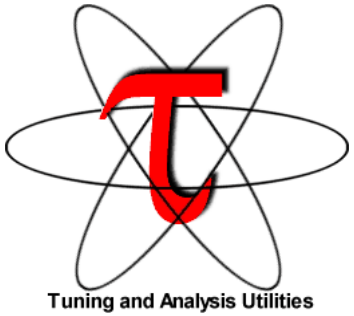

# TAU Performance System®

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# 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
  - …

# Installation (*Archer*)

- Setup preferred program environment compilers

```
% ssh -Y login.archer.ac.uk -l <USER>
% module switch PrgEnv-cray PrgEnv-gnu
% cd /work/ta002/ta002/$USER
% tar zxvf /work/ta002/ta002/shared/NPB3.3-MZ-MPI.tar.gz
% cd NPB3.3-MZ-MPI
% source /home/ta002/ta002/uosameer/pkgs/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 Jureca:
    - 2 compute nodes
    - 8 MPI processes with 6 OpenMP threads each
  - bt-mz_C.8 should run in less than 20 seconds

# 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
#---------------------------------------------------------------------------
MPIF77 = mpif77# CRAY MPICH with GNU compiler

# Alternative variant to perform instrumentation
# MPIF77= tau_f90.sh
# PREP is a generic preposition macro for instrumentation preparation
# MPIF77= $(PREP) mpif77
# MPIF77 = scorep …

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

Default (no instrumentation)

Uncomment mpif77 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=8                           *
 ***************************************************************
```

- Type "make" for instructions
- Type:
  % make suite
  to build

# Building an NPB-MZ-MPI Benchmark

```
% make bt-mz CLASS=C NPROCS=8
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 8 C
make[2]: Entering directory `../BT-MZ'
mpif77 -c  -O3 -fopenmp       bt.f
[…]
mpif77 -c  -O3 -fopenmp       mpi_setup.f
cd ../common;  mpif77  -c  -O3 -fopenmp        print_results.f
cd ../common;  mpif77  -c  -O3 -fopenmp        timers.f
mpif77 -O3 -fopenmp   -o ../bin/bt-mz_C.8 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.8
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 Archer (Cray XC30)

```
% cd bin
% cp ../jobscript/archer/run.pbs .
% qsub ./run.pbs
% less mzmpibt.o*
 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:     8
 Total number of threads:       48 (  6.0 threads/process)

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

 BT-MZ Benchmark Completed.
 Time in seconds = 19.66
```

- 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

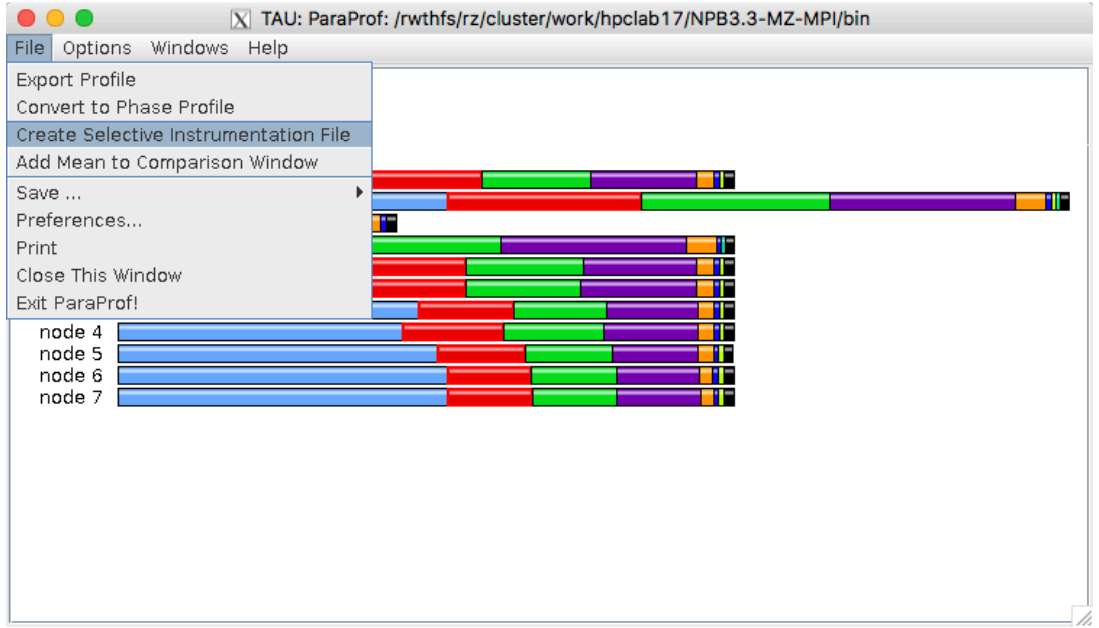
# Create selective instrumentation file

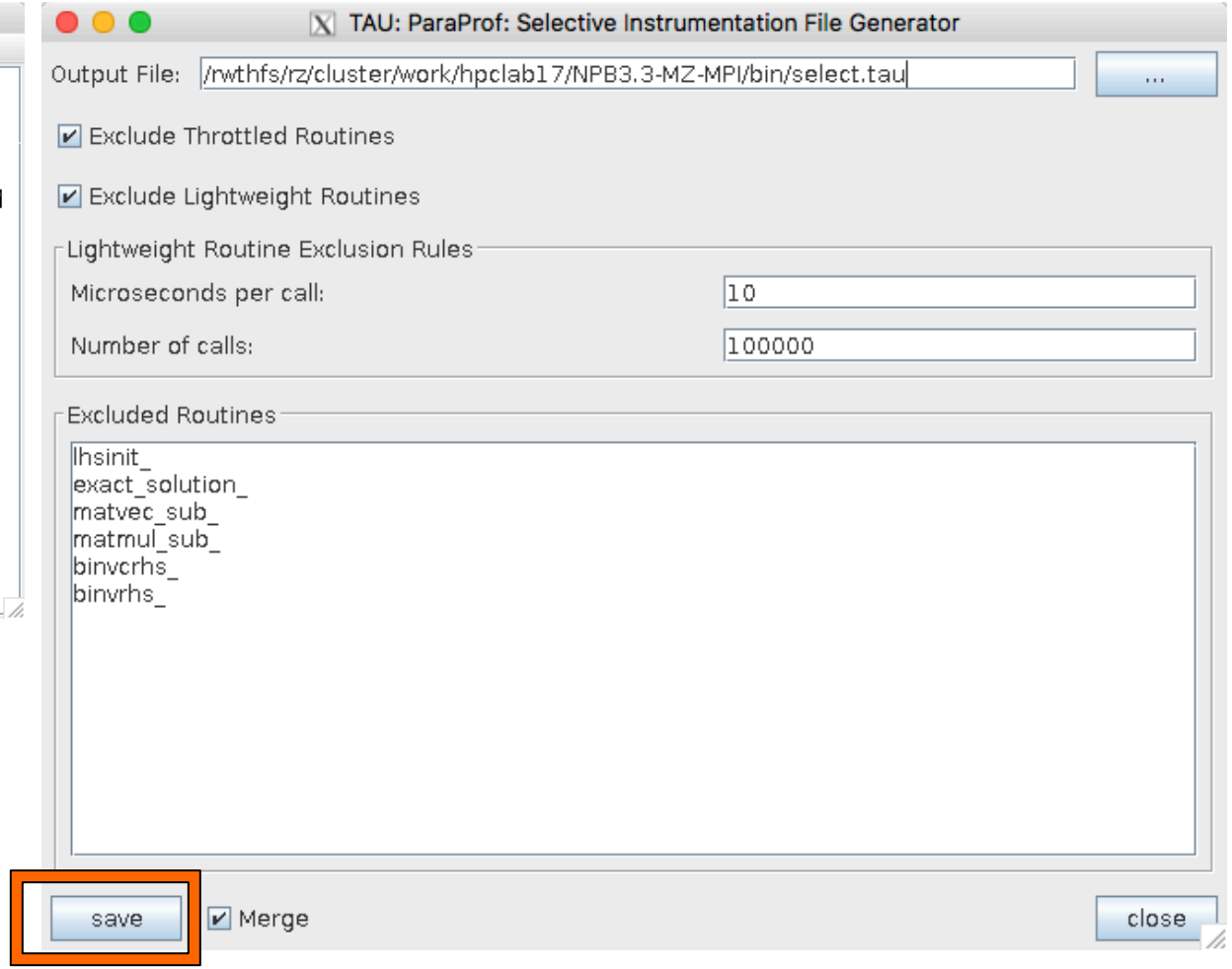
```
% source /home/ta002/ta002/uosameer/pkgs/tau.bashrc
% cd NPB3.3-MZ-MPI
% echo $TAU_MAKEFILE
/home/ta002/ta002/uosameer/pkgs/tau-2.29.1//craycnl/lib/
 Makefile.tau-gnu-papi-mpi-pdt-openmp-opari
% make suite MPIF77=tau_f77.sh
% cd bin.tau
% cp ../jobscript/archer/run.pbs  .
% qsub ./run.pbs
% pprof -a –m | more
% grep seconds mzmpibt.o*
mzmpibt.o7154184: Time in seconds =                    24.00
# To launch locally:
% paraprof
% paraprof --pack default.ppk
SCP to laptop where you may open it with:
% paraprof default.ppk
```

- 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

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




% paraprof

# 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'

- 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)
```

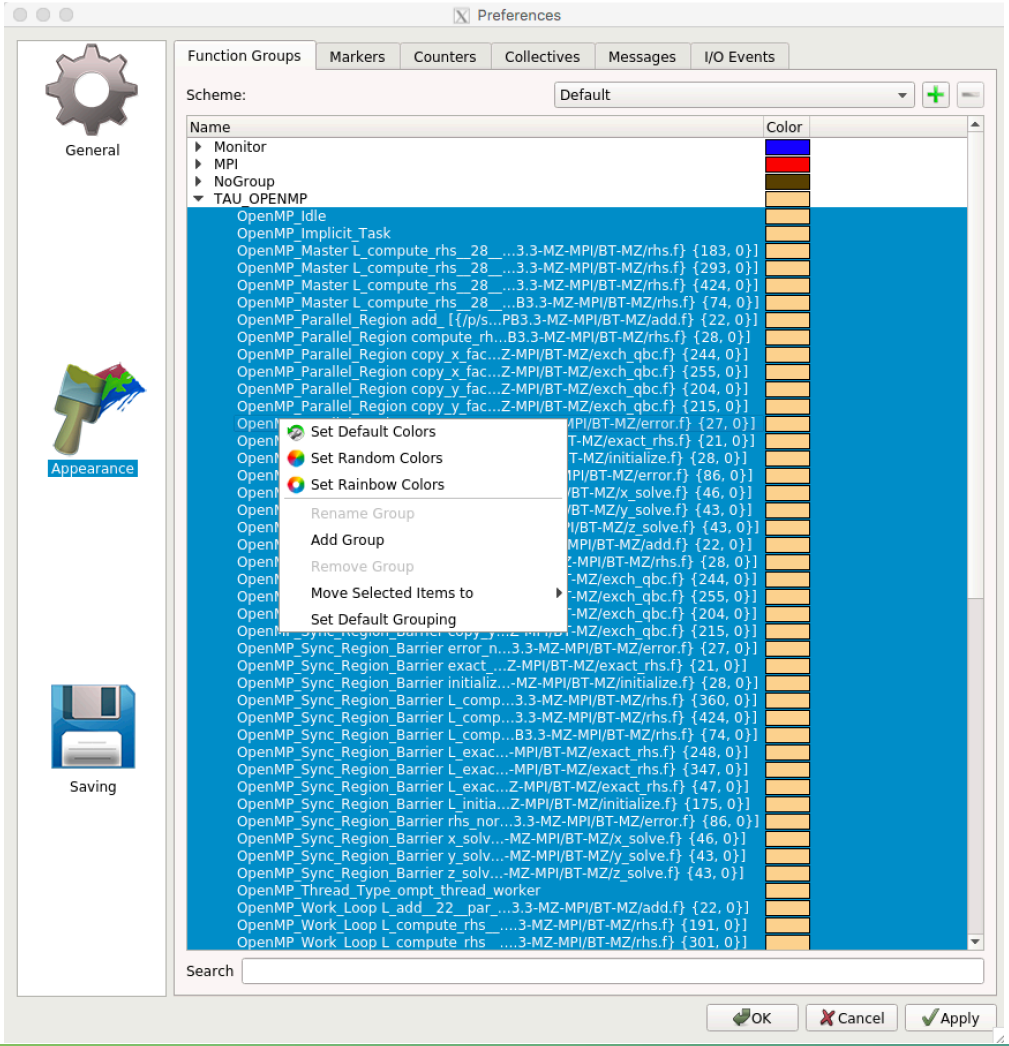
# Re-compile with selective instrumentation file, generate accurate results

```
% tau_f77.sh  | grep Select
 % setenv TAU_OPTIONS -optVerbose -optTauSelectFile=select.tau
  -optTauSelectFile="" Specify selective instrumentation file for tau_instrumentor
% export TAU_OPTIONS=' -optVerbose -optTauSelectFile=select.tau'
% cp select.tau NPB3.3-MZ-MPI/BT-MZ
% make clean
% make suite MPIF77=tau_f77.sh
% cd bin.tau
% rm prof*; qsub run.pbs
# After it runs:
% grep seconds *.o*
mzmpibt.o7154187: Time in seconds =                    20.27
% pprof -a | more
% paraprof --pack optimized.ppk
% paraprof default.ppk optimized.ppk &
```

# To generate OTF2 traces for Vampir [TU Dresden]

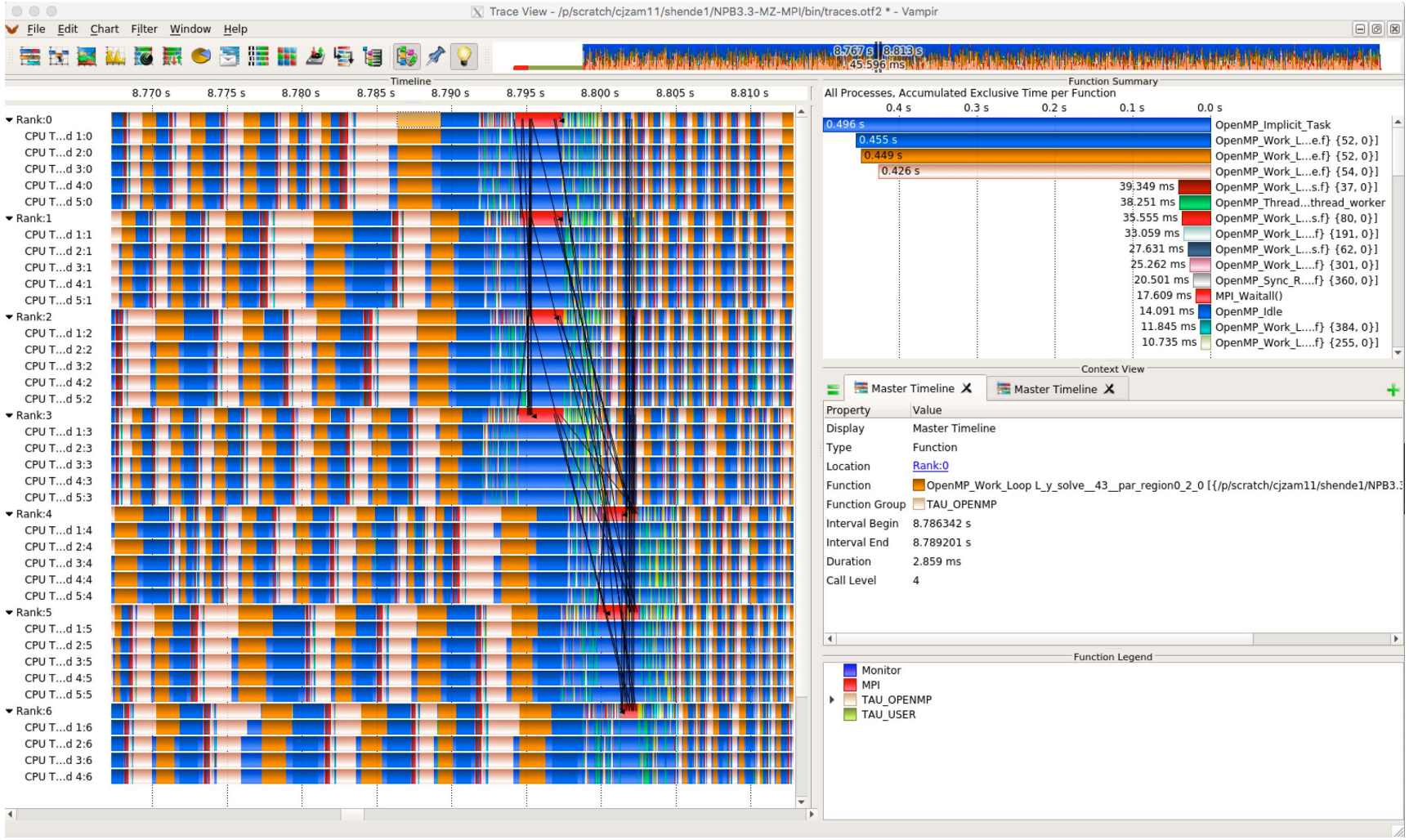
```
% vi run.pbs
#Add
export TAU_TRACE=1
export TAU_TRACE_FORMAT=otf2
# before aprun
% qsub run.pbs
# Copy over the traces* to a host that has Vampir:
% vampir traces.otf2
```

# Change Colors for Events in Vampir [TU Dresden]




- File -> Preferences -> Appearance
- Multi-select functions under TAU_OPENMP
- Select “Set Random Colors”
- Click Apply, OK

# Vampir [TU Dresden] Provides a Timeline Display




TAU generates OTF2 traces

% cat run.pbs
…
export TAU_TRACE=1
export TAU_TRACE_FORMAT=otf2

# 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 |

# Performance Research Lab, University of Oregon, Eugene, USA

# Support Acknowledgments


- US Department of Energy (DOE)
  - Office of Science contracts, ECP
  - SciDAC, LBL contracts
  - LLNL-LANL-SNL ASC/NNSA contract
  - Battelle, PNNL contract
  - ANL, ORNL contract
- Department of Defense (DoD)
  - PETTT, HPCMP
- National Science Foundation (NSF)
  - Glassbox, SI-2
- NASA
- CEA, France
- Partners:
  - University of Oregon
  - ParaTools, Inc., ParaTools, SAS
  - The Ohio State University
  - University of Tennessee, Knoxville
  - T.U. Dresden, GWT
  - Juelich Supercomputing Center











ParaTools



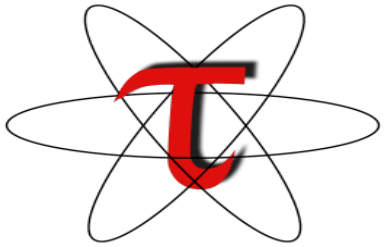





# Acknowledgement

This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation's exascale computing imperative.

# Download TAU from U. Oregon



**http://tau.uoregon.edu**

**http://www.hpclinux.com [LiveDVD, OVA]**

**https://e4s.io [Containers for Extreme-Scale Scientific Software Stack]**

**Free download, open source, BSD license**