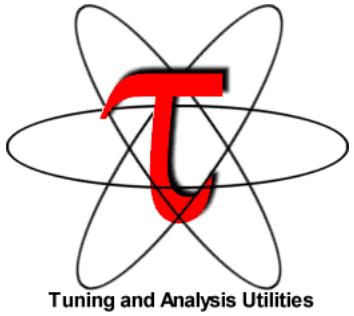
VI-HPS

TAU Performance System®
Hands-On



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BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación Lawrence Livermore National Laboratory TECHNISCHE UNIVERSITÄT DARMSTADT TUM Technische Universität München UNIVERSITY OF OREGON THE UNIVERSITY of TENNESSEE

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 (*Wrangler, TACC*)

- Setup preferred program environment compilers

```
% ssh -Y <login>@wrangler.tacc.utexas.edu
% source ~tg457572/tau.bashrc
% cp ~tg457572/pkgs/tar/NPB3.3-MZ-MPI.tar.gz $WORK;

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

For PerfExplorer:

```
% cp ~tg457572/pkgs/tar/data.tgz. ; tar zxf data.tgz; cd data
% cat README; cd tau; ./upload.sh; perfexplorer &
  and follow the steps
```

Local Installation (*Stampede2, TACC*)

- Setup preferred program environment compilers

```
% ssh -Y <login>@stampede2.tacc.utexas.edu
% source ~tg828282/Tutorial/vihps-intel.sh

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

For PerfExplorer:

```
% cp ~tg457572/pkgs/tar/data.tgz. ; tar zxf data.tgz; cd data
% cat README; cd tau; ./upload.sh; perfexplorer &
  and follow the steps
```

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.32 should run in less than 30 seconds

Compiler and MPI modules (On Wrangler, TACC)

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

```
. ~tg457572/tau.bashrc
```

- Copy tutorial sources to your scratch directory

```
% cd $WORK
% tar zxvf ~tg457572/pkgs/tar//NPB3.3-MZ-MPI.tar.gz
% cd NPB3.3-MZ-MPI
```

Compiler and MPI modules (On Stampede2, TACC)

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

```
. ~tg828282/Tutorial/vihps-intel.sh
```

- Copy tutorial sources to your scratch directory

```
% cd $SCRATCH
% tar zxvf ~tg828282/Tutorial/NPB3.3-MZ-MPI.tar.gz
% cd NPB3.3-MZ-MPI
```

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 # OpenMPI with Intel compiler
MPIF77 = mpif77
# Alternative variant to perform instrumentation
# MPIF77 = tau_f90.sh
# PREP is a generic preposition macro for instrumentation preparation
#MPIF77 = $(PREP) mpif77 -f77=ifort
#MPIF77 = scorep …
...
```

Default (no instrumentation)

Uncomment MPIF77 and comment Score-P's compiler wrapper to generate uninstrumented binary!

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

Building an NPB-MZ-MPI Benchmark (Wrangler)

```
% make bt-mz CLASS=B 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 B
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_B.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_B.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=**32**
  - the benchmark class (S, W, A, B, C, D, E): CLASS=**C**

Shortcut: % **make suite**

NPB-MZ-MPI / BT reference execution (Wrangler)

```
% cd bin
% cp ../jobscript/wrangler/reference.sbatch .
% less reference.sbatch
% sbatch reference.sbatch
% less mzmpibt.o<job_id>
 NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:   8 x   8
 Iterations: 200    dt:   0.000300
 Number of active processes:    16
 Use the default load factors with threads
 Total number of threads:     64  (  4.0 threads/process)
 Calculated speedup =     62.56
 Time step    1
 Time step   20
  [...]
 Time step  180
 Time step  200
 Verification Successful

 BT-MZ Benchmark Completed.
 Time in seconds = 5.45
```

- 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 (Stampede2)

```
% cd bin
% cp ../jobscript/stampede2/reference.sbatch .
% less reference.sbatch
% sbatch reference.sbatch
% 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 OMPT replacement library (tau_exec –T ompt)

```
% cd bin
% cp ../jobscript/stampede2/tau.sbatch .
% sbatch ./tau.sbatch
% cat mzmpibt.o<job_id>
 NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:   8 x   8
 Iterations: 200    dt:   0.000300
 Number of active processes:    16
 Use the default load factors with threads
 Total number of threads:     64  (  4.0 threads/process)
 Calculated speedup =     62.56
 Time step    1
 Time step   20
  [...]
 Time step  180
 Time step  200
 Verification Successful

 BT-MZ Benchmark Completed.
 Time in seconds = 5.45
% 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 Sampling (tau_exec –ompt -ebs)

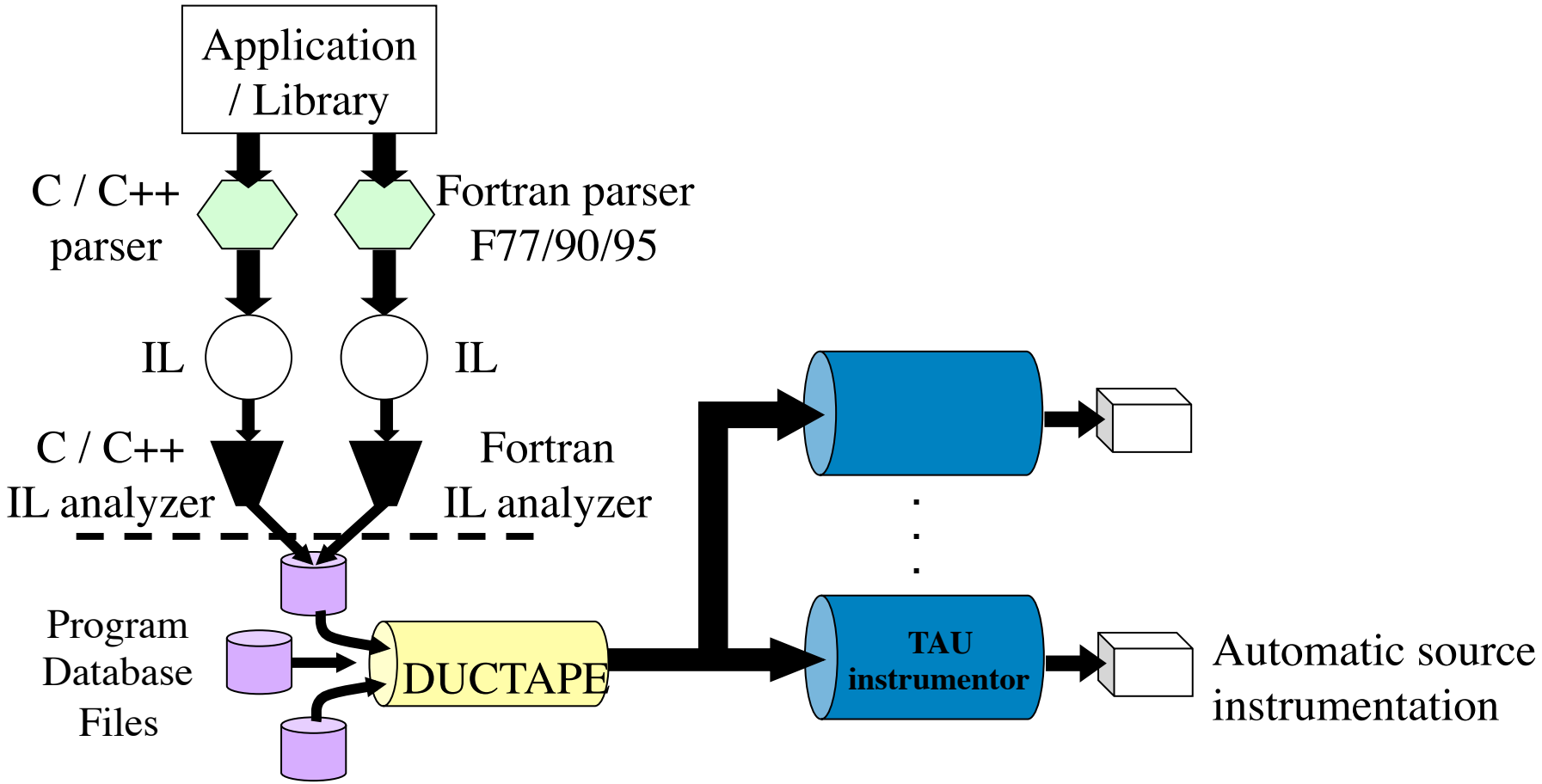
```
% cd bin
% cp ../jobscript/stampede2/tau.sbatch .
# Uncomment the -ebs line at the end and
% sbatch ./tau.sbatch
% cat mzmpibt.o<job_id>
 NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:  16 x  16
 Iterations:  200   dt:   0.000100
 Number of active processes:    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 = 24
% 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!

TAU's Source Instrumentation

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



Source instrumentation using TAU

```
Uncomment the MPIF77 line for TAU in config/make.def
% vi config/make.def
MPIF77 = mpiifort

# Alternative variants to perform instrumentation
#MPIF77 = psc_instrument -t user,mpi,omp -s ${PROGRAM}.sir  mpiifort
#MPIF77 = scalasca -instrument  mpiifort
#MPIF77 = tau_f90.sh -tau_makefile=/home/00494/tg457572/pkgs/tau_latest/x86_64/lib/Makefile.tau-icpc-ompt-tr6
#MPIF77 = vtf77 -vt:hyb -vt:f77  mpiifort

% make clean; make suite
% cd bin.tau
% cp ../jobscript/tau.sbatch .
% sbatch tau.sbatch
% paraprof &
OR

% paraprof --pack bt.ppk
(scp bt.ppk to your laptop and use paraprof locally)
You may install from http://tau.uoregon.edu/tau.dmg or tau.exe
% paraprof bt.ppk
```

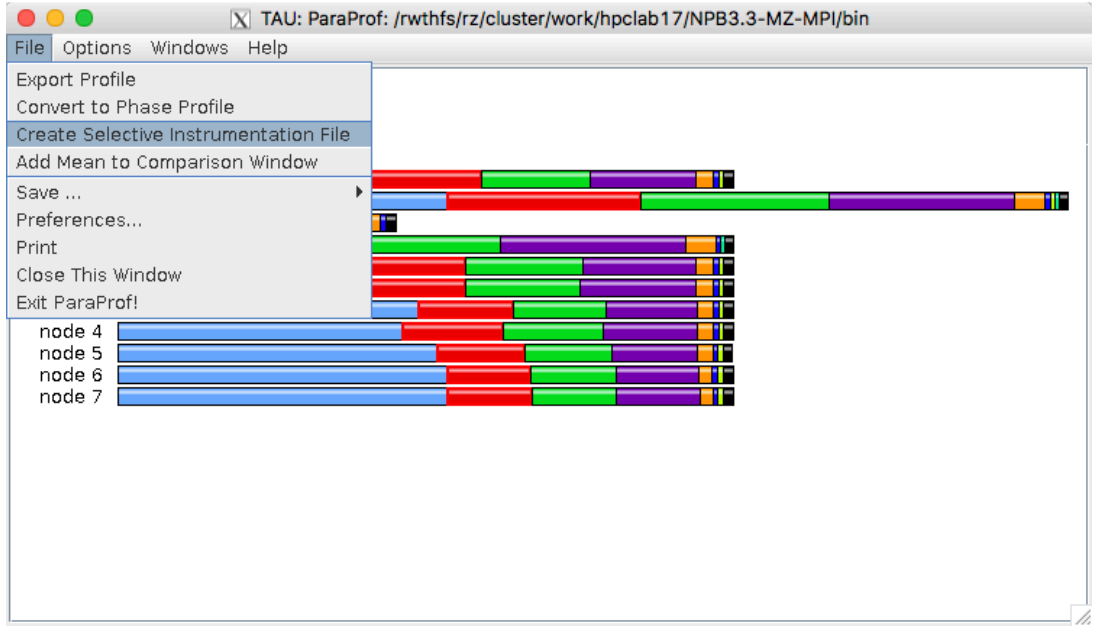
- Copy jobscript and launch as a hybrid MPI+OpenMP application

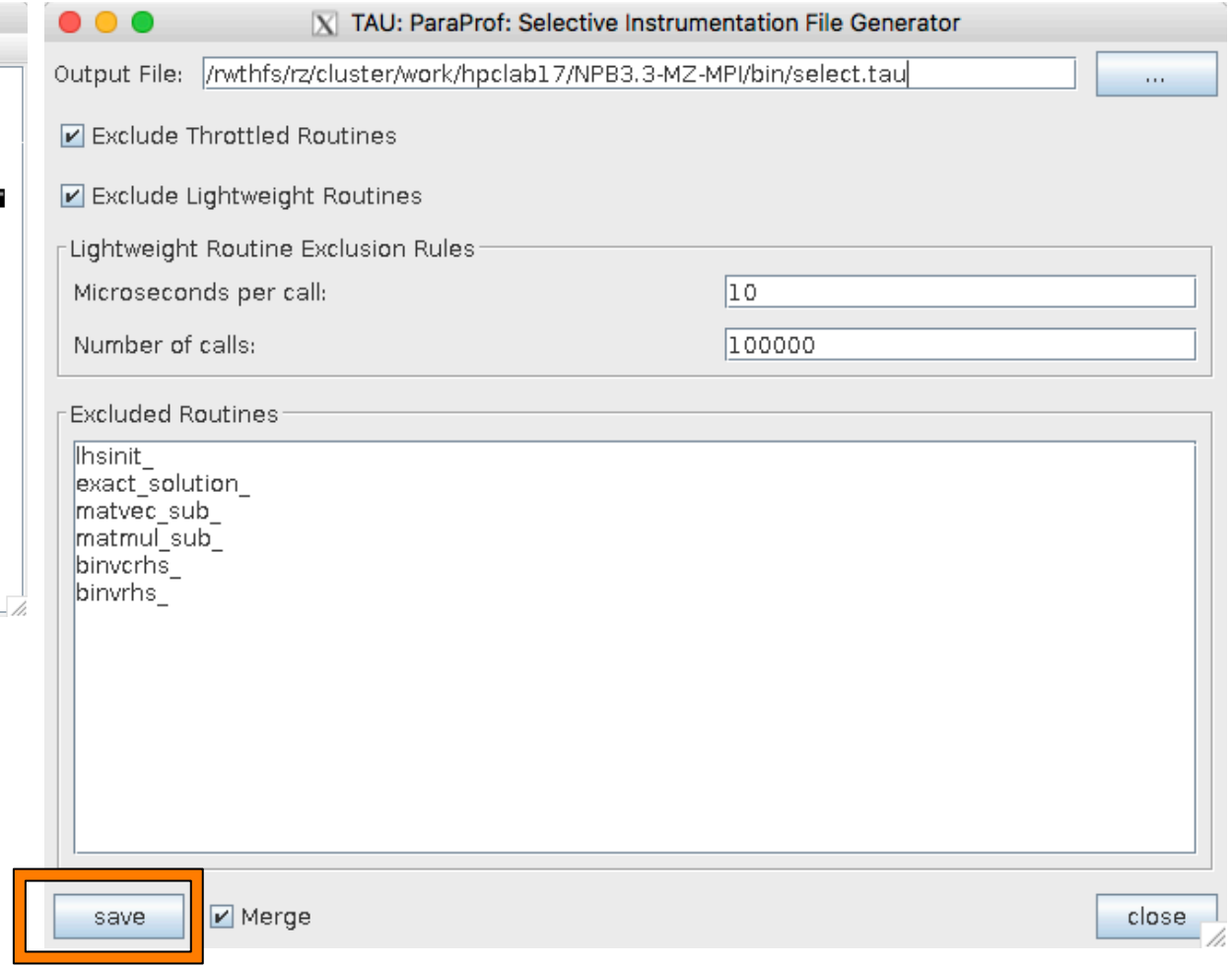
Hint: save the benchmark output (or note the run time) to be able to refer to it later

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

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

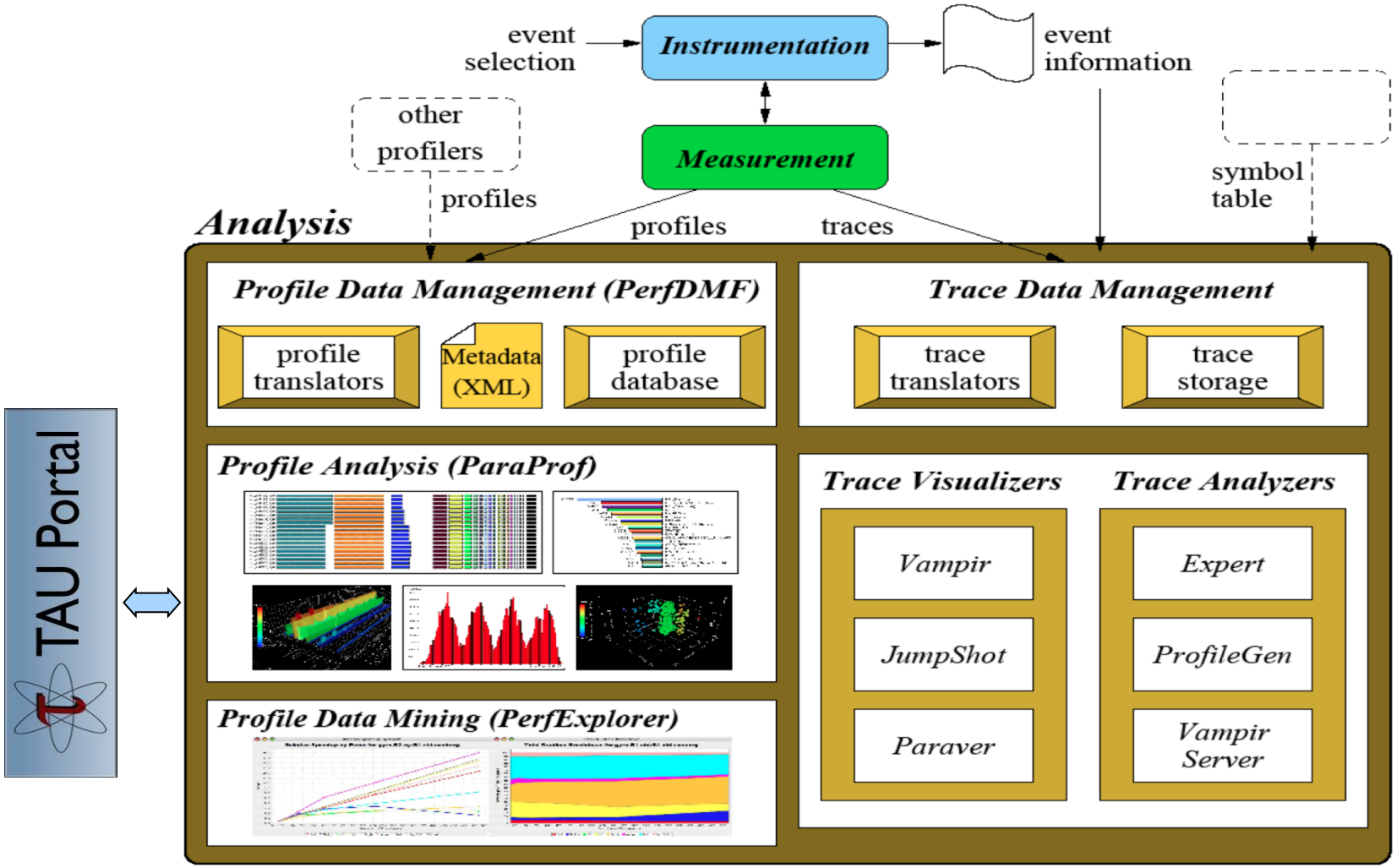
Environment Variable	Default	Description
TAU_TRACE	0	Setting to 1 turns on tracing
TAU_TRACE_FORMAT	Default	Setting to “otf2” turns on TAU’s native OTF2 trace generation (configure with –otf=download)
TAU_EBS_UNWIND	0	Setting to 1 turns on unwinding the callstack during sampling (use with tau_exec –ebs 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

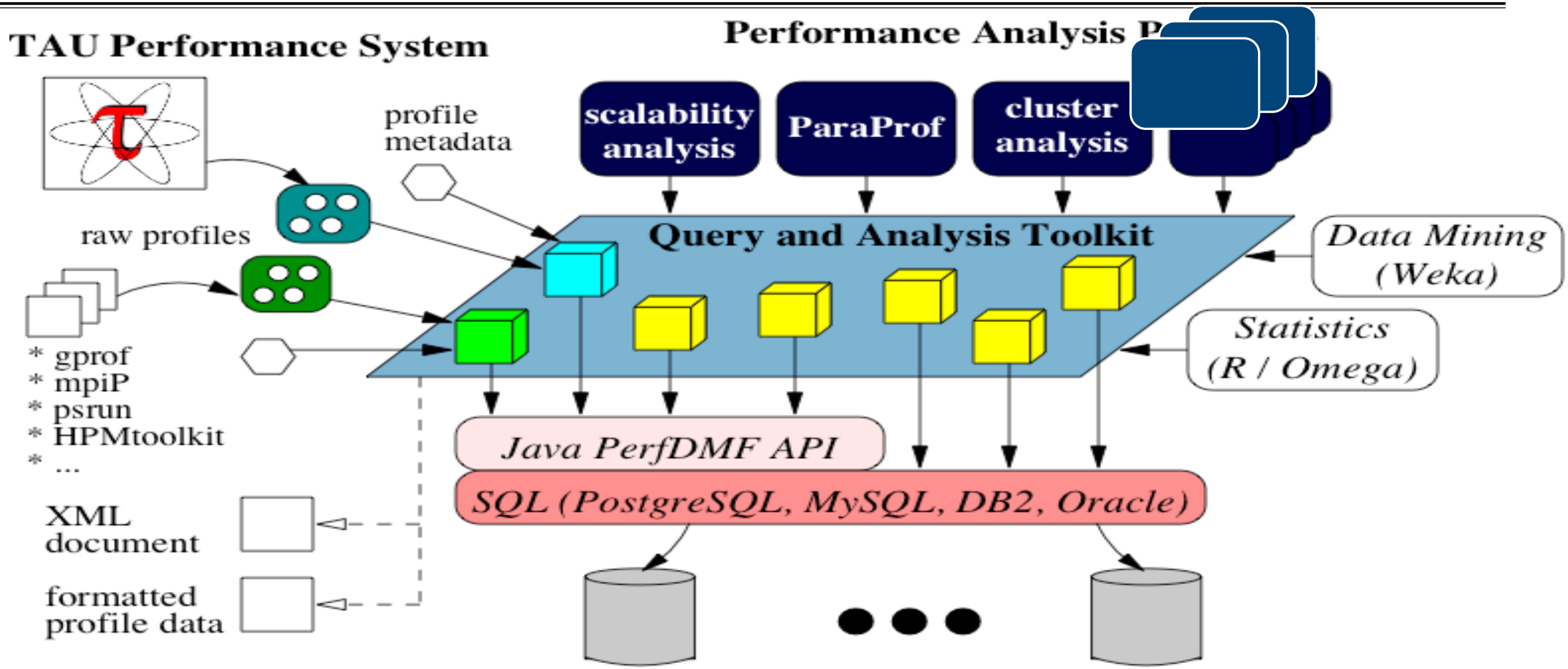
Environment Variable	Default	Description
TAU_TRACK_MEMORY_LEAKS	0	Tracks allocates that were not de-allocated (needs –optMemDbg or tau_exec –memory)
TAU_EBS_SOURCE	TIME	Allows using PAPI hardware counters for periodic interrupts for EBS (e.g., TAU_EBS_SOURCE=PAPI_TOT_INS when TAU_SAMPLING=1)
TAU_EBS_PERIOD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

TAU Analysis



TAUdb: Performance Data Management Framework



Using TAUdb

- Configure TAUdb (Done by each user)

  % taudb_configure --create-default
  - Choose derby, PostgreSQL, MySQL, Oracle or DB2
  - Hostname
  - Username
  - Password
  - Say yes to downloading required drivers (we are not allowed to distribute these)
  - Stores parameters in your ~/.ParaProf/taudb.cfg file
- Configure PerfExplorer (Done by each user)

  % perfexplorer_configure
- Execute PerfExplorer

  % perfexplorer

Local Installation (*Stampede2*)

- Setup preferred program environment compilers

```
% . ~tg828282/Tutorial/vihps-intel.sh
% cp ~tg457572/pkgs/tar/data.tgz . ; tar zxf data.tgz
% cd data
% cat README
  and follow the steps
% cd tau
% ./upload.sh
% perfexplorer
```

Local Installation (*Wrangler, Stampede*)

- Setup preferred program environment compilers

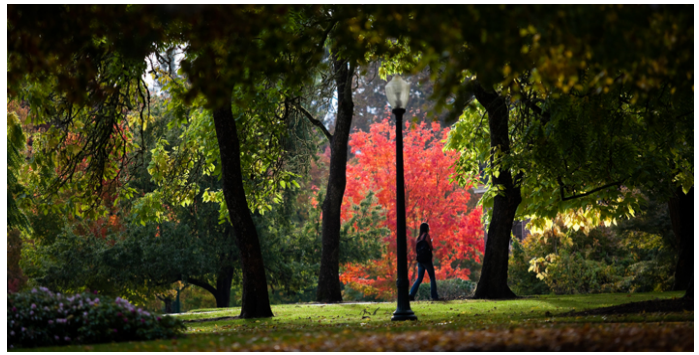
```
% source ~tg457572/tau.bashrc
% cp ~tg457572/pkgs/tar/data.tgz . ; tar zxf data.tgz
% cd data
% cat README
  and follow the steps
% cd tau
% ./upload.sh
% perfexplorer &
```

Local Installation (*Stampede2, TACC*)

- Setup preferred program environment compilers

```
% . ~tg828282/Tutorial/vihps-intel.sh
% cp ~tg457572/pkgs/tar/data.tgz . ; tar zxf data.tgz
% cd data
% cat README
  and follow the steps
% cd tau
% ./upload.sh
% perfexplorer
```

Performance Research Lab, University of Oregon, Eugene, USA



Support Acknowledgments

- US Department of Energy (DOE)
  - Office of Science contracts
  - 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

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]

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

Free download, open source, BSD license