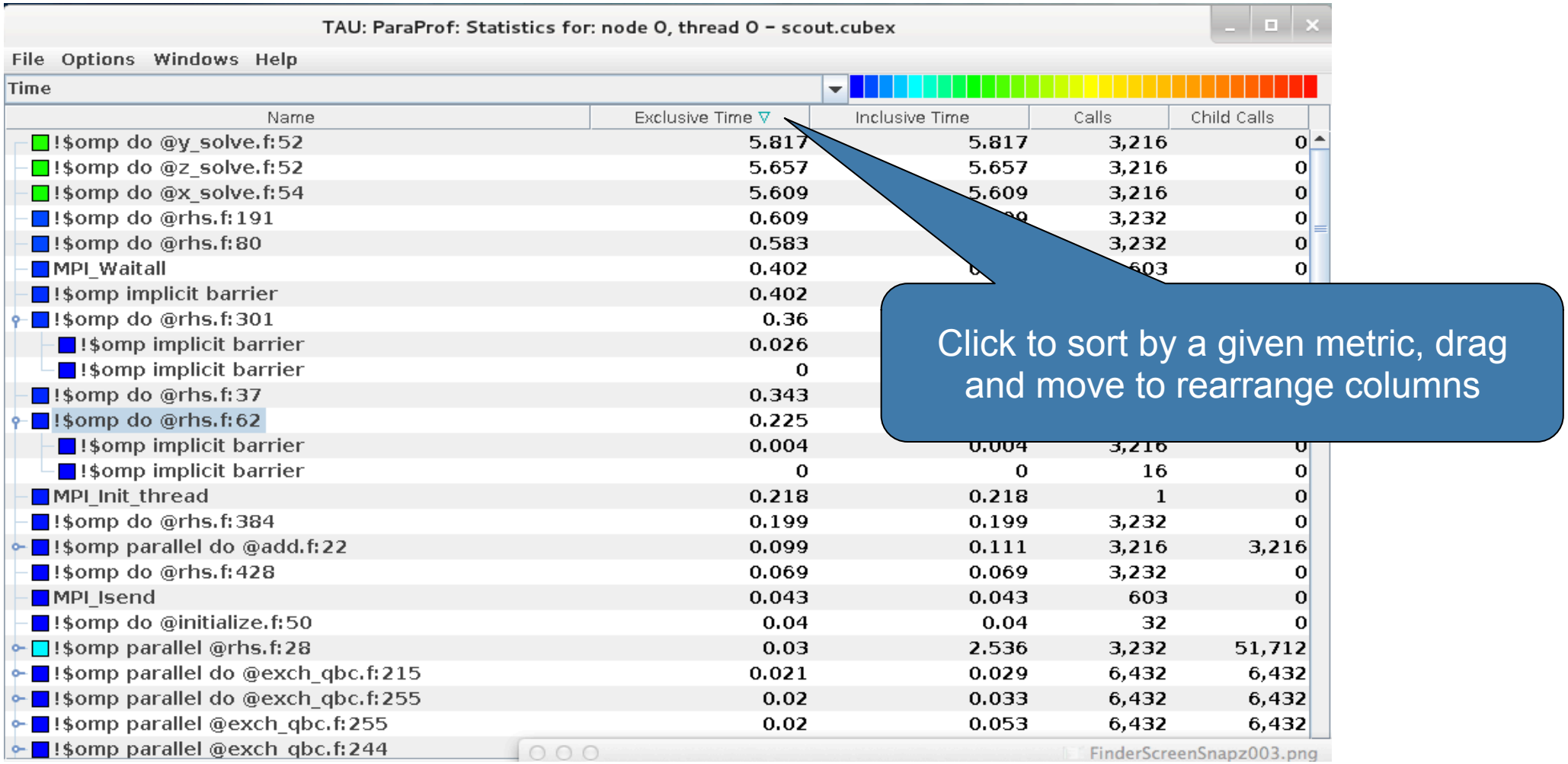


Paraprof Thread Statistics Table with TAU_SAMPLING=1



Right click here

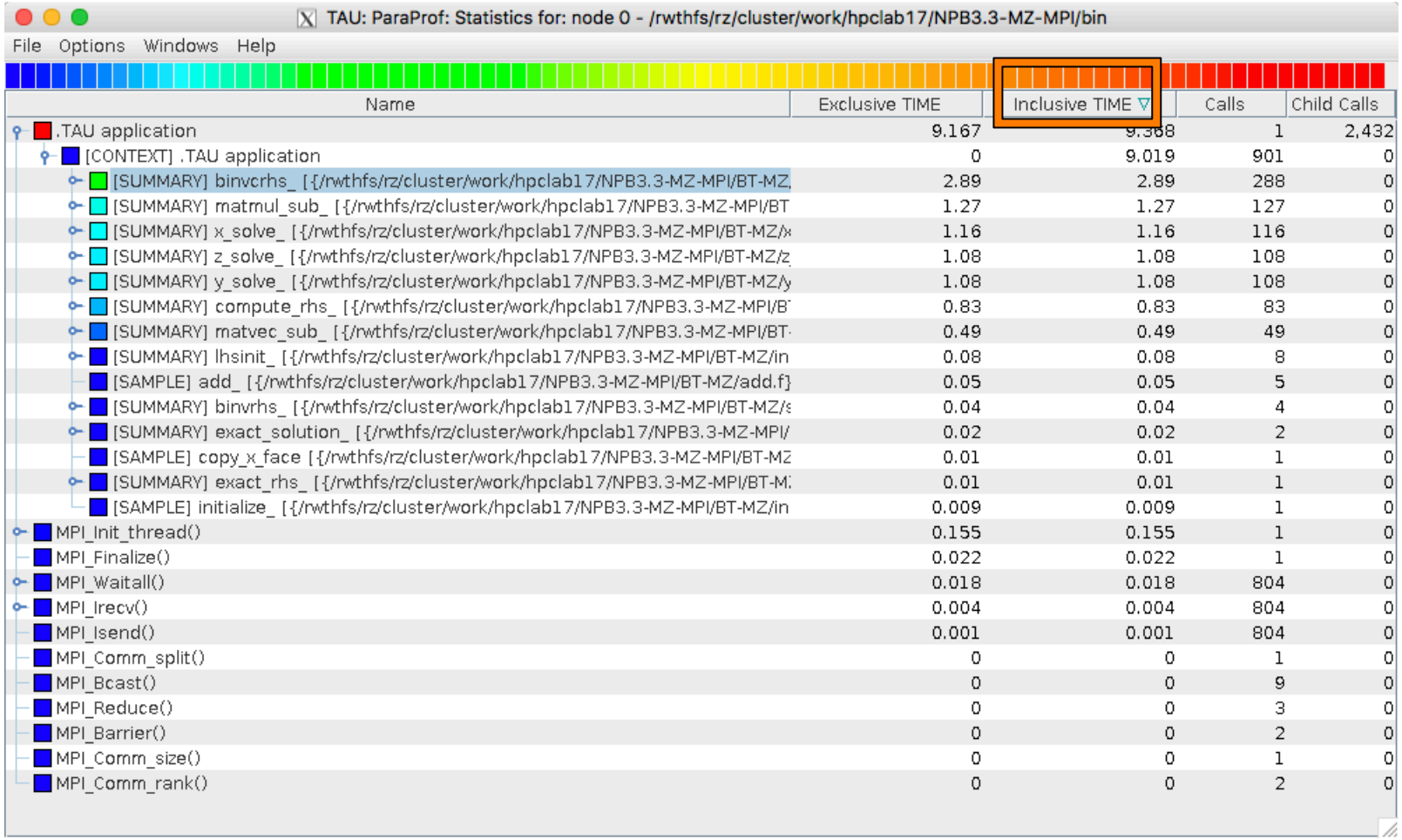
ParaProf: Thread Statistics Table



ParaProf

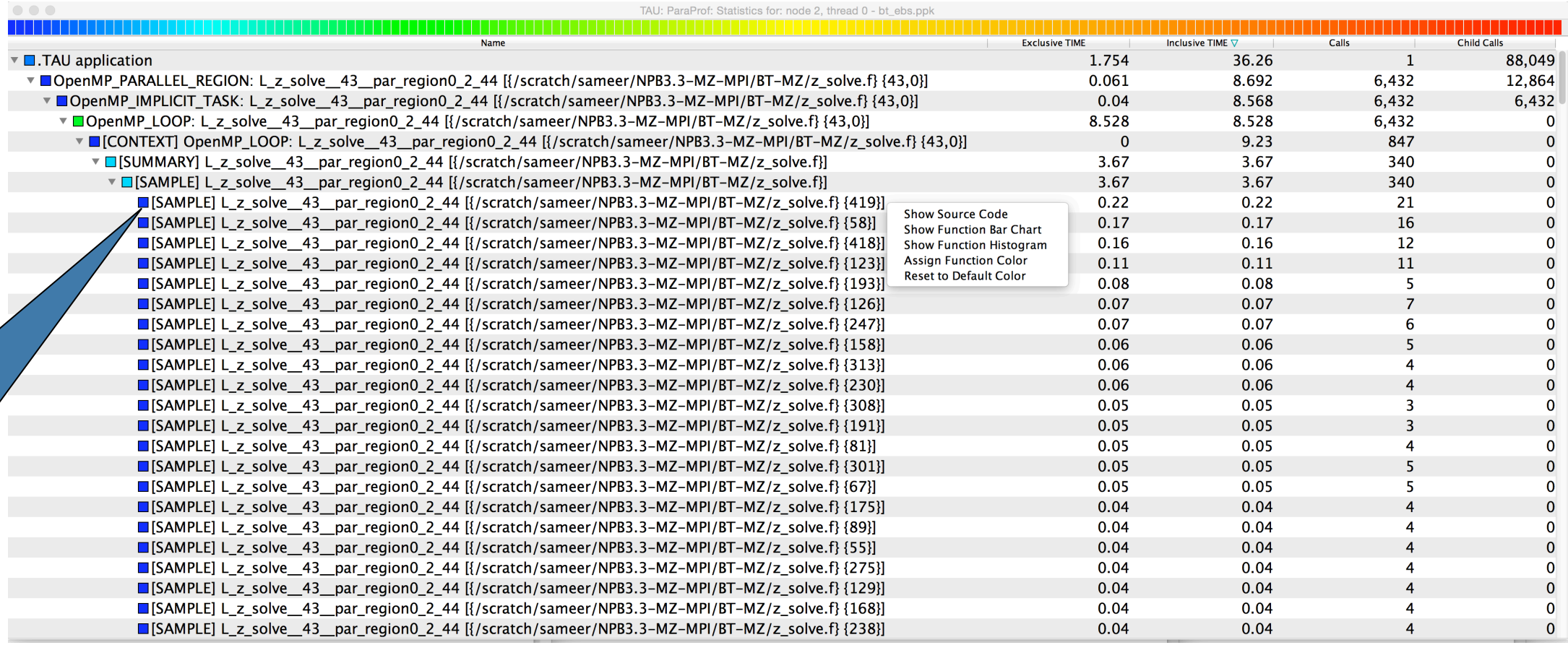
- Click on Columns:
- to sort by incl time

- Open binvcrhs
- Click on Sample



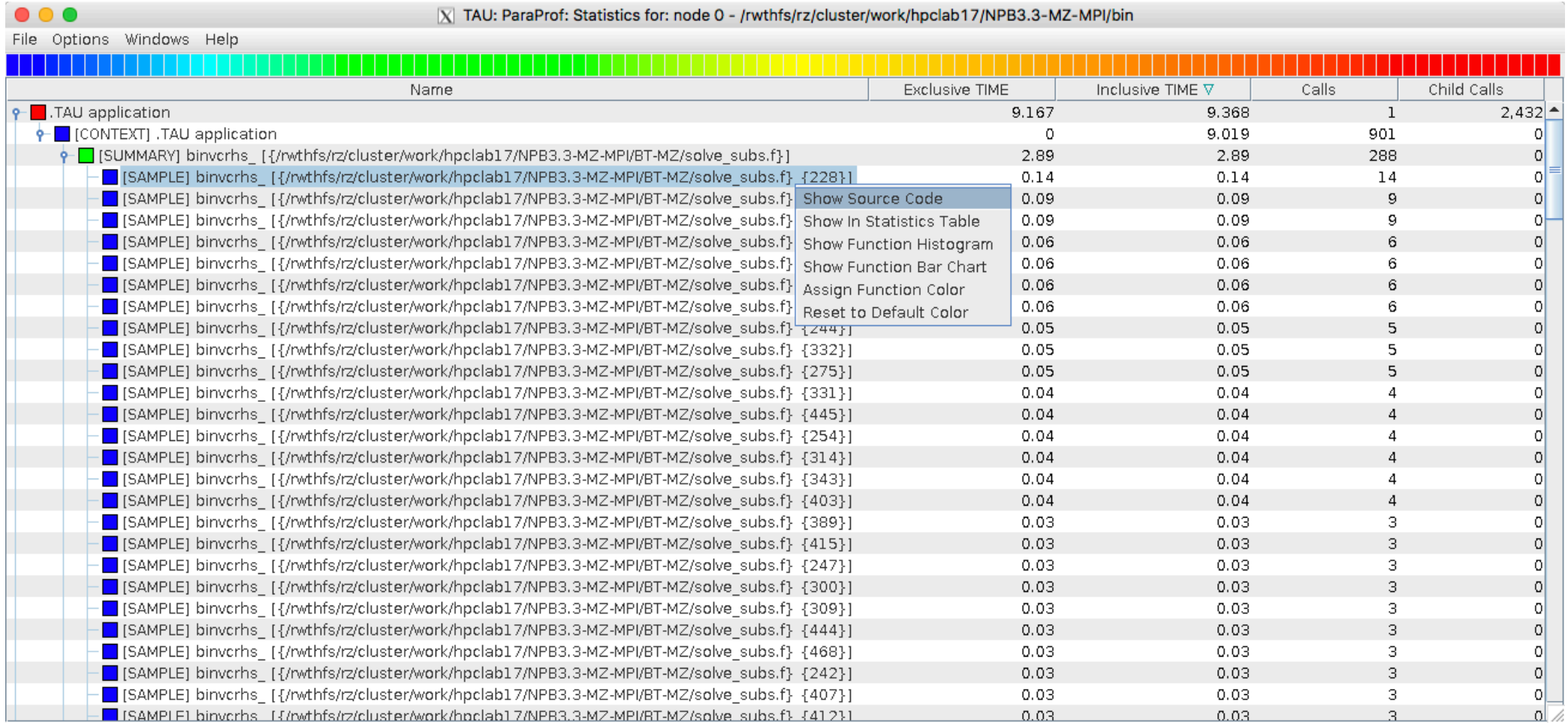
Name	Exclusive TIME	Inclusive TIME ▽	Calls	Child Calls
.TAU application	9.167	9.368	1	2,432
[CONTEXT] .TAU application	0	9.019	901	0
[SUMMARY] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ	2.89	2.89	288	0
[SUMMARY] matmul_sub_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT	1.27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

Paraprof Thread Statistics Table



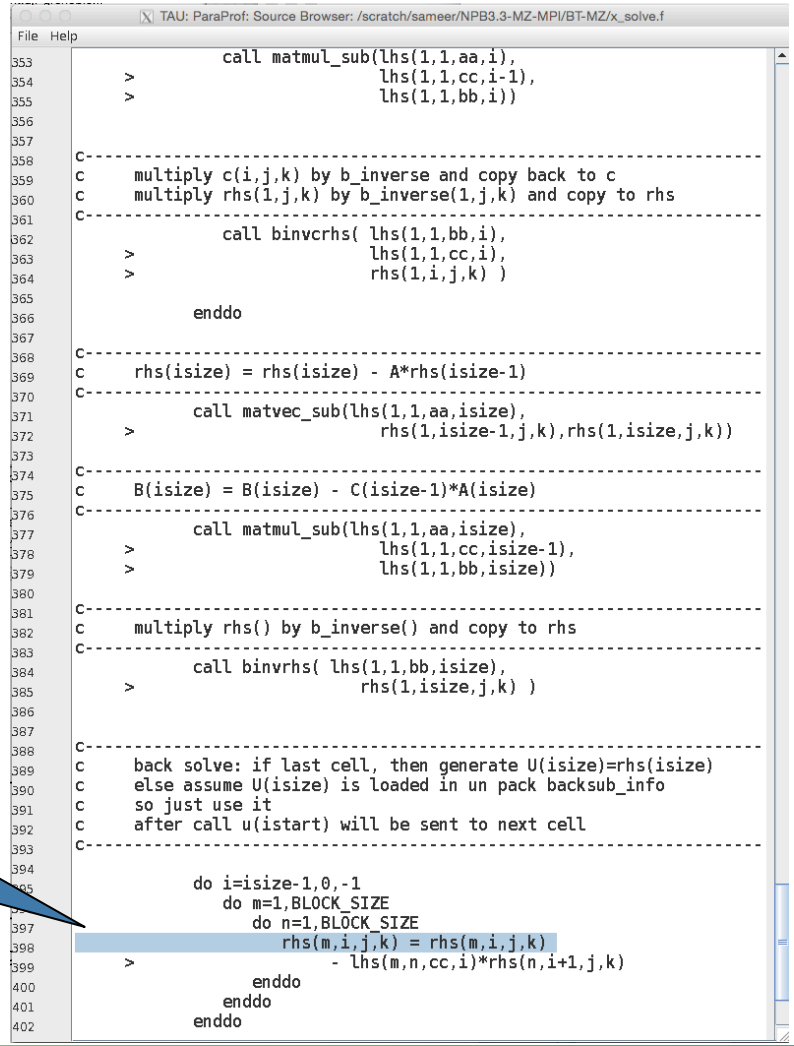
Right click here and choose “Show Source Code” for a sample

ParaProf

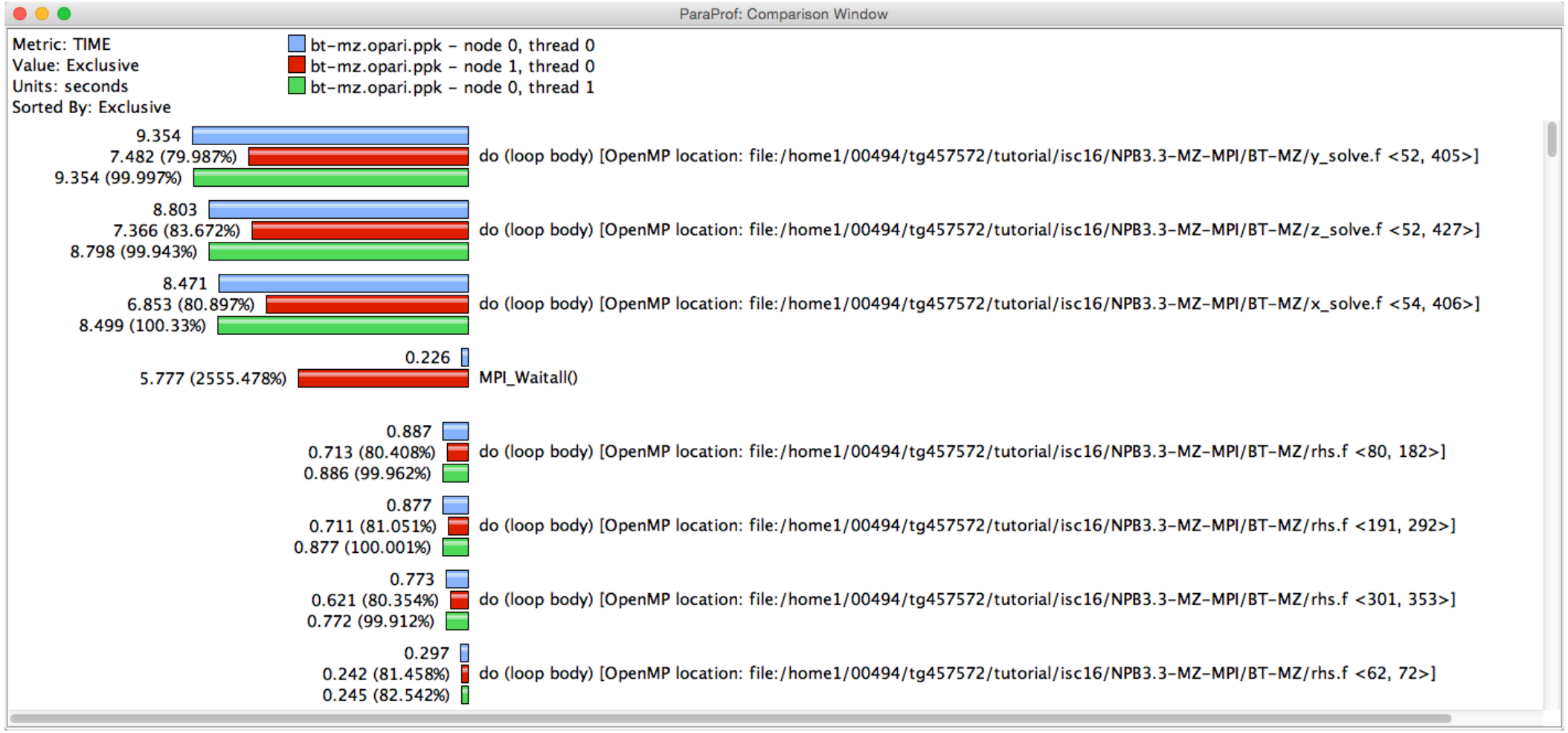

TAU: ParaProf: Statistics for: node 0 - /rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/bin
File Options Windows Help
Name Exclusive TIME Inclusive TIME Calls Child Calls
.TAU application 9.167 9.368 1 2,432
[CONTEXT] .TAU application 0 9.019 901 0
[SUMMARY] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f}] 2.89 2.89 288 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {228}] 0.14 0.14 14 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {332}] 0.05 0.05 5 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {275}] 0.05 0.05 5 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {331}] 0.04 0.04 4 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {445}] 0.04 0.04 4 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {254}] 0.04 0.04 4 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {314}] 0.04 0.04 4 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {343}] 0.04 0.04 4 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {403}] 0.04 0.04 4 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {389}] 0.03 0.03 3 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {415}] 0.03 0.03 3 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {247}] 0.03 0.03 3 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {300}] 0.03 0.03 3 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {309}] 0.03 0.03 3 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {444}] 0.03 0.03 3 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {468}] 0.03 0.03 3 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {242}] 0.03 0.03 3 0
[SAMPLE] binvcrhs_ [{/rwthfs/rz/cluster/work/hpclab17/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f} {407}] 0.03 0.03 3 0
Show Source Code
Show In Statistics Table
Show Function Histogram
Show Function Bar Chart
Assign Function Color
Reset to Default Color

Statement Level Profiling with TAU

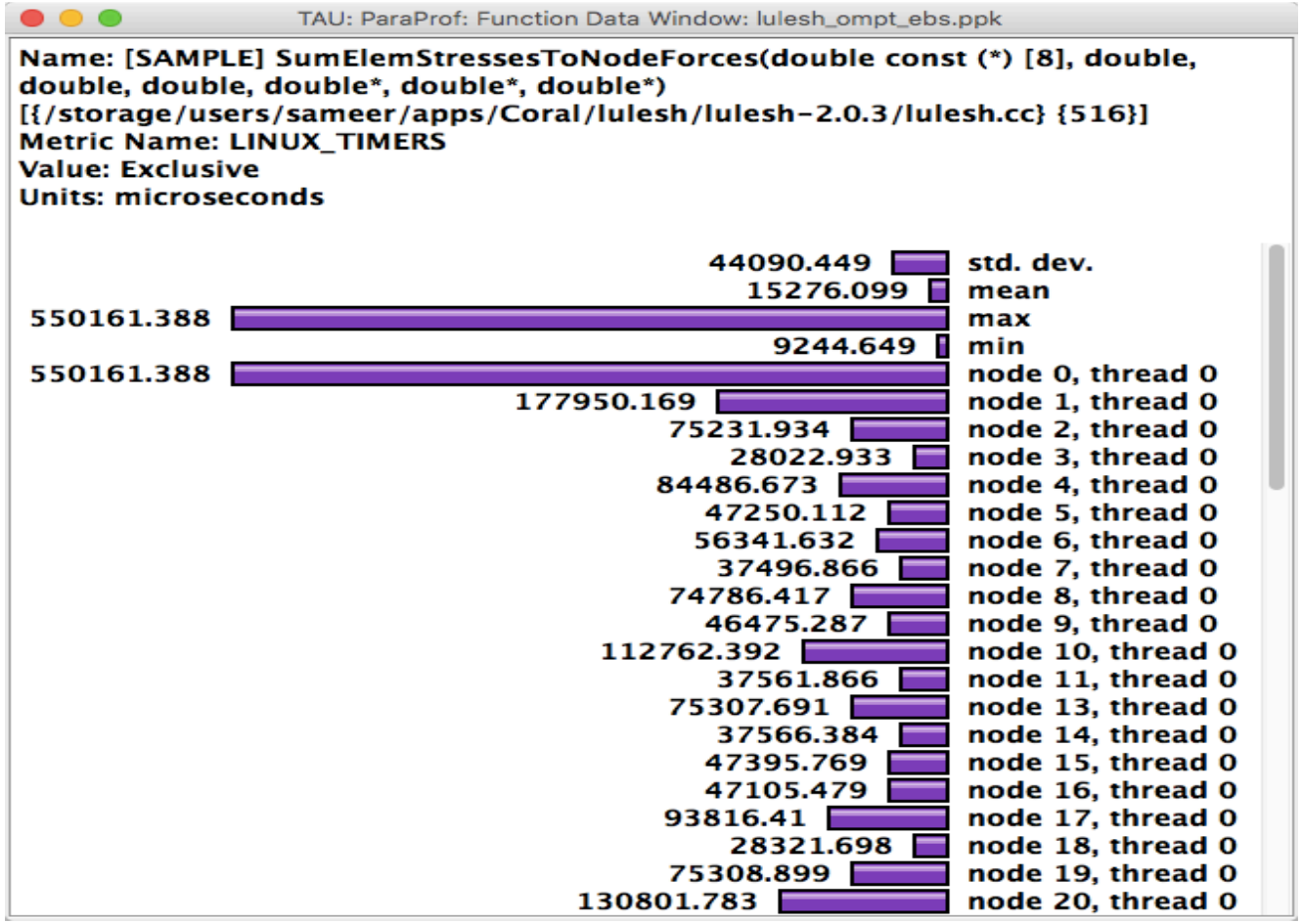
Source location where samples are taken. Compute intensive region.



ParaProf Comparison Window



TAU – Event Based Sampling (EBS)



% export TAU_SAMPLING=1

Examples: 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

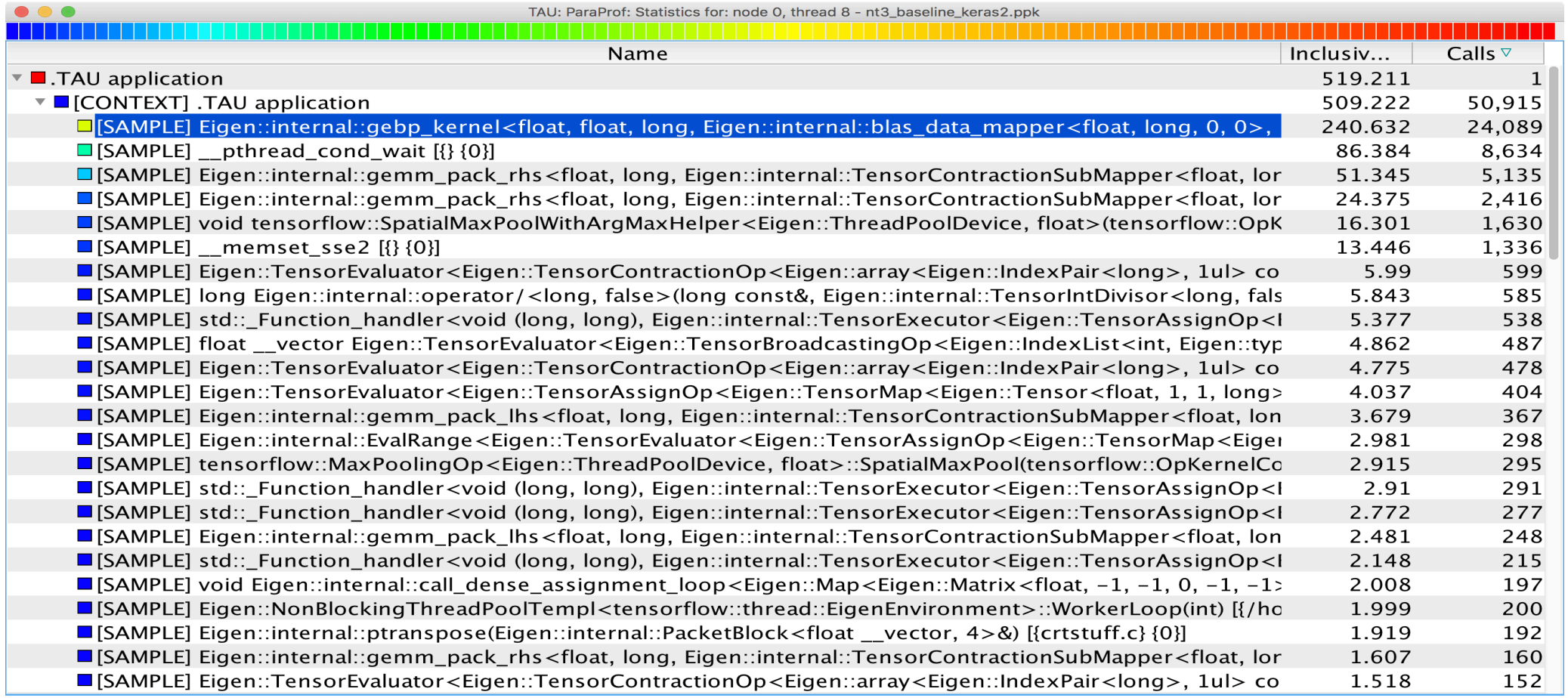
UNWINDING CALLSTACKS

% export TAU_SAMPLING=1; export TAU_EBS_UNWIND=1

UNWINDING CALLSTACKS

Name	Inclusive TIME	Calls
.TAU application	79.592	1
MPI_Recv()	75.607	6,870
[CONTEXT] MPI_Recv()	74.848	1,497
[UNWIND] /gpfs/mira-home/sameer/gamess-theta-tau/object/unport.f.410 [@] MAIN__ [{/gpfs/mira-home/sameer/gamess-theta-	26.196	524
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_fortran.c.67 [@] beging_ [{/gpfs/mira-home/sameer/g	21.7	434
[UNWIND] /gpfs/mira-home/sameer/gamess-theta-tau/object/gamess.f.538 [@] main [{/gpfs/mira-home/sameer/gamess-theta-ta	11.85	237
[UNWIND] /gpfs/mira-home/sameer/gamess-theta-tau/object/unport.f.410 [@] MAIN__ [{/gpfs/mira-home/sameer/gamess-thet	11.85	237
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_fortran.c.67 [@] beging_ [{/gpfs/mira-home/sam	11.85	237
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_init.c.113 [@] ddi_init_ [{/gpfs/mira-home/yur	11.85	237
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_server.c.99 [@] DDI_Init [{/gpfs/mira-home/	11.85	237
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_recv.c.65 [@] DDI_Server [{/gpfs/mira-ho	11.85	237
[UNWIND] /lus/theta-fs0/software/perftools/tau/tau-2.26.3/src/Profile/TauMpi.c.2371 [@] DDI_Recv_request [{/gpfs	11.85	237
[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-fs(	11.85	237
[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,	11.7	234
[SAMPLE] MPIDI_CH3I_Progress [{/opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1} {0	11.3	226
[SAMPLE] MPIDU_Sched_are_pending [{/opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0	0.2	4
[SAMPLE] MPID_nem_gni_poll [{/opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1} {0}]	0.15	3
[SAMPLE] MPID_nem_network_poll [{/opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1	0.05	1
[UNWIND] ch3_progress.c.0 [@] PMPI_Recv [{/opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.	0.15	3
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_init.c.113 [@] ddi_init_ [{/gpfs/mira-home/yuri/dist/G	8.701	174
[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_server.c.99 [@] DDI_Init [{/gpfs/mira-home/yuri/dist/(	5.75	115
[UNWIND] /lib64/libc-2.22.so.0 [@] _start [{/home/abuild/rpmbuild/BUILD/glibc-2.22/csu/../sysdeps/x86_64/start.S} {118}]	0.2	4
[SAMPLE] GNII_DlaProgress [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0} {0}]	0.2	4
[UNWIND] [/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0.0] [@] UNRESOLVED UNKNOWN	0.15	3
[SAMPLE] GNI_CqGetEvent [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0} {0}]	0.051	1
[UNWIND] /opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1.0 [@] MPIDI_CH3I_Progress [{/opt/cray/pe/mpt/	0.05	1
MPI_Finalize()	3.601	1
MPI_Send()	0.122	6,866
MPI_Init_thread()	0.112	1
[CONTEXT] .TAU application	0.05	1

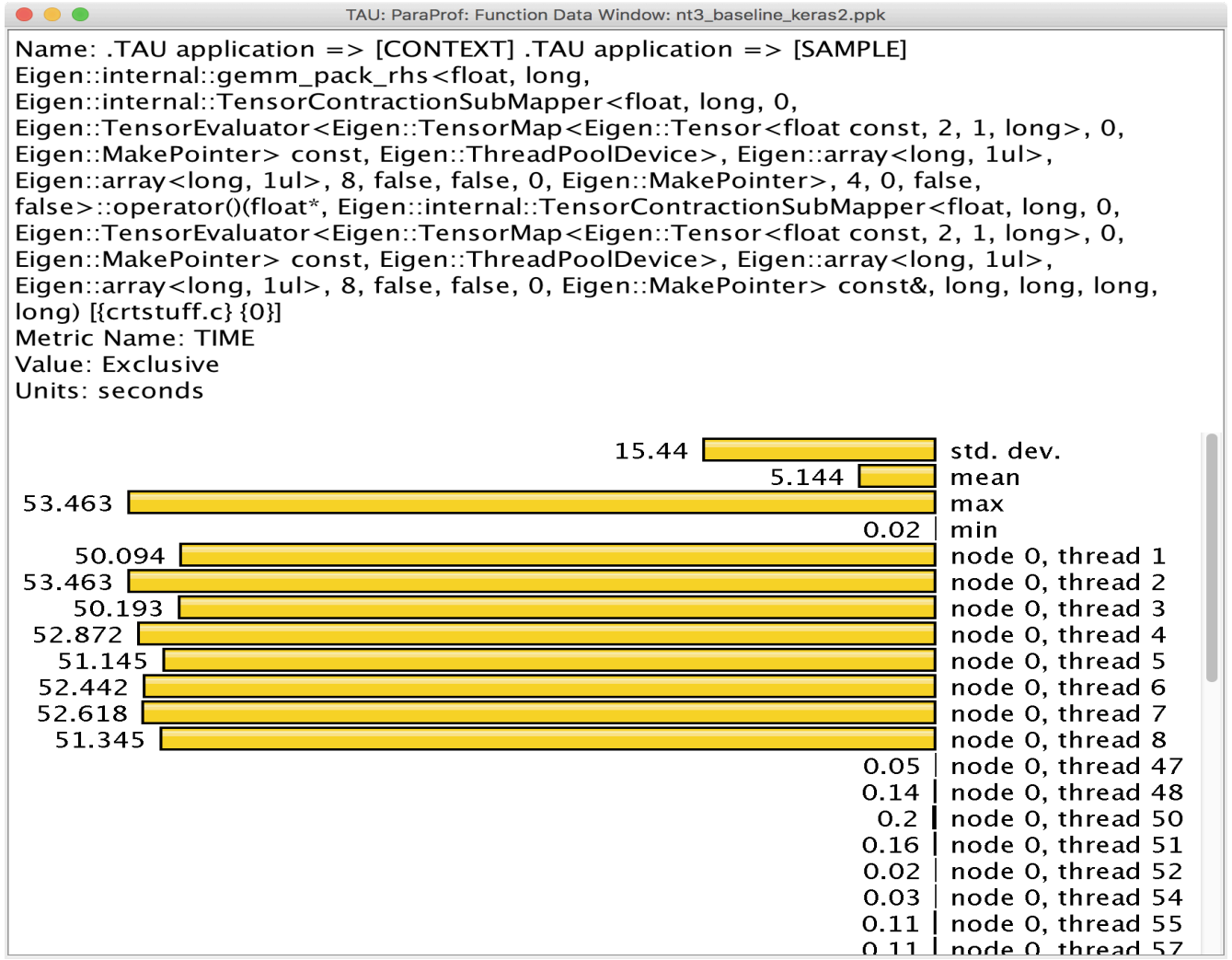
Deep Learning: Tensorflow



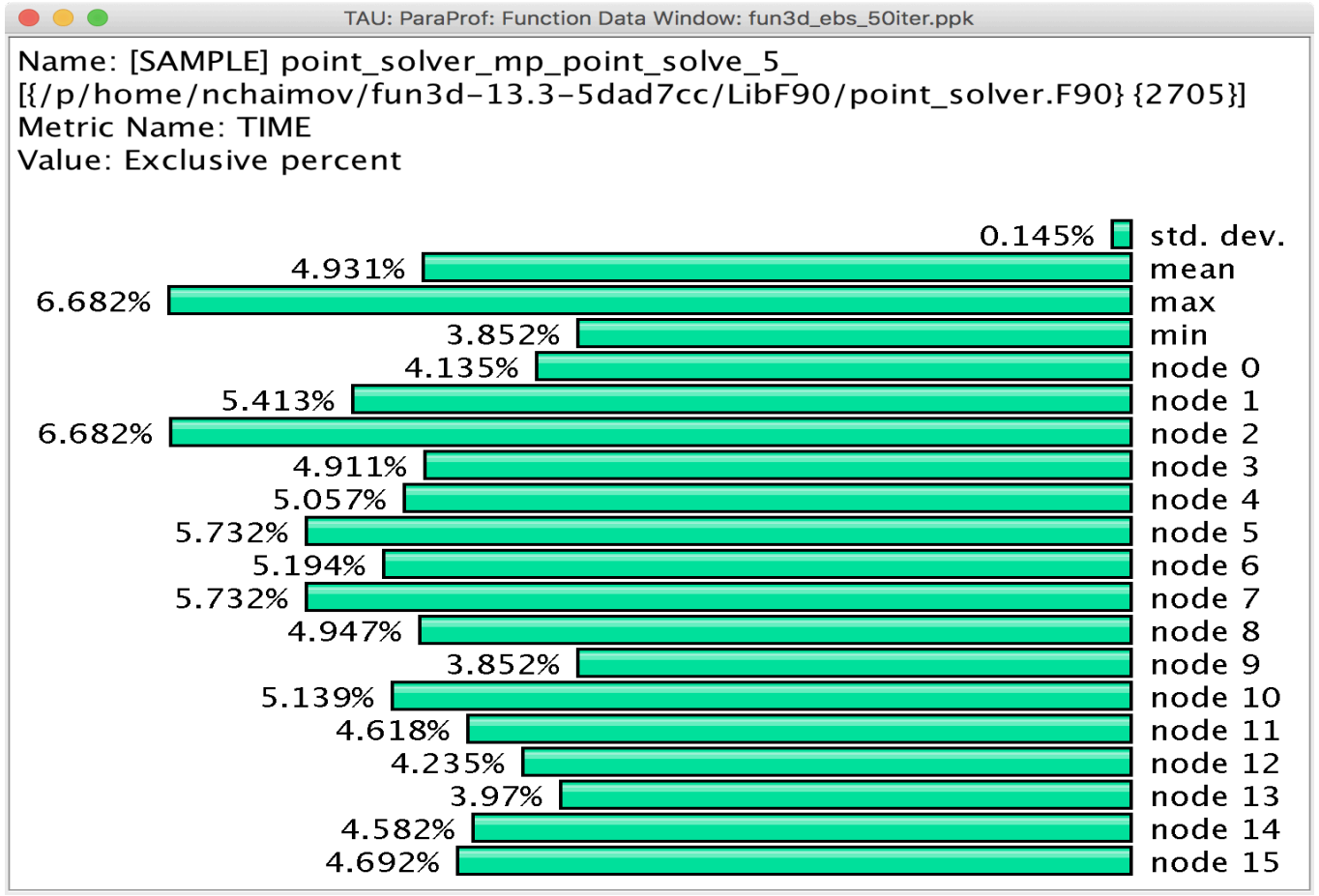
Name	Inclusiv...	Calls
.TAU application	519.211	1
[CONTEXT] .TAU application	509.222	50,915
[SAMPLE] Eigen::internal::gebp_kernel<float, float, long, Eigen::internal::blas_data_mapper<float, long, 0, 0>,	240.632	24,089
[SAMPLE] __pthread_cond_wait [{} {0}]	86.384	8,634
[SAMPLE] Eigen::internal::gemm_pack_rhs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

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

Sampling Tensorflow



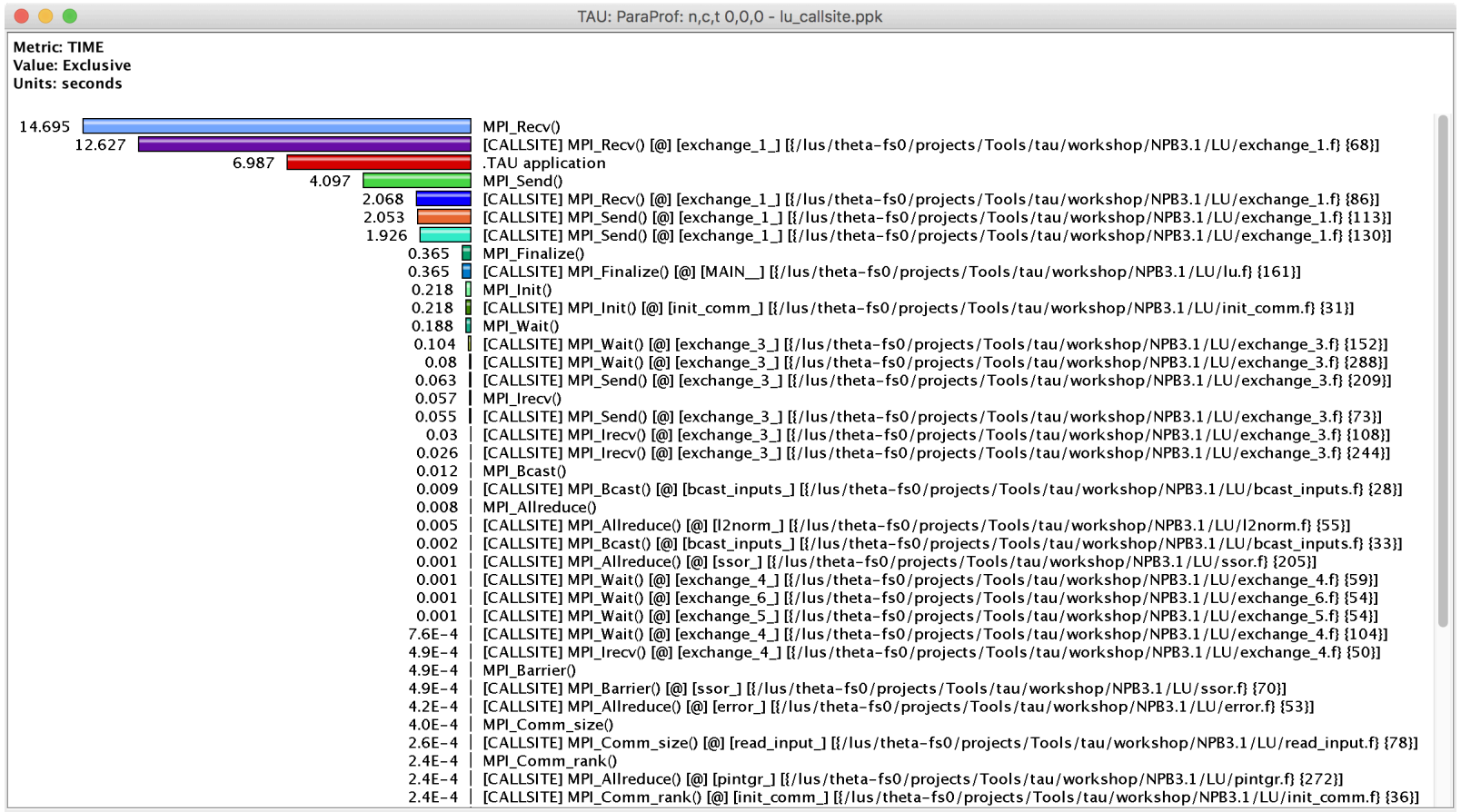
Event Based Sampling (EBS)



Uninstrumented!

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

Callsite Profiling and Tracing



% export TAU_CALLSITE=1

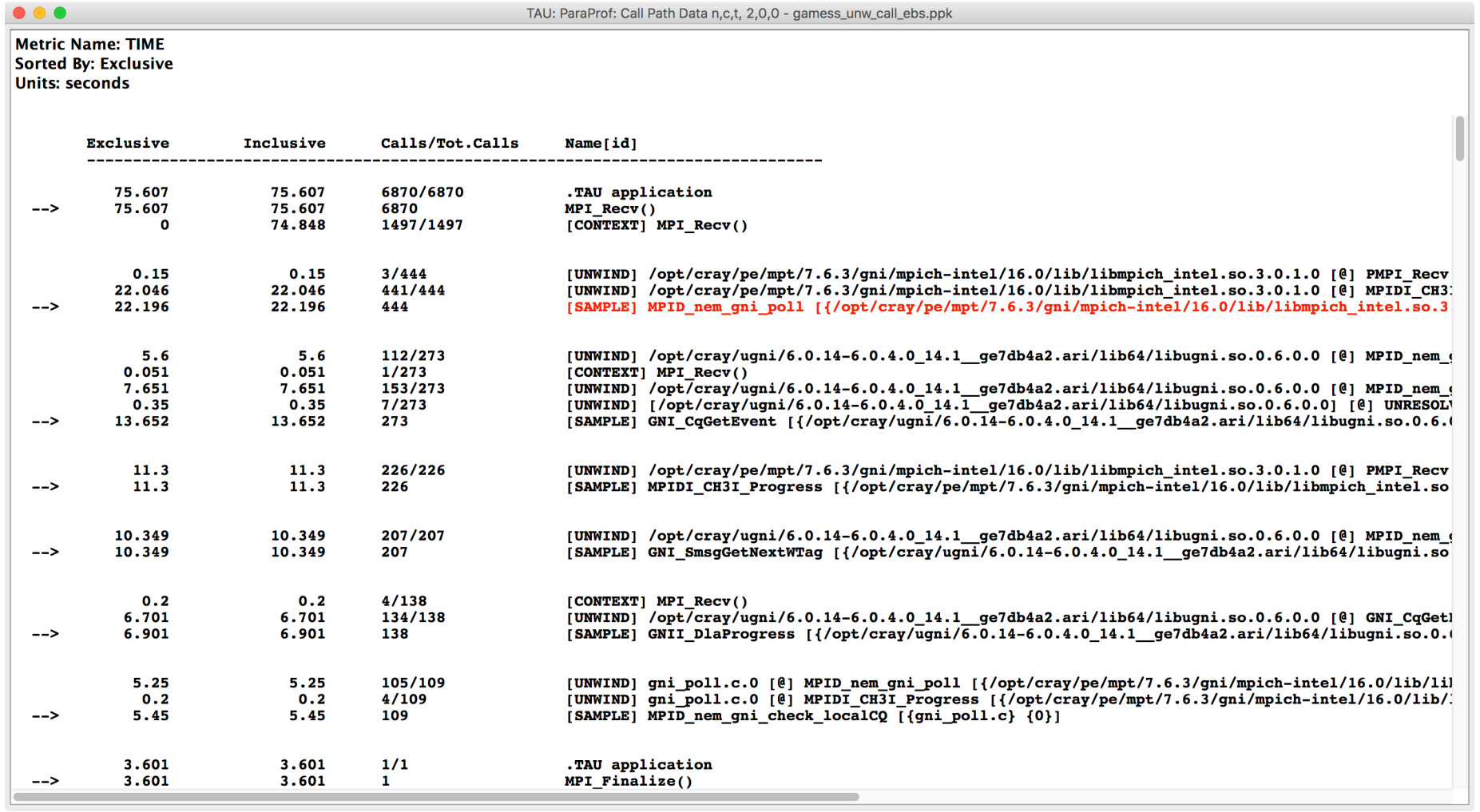
CALLPATH THREAD RELATIONS WINDOW

TAU: ParaProf: Call Path Data n,c,t, 2,0,0 - gamess_unw_call_ebs.ppk

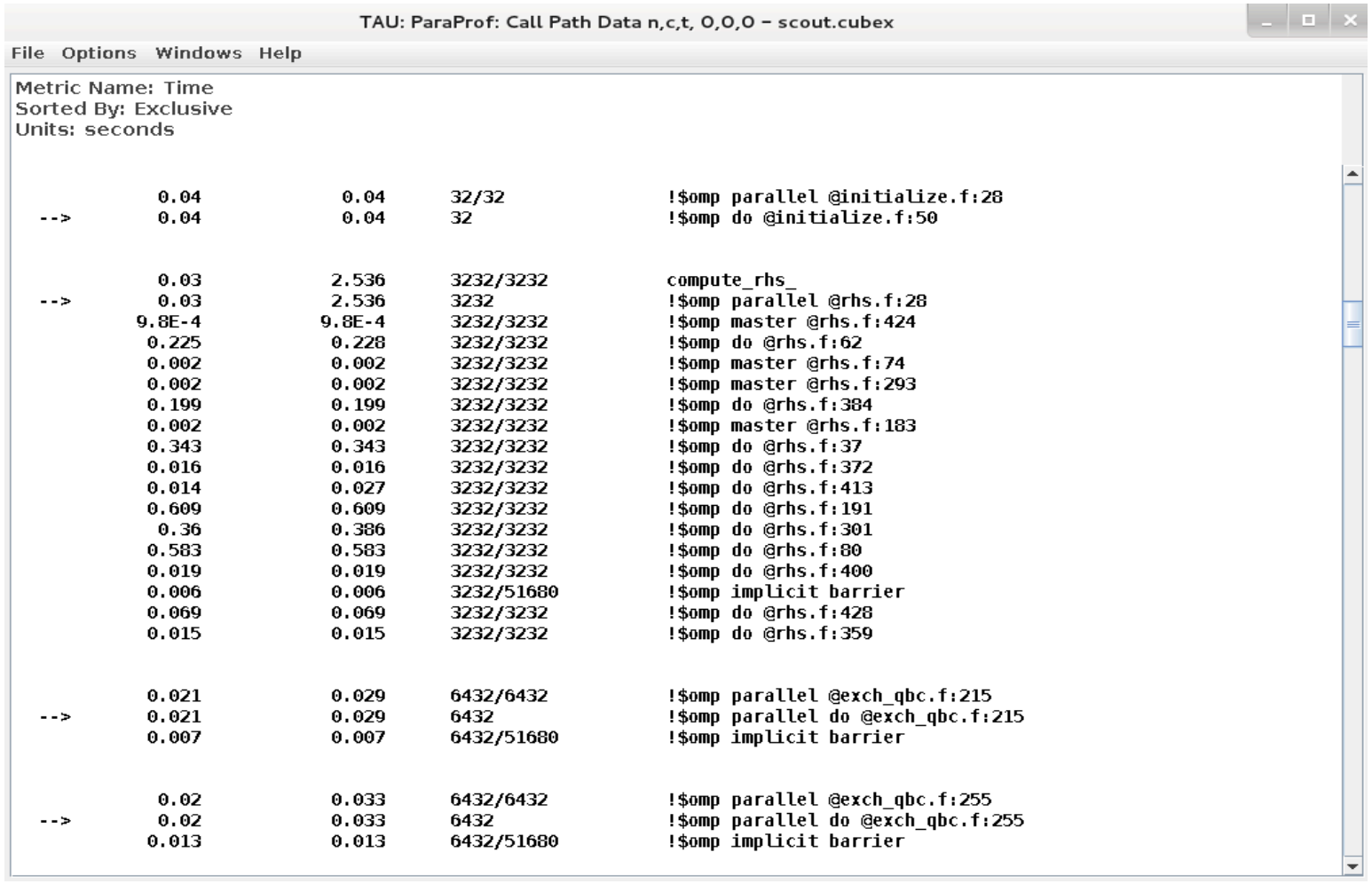
Metric Name: TIME
Sorted By: Inclusive
Units: seconds

	Exclusive	Inclusive	Calls/Tot.Calls	Name[id]
-->	0.121	79.592	1	.TAU application
	0.002	0.002	1/1	MPI_Gather()
	0.004	0.004	3/3	MPI_Allgather()
	0.122	0.122	6866/6866	MPI_Send()
	0.002	0.002	1/1	MPI_Comm_split()
	8.9E-5	8.9E-5	2/2	MPI_Comm_size()
	4.6E-4	4.6E-4	3/3	MPI_Group_incl()
	75.607	75.607	6870/6870	MPI_Recv()
	0.002	0.002	4/4	MPI_Comm_create()
	9.5E-5	9.5E-5	6/6	MPI_Comm_rank()
	5.4E-4	5.4E-4	1/1	MPI_Comm_group()
	0.003	0.003	7/7	MPI_Barrier()
	0.112	0.112	1/1	MPI_Init_thread()
	6.3E-4	6.3E-4	1/1	MPI_Group_intersection()
	0	0.05	1/1	[CONTEXT] .TAU application
	3.601	3.601	1/1	MPI_Finalize()
	0.014	0.014	6/6	MPI_Bcast()
	75.607	75.607	6870/6870	.TAU application
-->	75.607	75.607	6870	MPI_Recv()
	0	74.848	1497/1497	[CONTEXT] MPI_Recv()
	0	74.848	1497/1497	MPI_Recv()
-->	0	74.848	1497	[CONTEXT] MPI_Recv()
	0	8.701	174/1371	[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_init.c.113 [@] ddi_i
	0	26.196	524/763	[UNWIND] /gpfs/mira-home/sameer/gamess-theta-tau/object/unport.f.410 [@] MAIN__ [{/gpfs/mir
	0.2	0.2	4/138	[SAMPLE] GNII_DlaProgress [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.s
	0	5.75	115/1484	[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_server.c.99 [@] DDI_
	0	0.2	4/5	[UNWIND] /lib64/libc-2.22.so.0 [@] _start [{/home/abuild/rpmbuild/BUILD/glibc-2.22/csu/../s
	0	11.85	237/239	[UNWIND] /gpfs/mira-home/sameer/gamess-theta-tau/object/gamess.f.538 [@] main [{/gpfs/mira-
	0.051	0.051	1/273	[SAMPLE] GNI_CqGetEvent [{/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so
	0	0.05	1/1197	[UNWIND] /opt/cray/pe/mpt/7.6.3/gni/mpich-intel/16.0/lib/libmpich_intel.so.3.0.1.0 [@] MPID
	0	0.15	3/7	[UNWIND] [/opt/cray/ugni/6.0.14-6.0.4.0_14.1__ge7db4a2.ari/lib64/libugni.so.0.6.0.0] [@] UNI
	0	21.7	434/1197	[UNWIND] /gpfs/mira-home/yuri/dist/Github/gamess-theta-tau/ddi/src/ddi_fortran.c.67 [@] beg

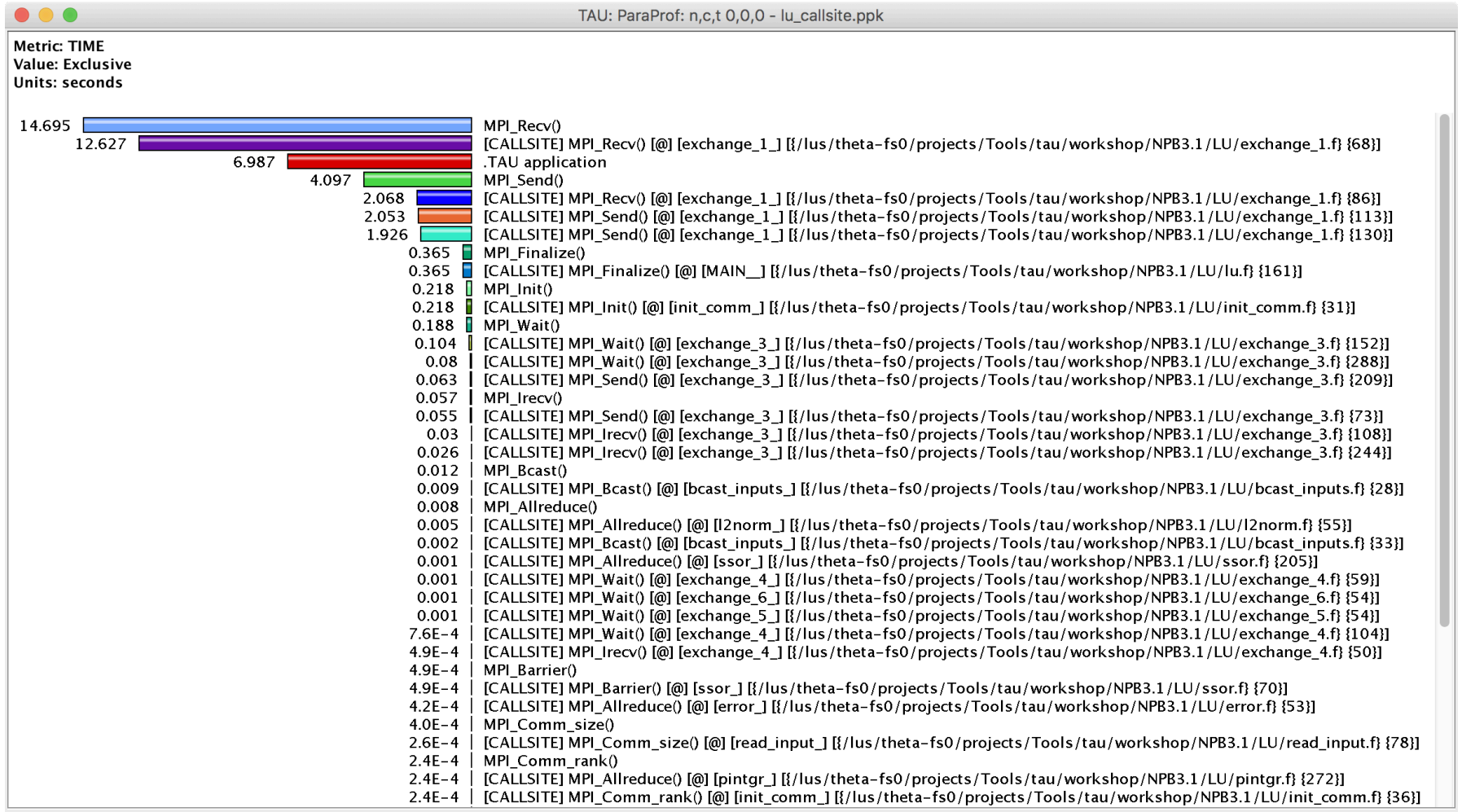
CALLPATH THREAD RELATIONS WINDOW



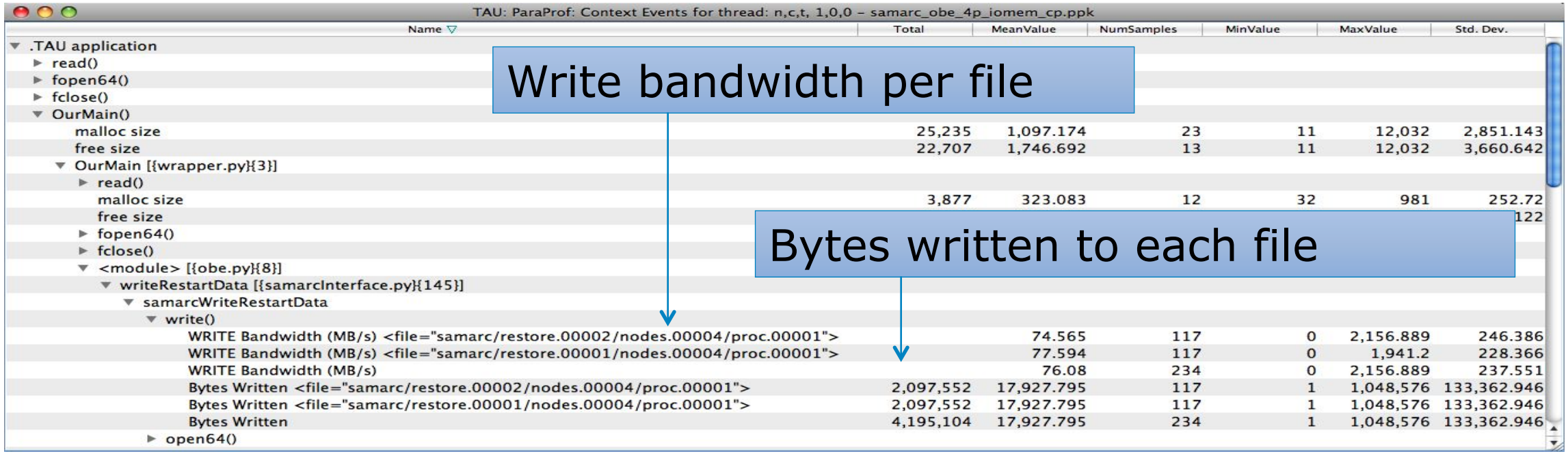
ParaProf: Callpath Thread Relations Window



Callsite Profiling and Tracing (TAU_CALLSITE=1)

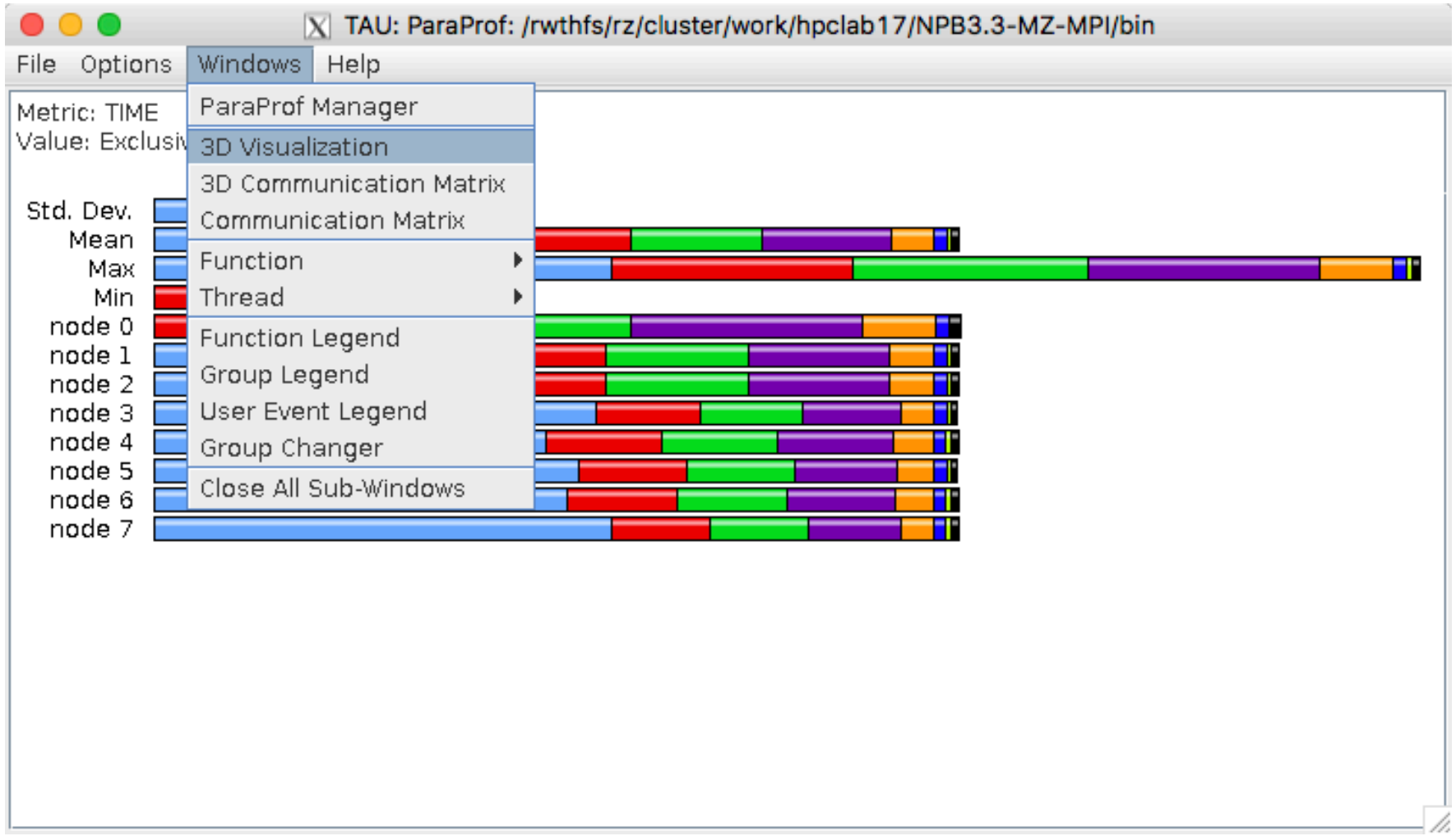


TAU – Context Events

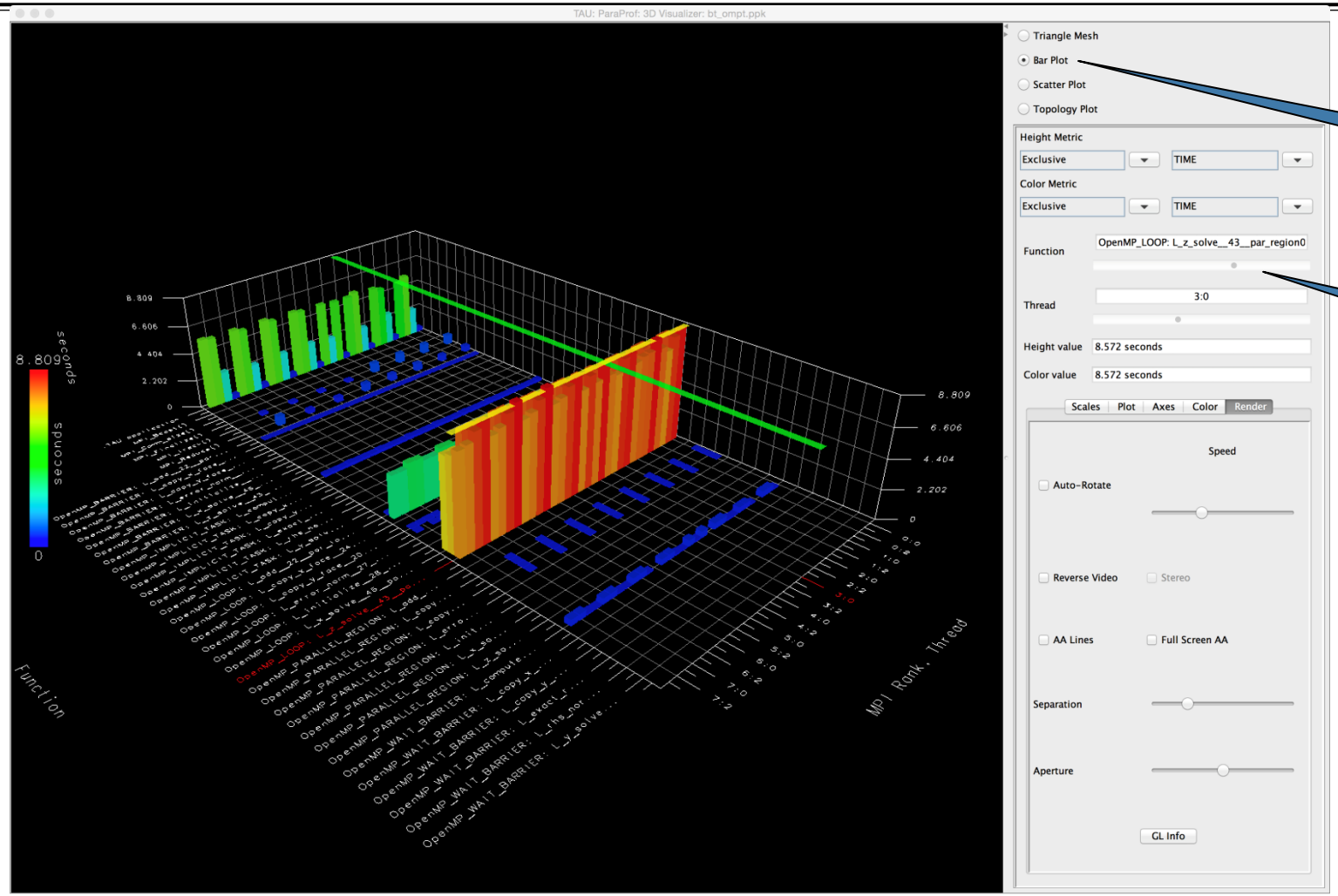


Name	Total	MeanValue	NumSamples	MinValue	MaxValue	Std. Dev.
.TAU application						
read()						
fopen64()						
fclose()						
OurMain()						
malloc size	25,235	1,097.174	23	11	12,032	2,851.143
free size	22,707	1,746.692	13	11	12,032	3,660.642
OurMain [{wrapper.py}{3}]						
read()						
malloc size	3,877	323.083	12	32	981	252.72
free size						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()						

ParaProf with Optimized Instrumentation



Paraprof 3D visualization window

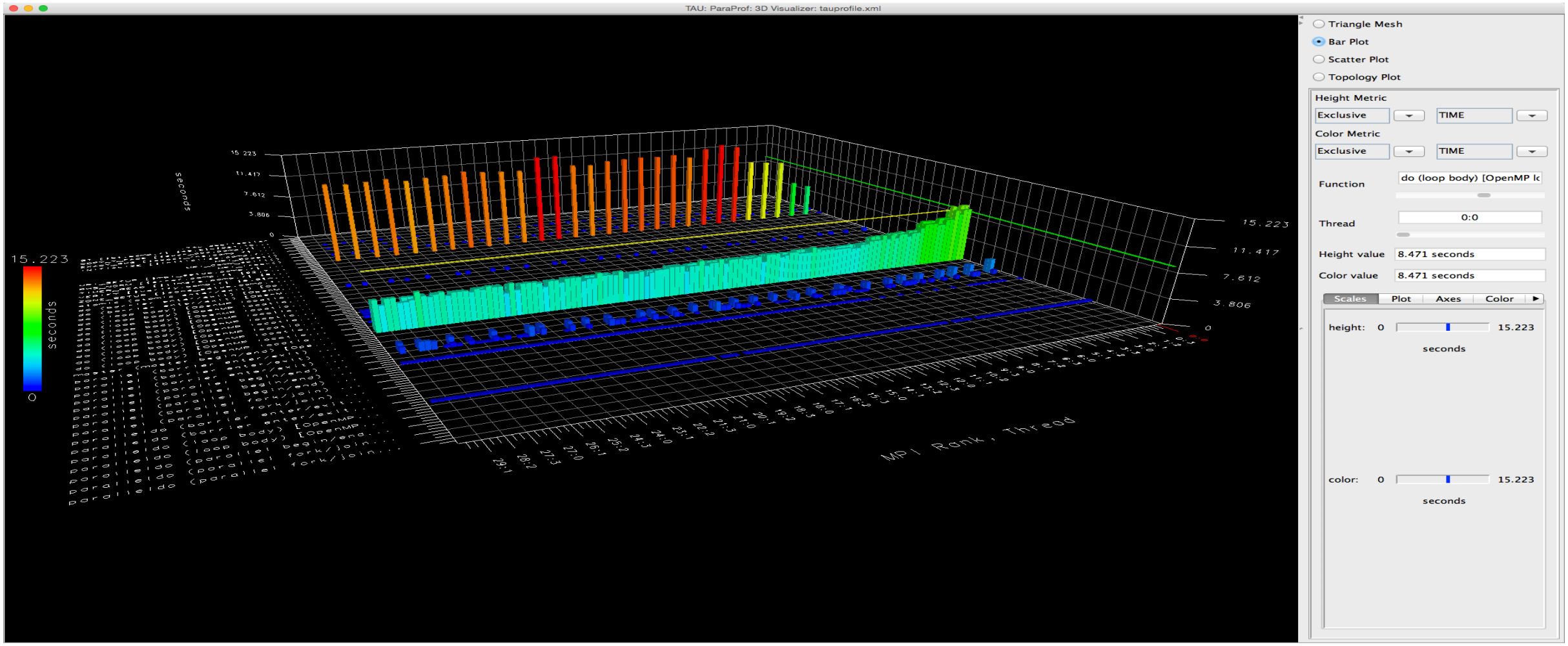


Click Bar Plot

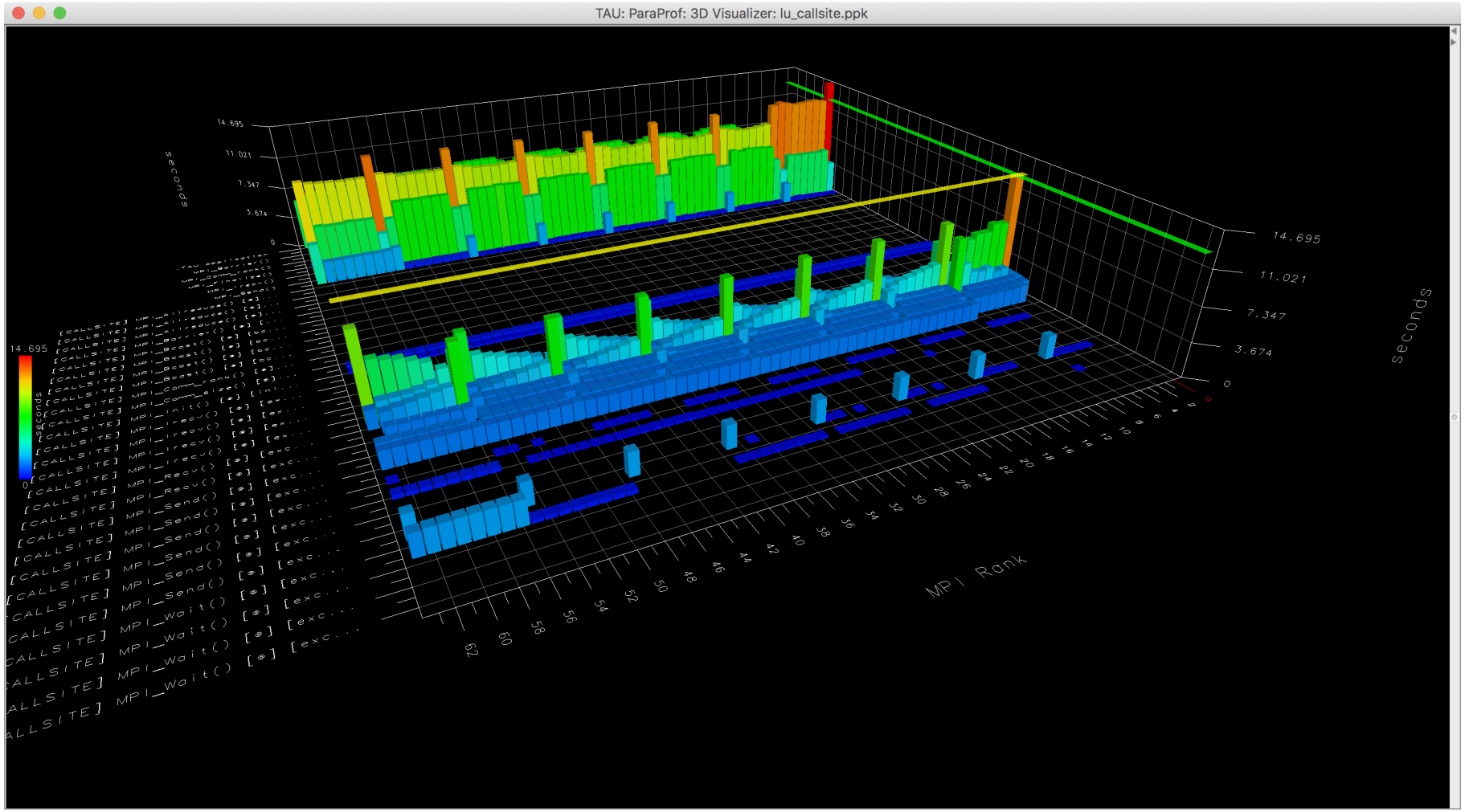
Move Function and Thread Sliders

Windows -> 3D visualization

ParaProf: 3D Visualization Window Showing Entire Profile



Callsite Profiling and Tracing



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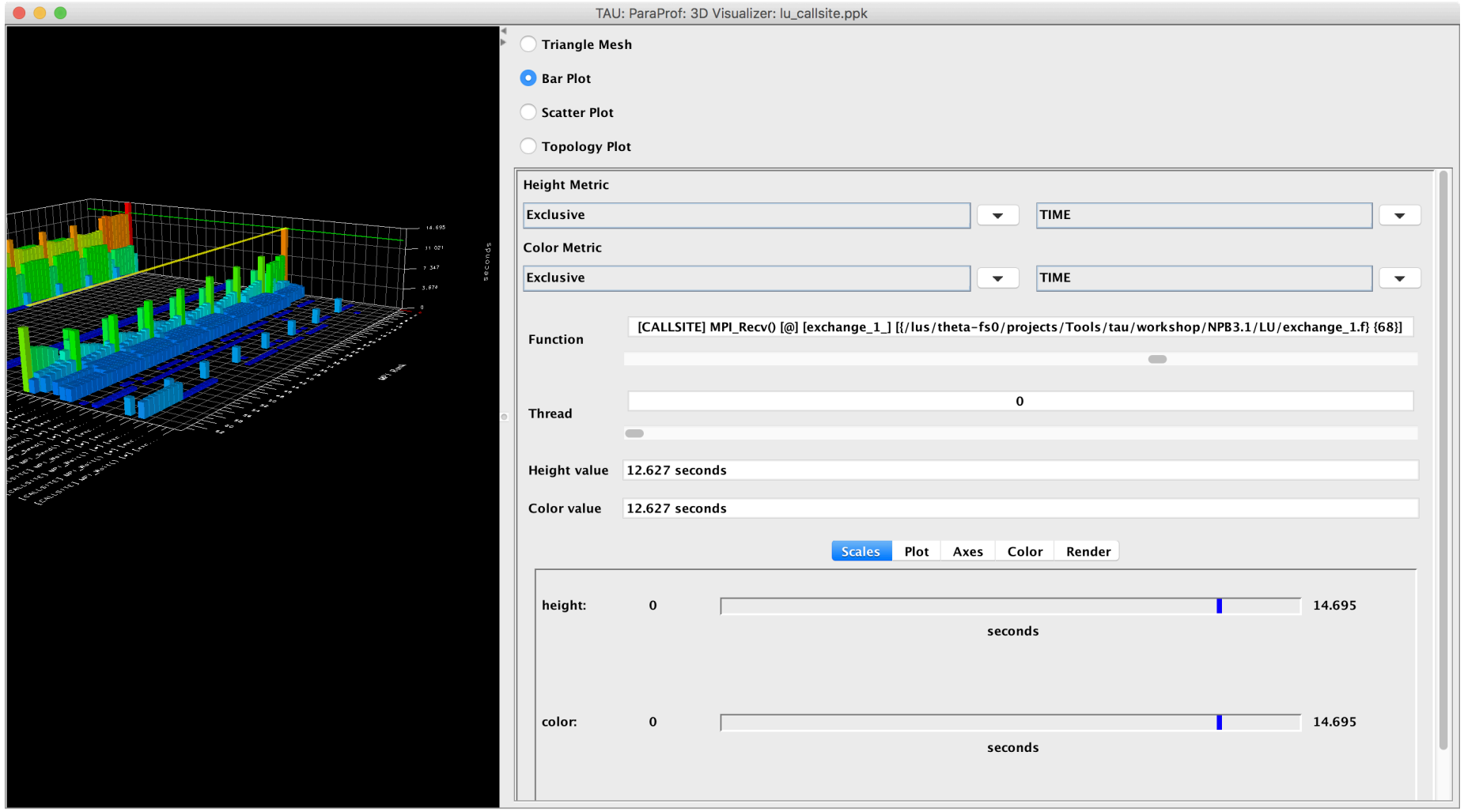
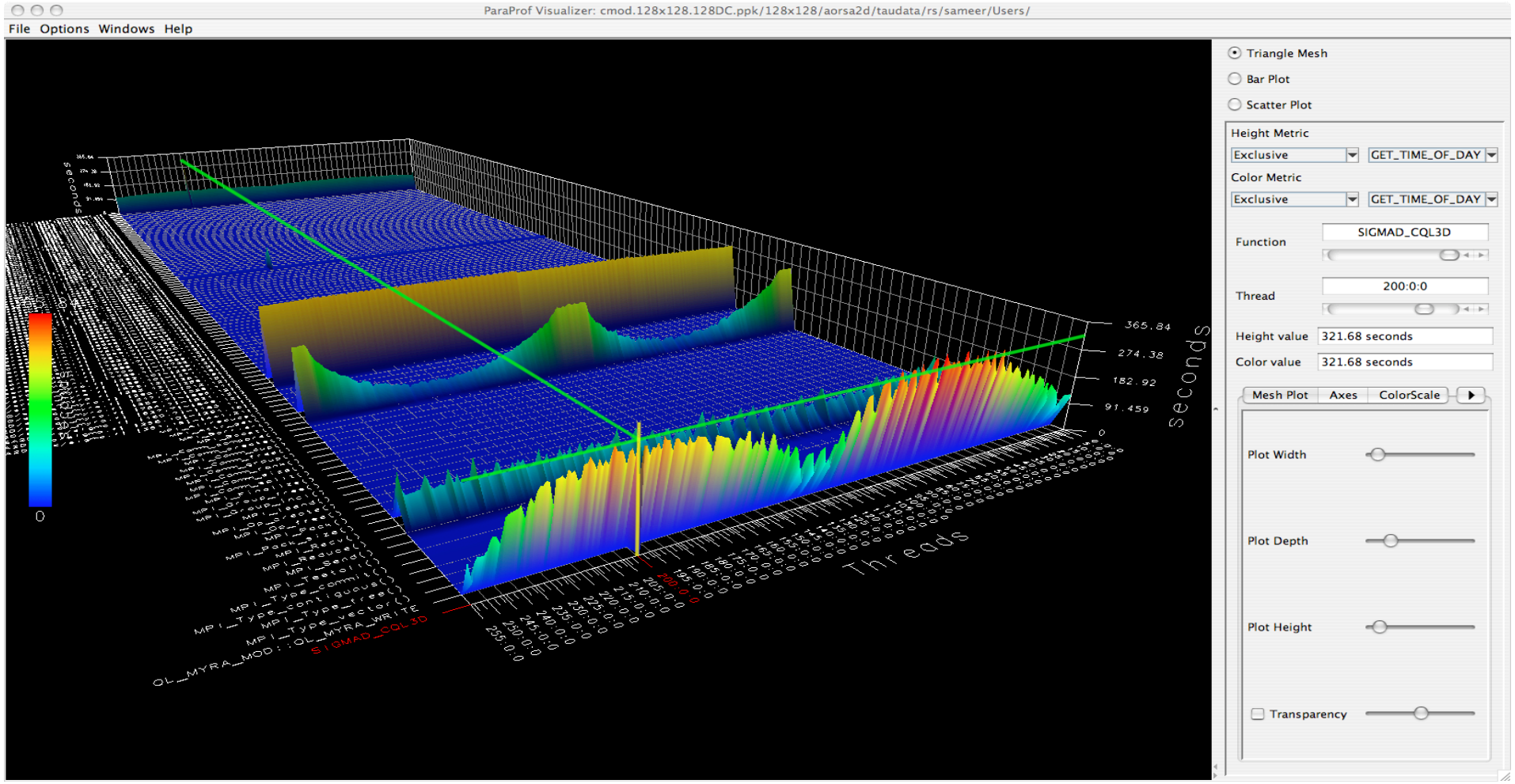
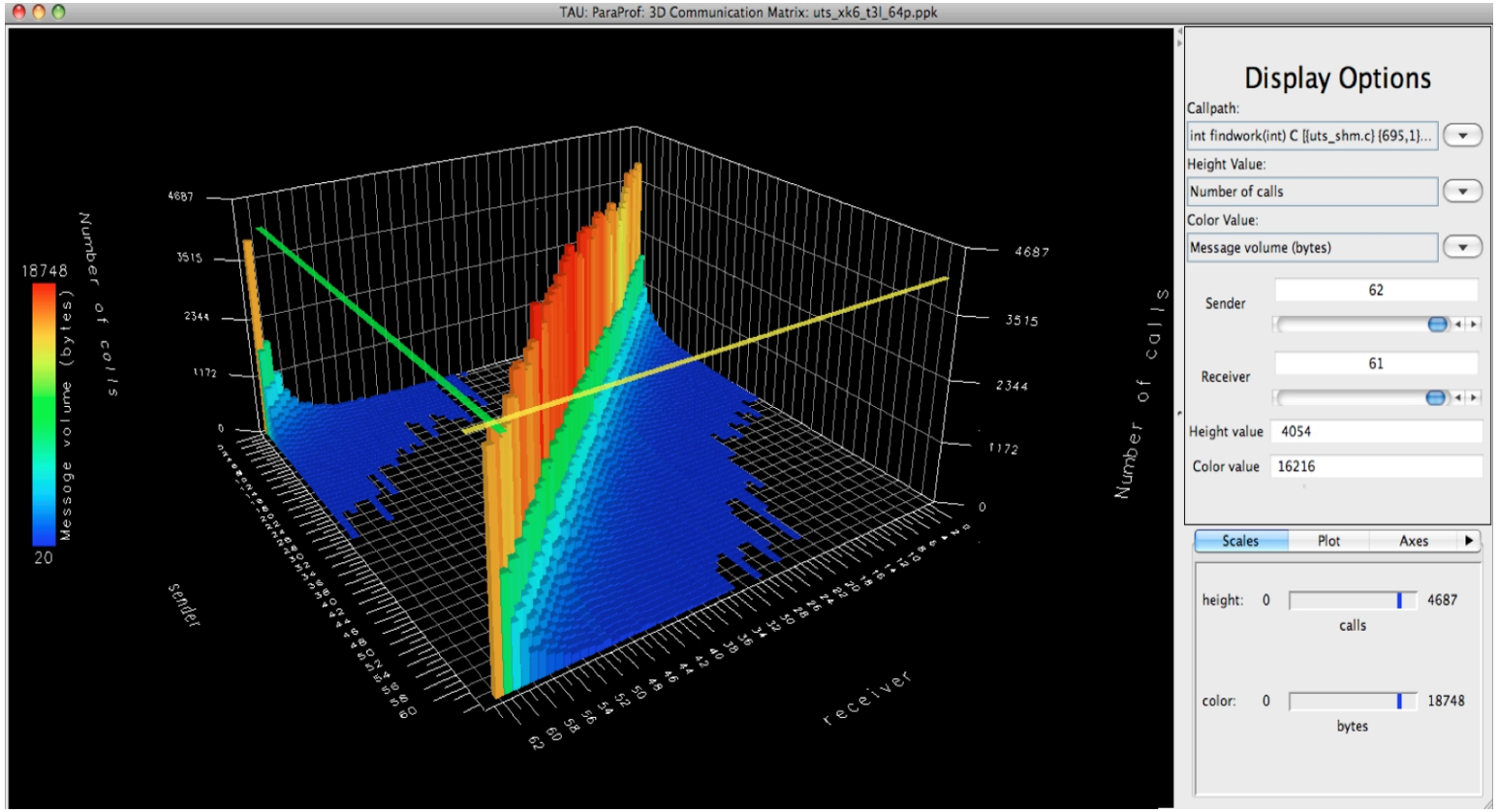


Parallel Profile Visualization: ParaProf

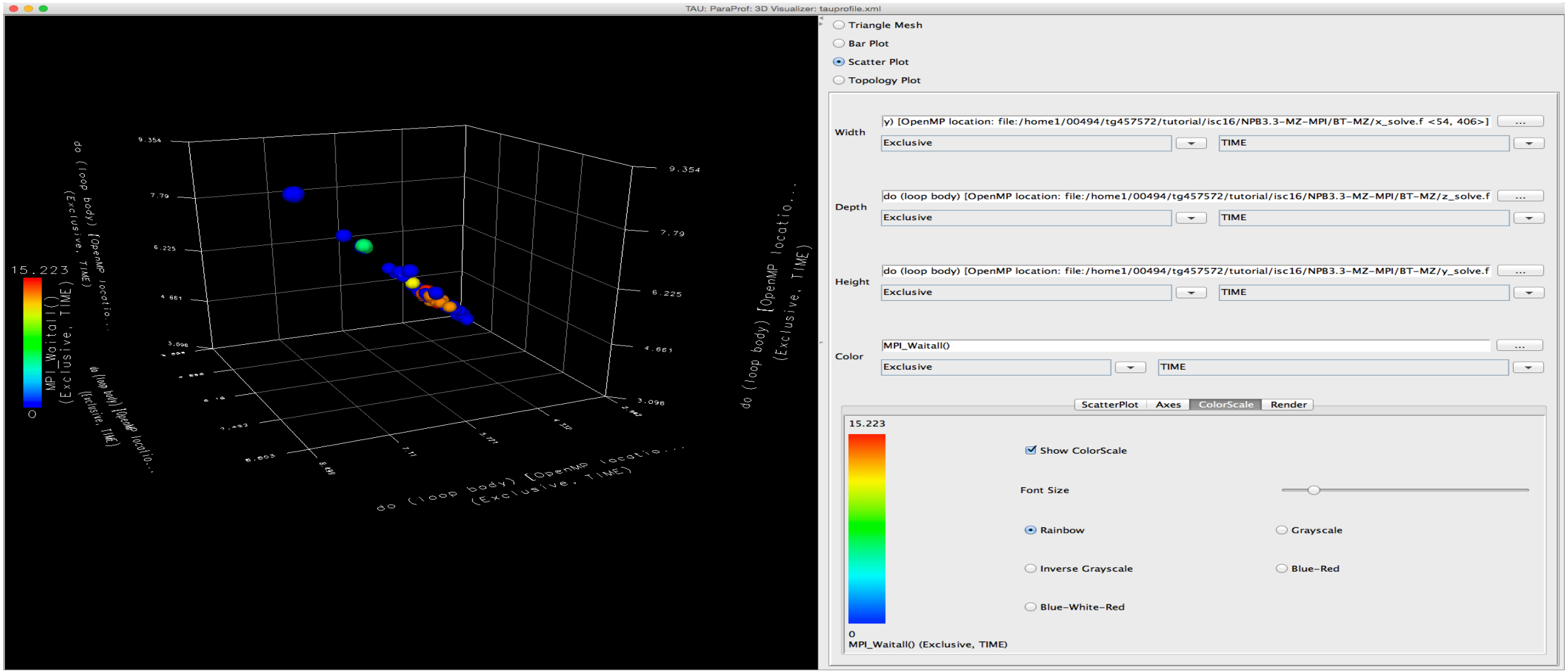


ParaProf 3D Communication Matrix

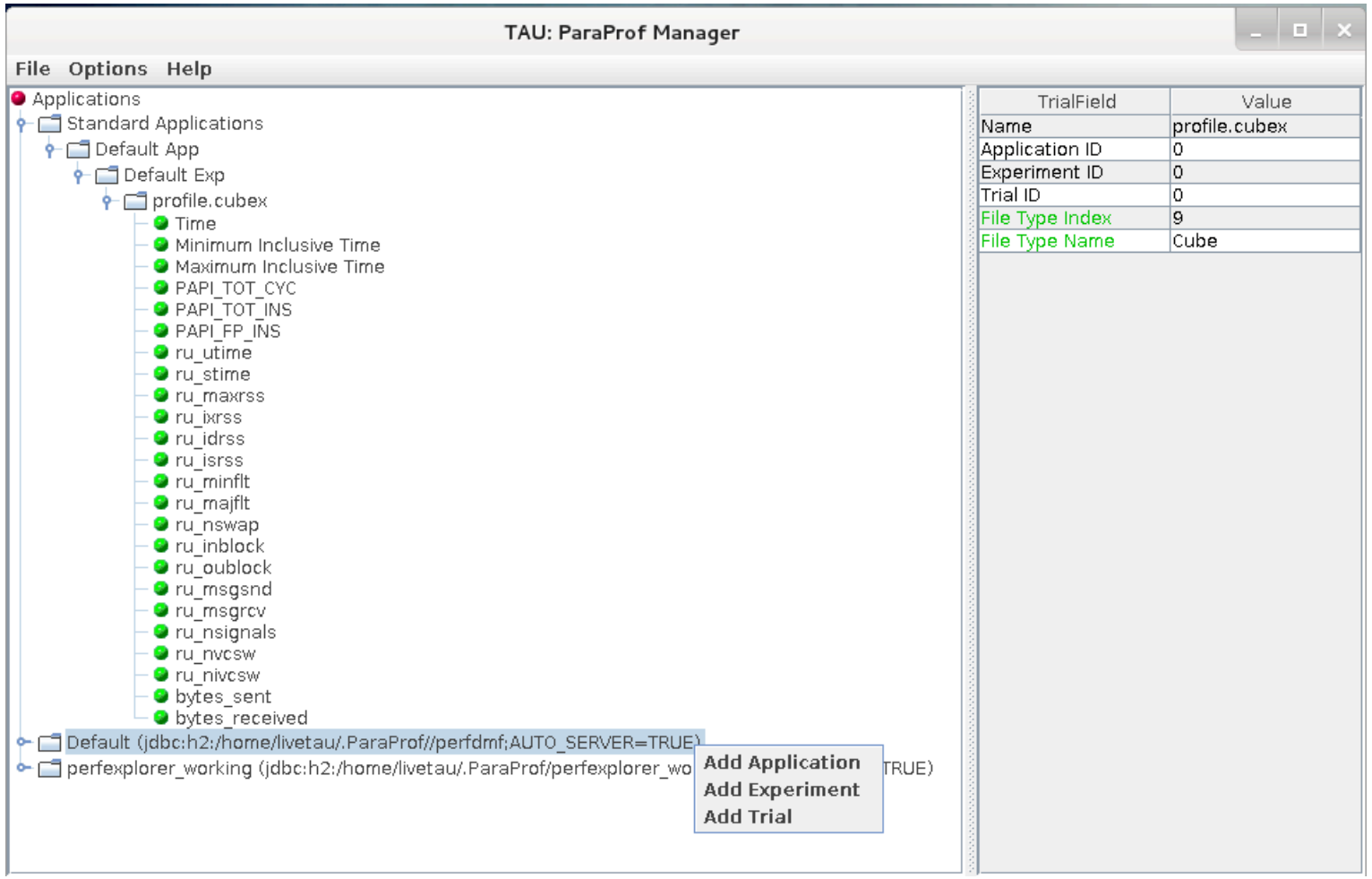


% export TAU_COMM_MATRIX=1

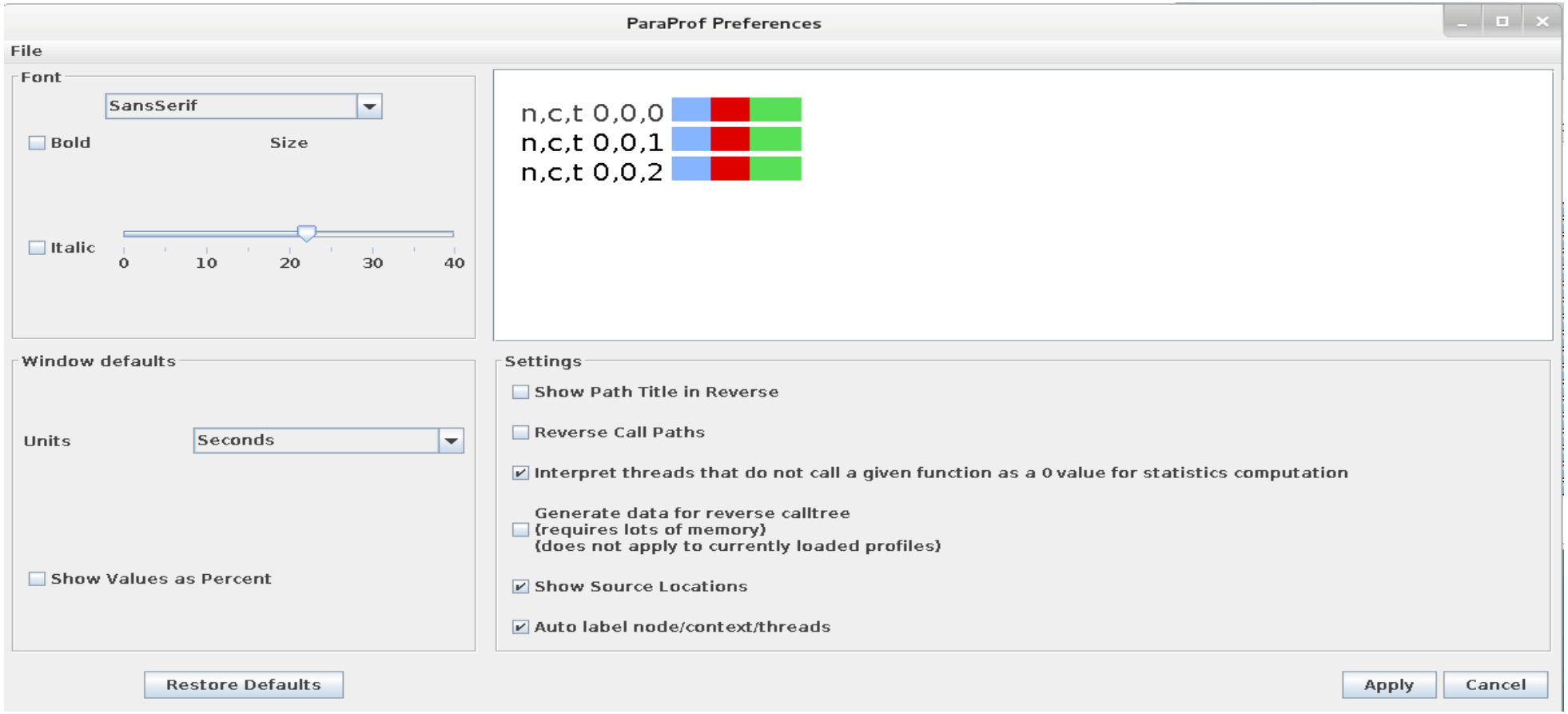
ParaProf: 3D Scatter Plot



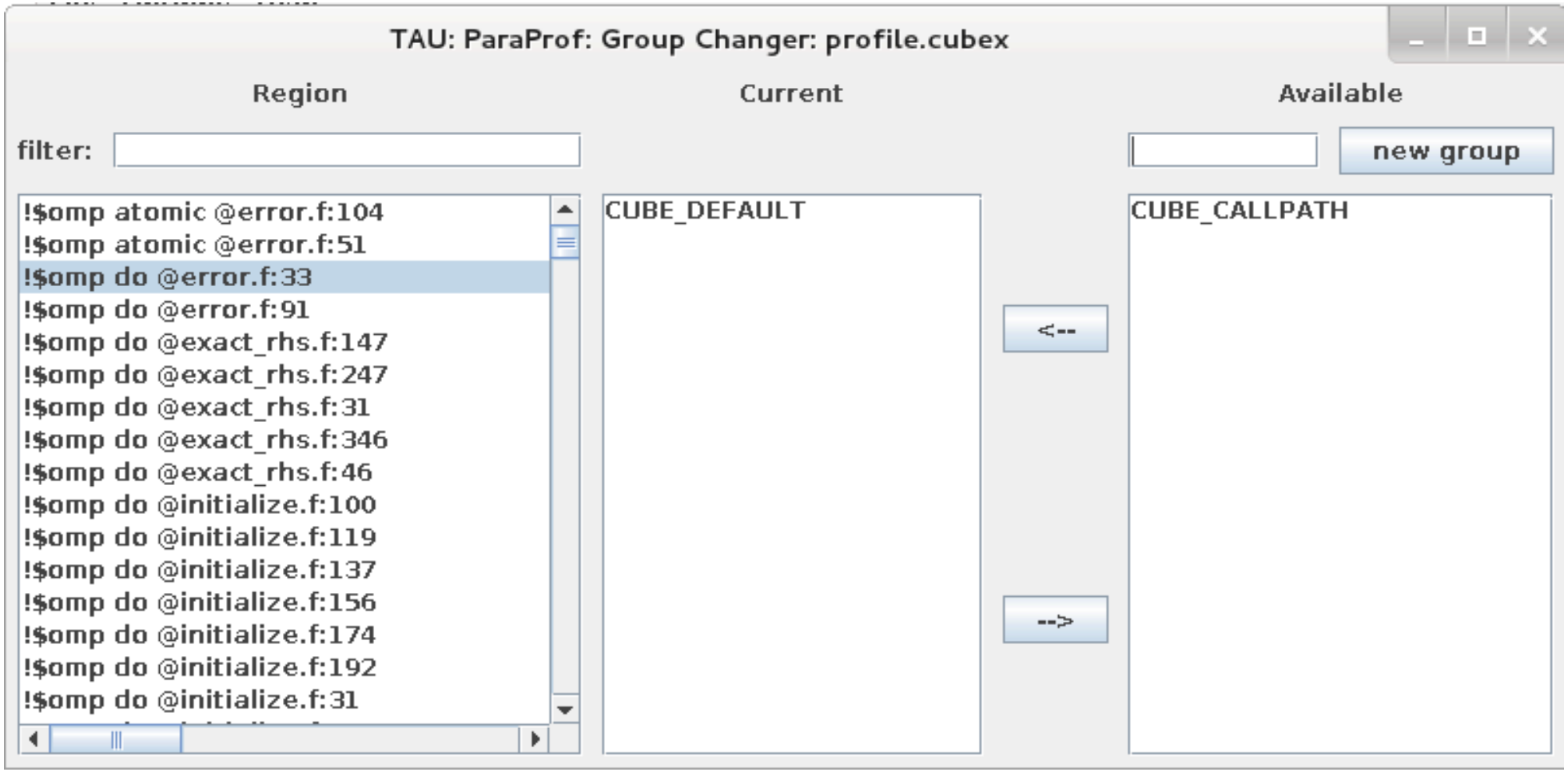
ParaProf: Score-P Profile Files, Database



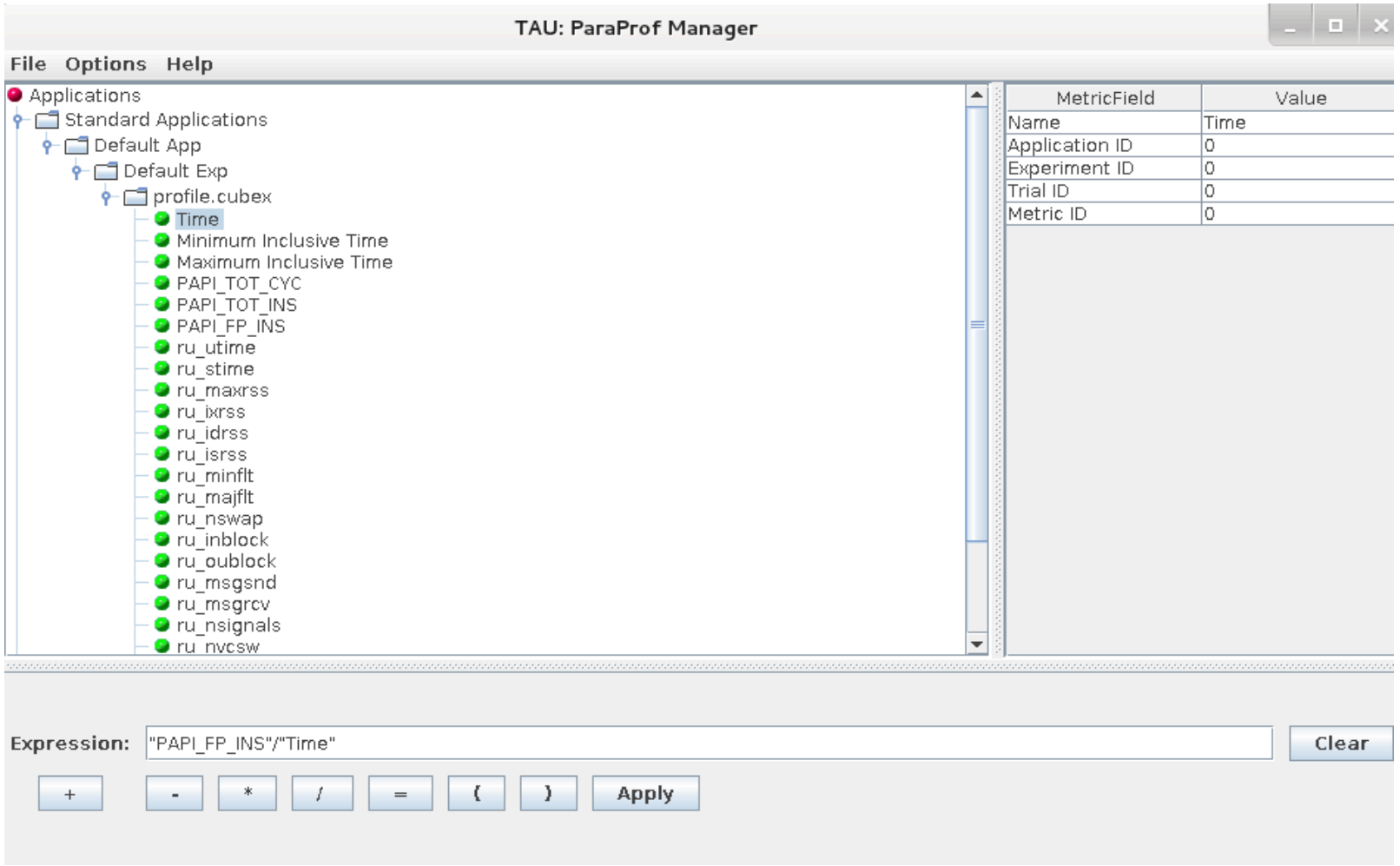
ParaProf: File Preferences Window



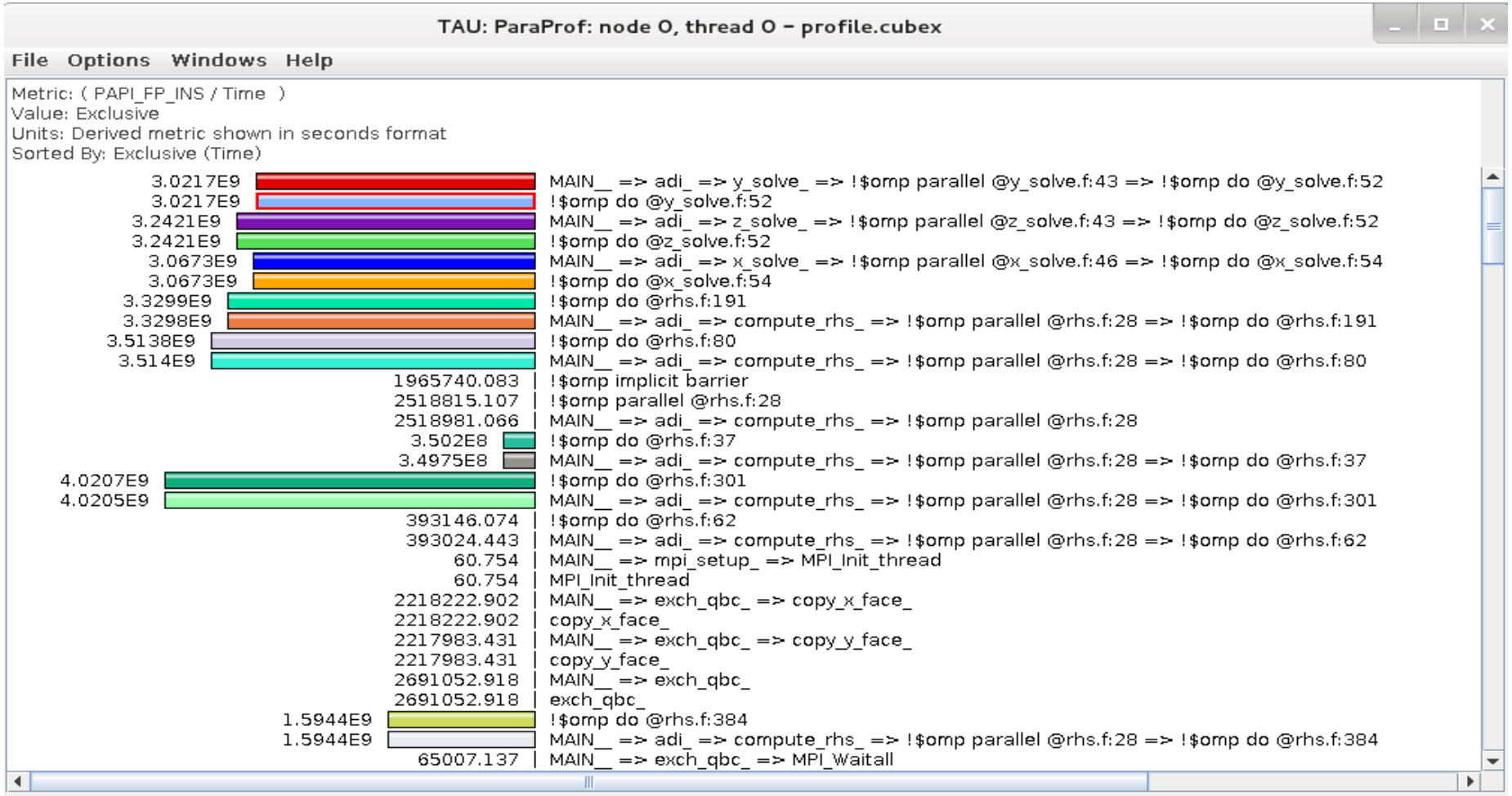
ParaProf: Group Changer Window



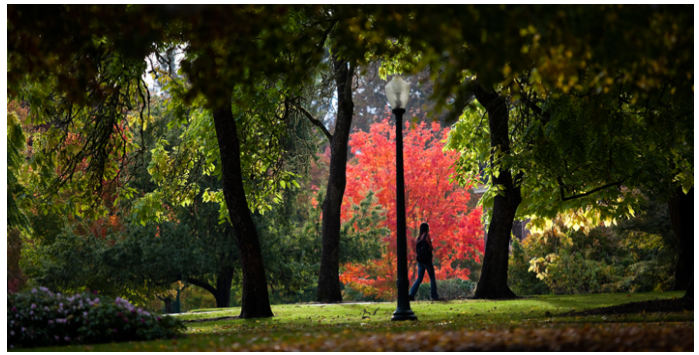
ParaProf: Derived Metric Panel in Manager Window



Sorting Derived FLOPS metric by Exclusive Time



Performance Research Lab, University of Oregon, Eugene, USA



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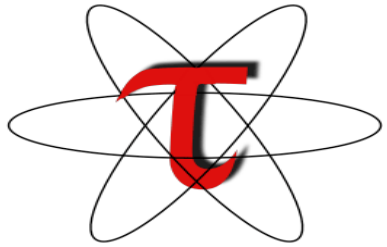

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