

The TAU Performance System

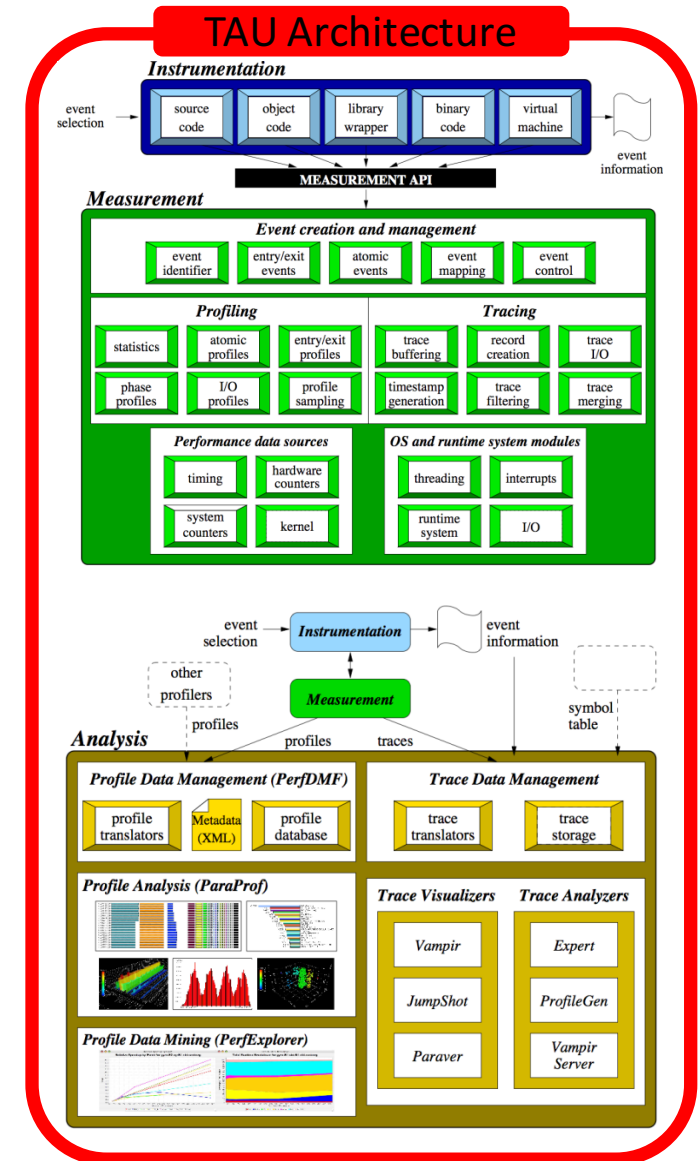
ParaTools, Inc.

John C. Linfood, Sameer Shende, et al.
{jlinford,sameer}@paratools.com

Scaling Your Science on Mira
24 May 2016, ALCF

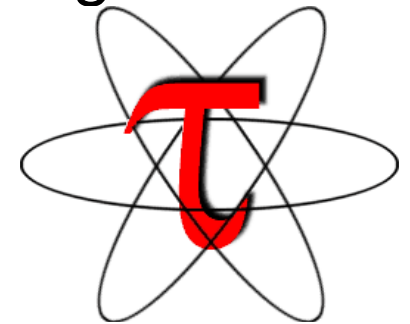
The TAU Performance System[®]

- *Integrated toolkit* for performance problem solving
 - Instrumentation, measurement, analysis, visualization
 - Portable profiling and tracing
 - Performance data management and data mining
- Direct and indirect measurement
- *Free, open source, BSD license*
- Available on all HPC platforms (and some non-HPC)
- <http://tau.uoregon.edu/>



The TAU Performance System[®]

- Tuning and Analysis Utilities (**20+ year project**)
- Comprehensive performance profiling and tracing
 - Integrated, scalable, flexible, portable
 - Targets all parallel programming/execution paradigms
- Integrated performance toolkit
 - Instrumentation, measurement, analysis, visualization
 - Widely-ported performance profiling / tracing system
 - Performance data management and data mining
 - Open source (BSD-style license)
- Integrates with application frameworks



TAU Supports All HPC Platforms

C/C++

Fortran

pthread

Intel GNU

MinGW

Insert
yours
here

CUDA

UPC

OpenACC

Intel MIC

LLVM

Linux

BlueGene

Android

GPI

Java

OpenMP

PGI

Windows

Fujitsu

MPC

Python

MPI

Sun

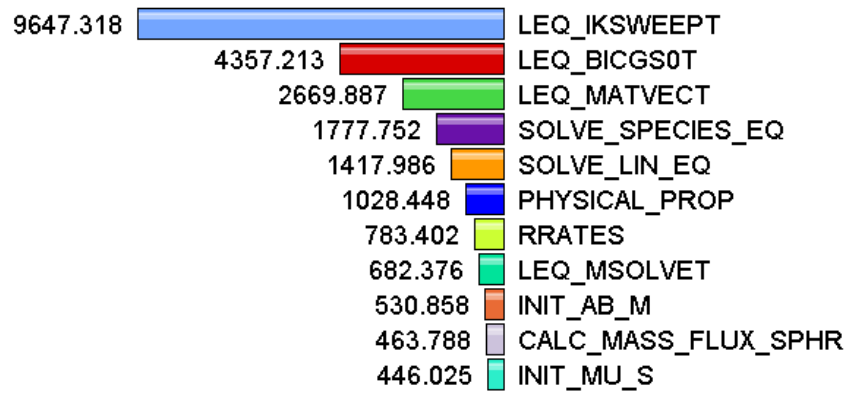
AIX

ARM

OS X

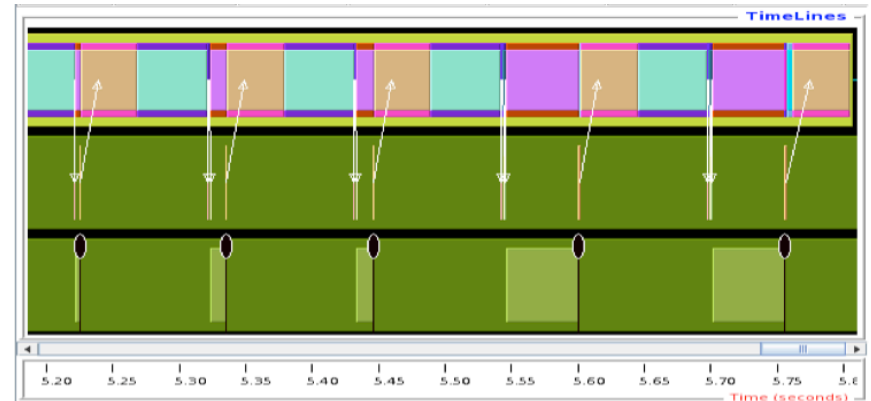
Measurement Approaches

Profiling



Shows
how much time
was spent in each
routine

Tracing

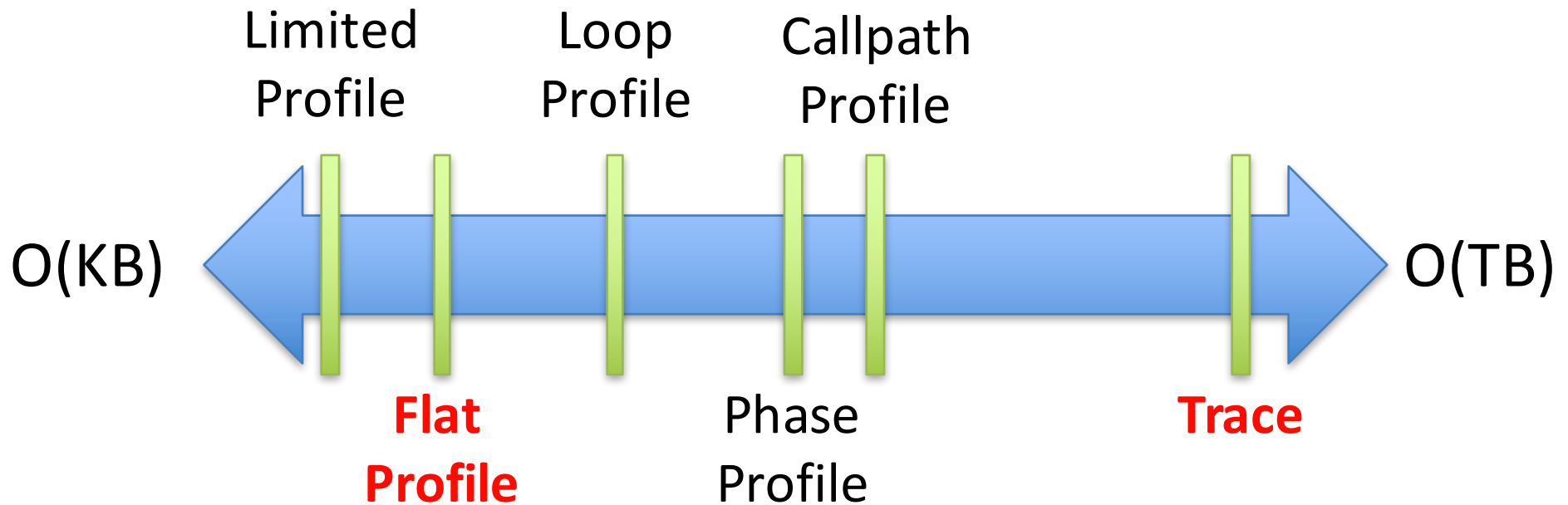


Shows
when events
take place on a
timeline

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_DEPTH** environment variable
- *Phase* profiles
 - Flat profiles under a phase (nested phases allowed)
 - Default “main” phase
 - Supports static or dynamic (e.g. per-iteration) phases

How much data do you want?



All levels support multiple metrics/counters

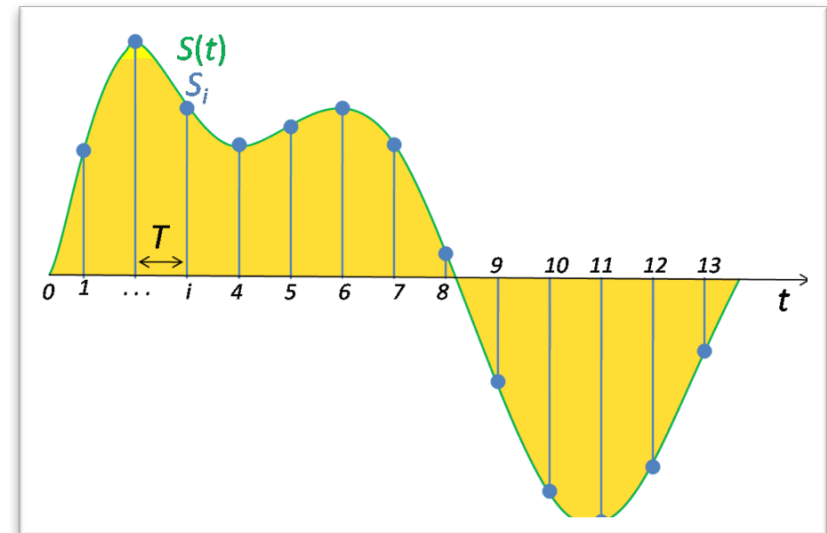
Performance Data Measurement

Direct via Probes

```
call TAU_START('potential')  
// code  
call TAU_STOP('potential')
```

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

Indirect via Sampling



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

Insert TAU API Calls Automatically

- Use TAU's compiler wrappers
 - Replace `cxx` with `tau_cxx.sh`, etc.
 - Automatically instruments source code, links with TAU libraries.
- Use `tau_cc.sh` for C, `tau_f90.sh` for Fortran, etc.

Makefile without TAU

```
CXX = mpicxx
F90 = mpif90
CXXFLAGS =
LIBS = -lm
OBJS = f1.o f2.o f3.o ... fn.o

app: $(OBJS)
    $(CXX) $(LDFLAGS) $(OBJS) -o $@
    $(LIBS)
.cpp.o:
    $(CXX) $(CXXFLAGS) -c $<
```

Makefile with TAU

```
CXX = tau_cxx.sh
F90 = tau_f90.sh
CXXFLAGS =
LIBS = -lm
OBJS = f1.o f2.o f3.o ... fn.o

app: $(OBJS)
    $(CXX) $(LDFLAGS) $(OBJS) -o $@
    $(LIBS)
.cpp.o:
    $(CXX) $(CXXFLAGS) -c $<
```

ALCF Quick Start

1. Choose an appropriate TAU_MAKEFILE:

```
% soft add +tau-latest
```

```
% export TAU_MAKEFILE=/soft/perf-tools/tau/tau_latest/  
bgq/lib/Makefile.tau-bgqtimers-mpi-pdt
```

```
% export TAU_OPTIONS='-optVerbose ...'  
# (see tau_compiler.sh -help for more options)
```

2. Use `tau_f90.sh`, `tau_cxx.sh`, etc. as Fortran, C++, etc. compiler:

```
% mpixlf90_r foo.f90
```

changes to

```
% tau_f90.sh foo.f90
```

3. Execute application:

```
% qsub -A <queue> -q R.bc -n 256 -t 10 ./a.out
```

Note: If TAU_MAKEFILE has “`papi`” in its name, set **TAU_METRICS**:

```
% qsub --env TAU_METRICS=BGQ_TIMERS:PAPI_L2_DCM...
```

4. Analyze performance data:

pprof (for text based profile display)

paraprof (for GUI)

TAU Configurations on Mira

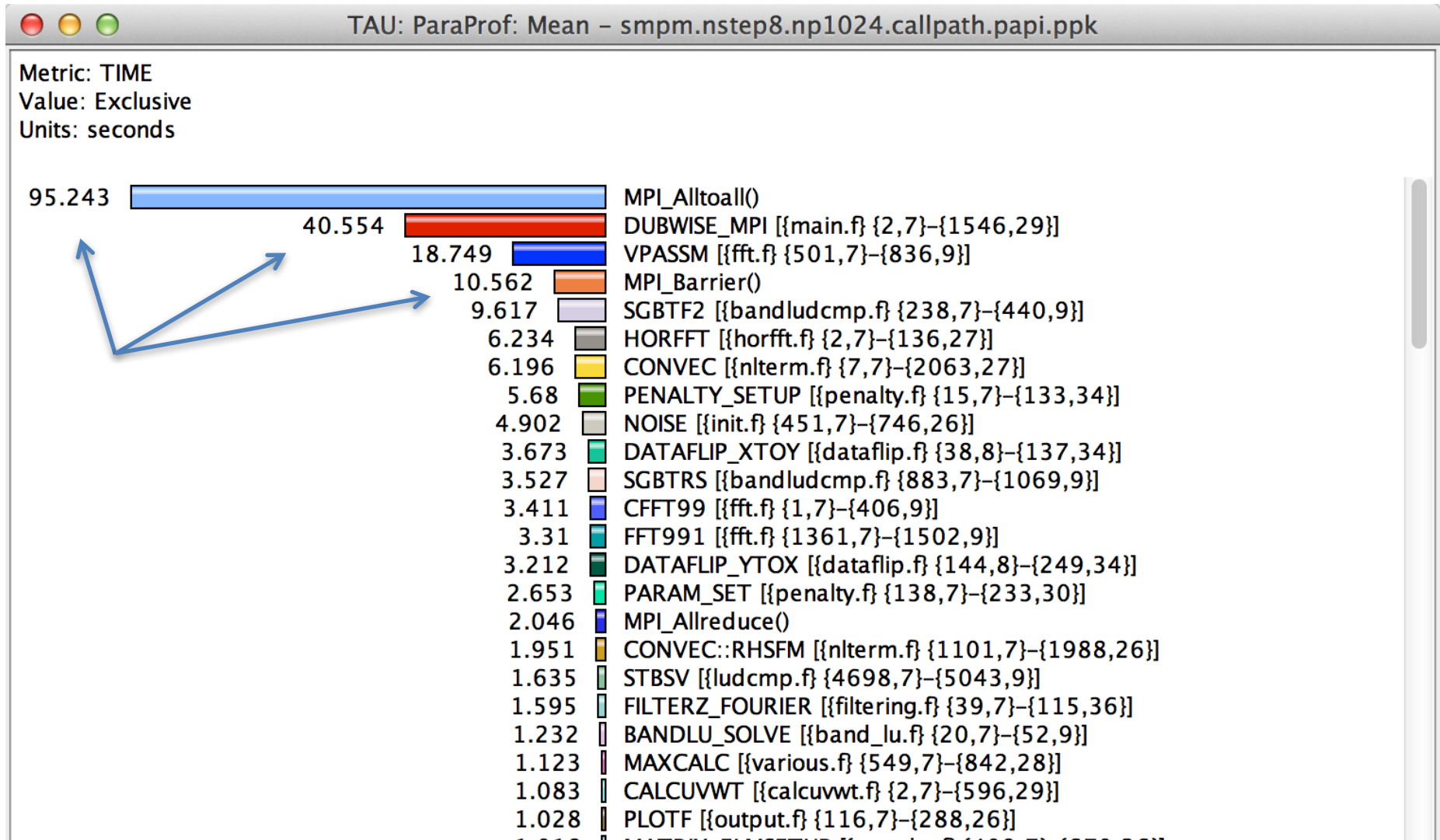
- Each configuration of TAU corresponds to a unique stub makefile (*TAU_MAKEFILE*) in the TAU installation directory

```
% ls /soft/perftools/tau/tau_latest/bgq/lib/Makefile.*  
Makefile.tau-bgqtimers-mpi-pdt-openmp-opari  
Makefile.tau-bgqtimers-mpi-pthread-pdt  
Makefile.tau-bgqtimers-papi-mpi-pdt  
Makefile.tau-bgqtimers-papi-mpi-pdt-openmp-opari  
Makefile.tau-bgqtimers-papi-mpi-pthread-pdt  
Makefile.tau-bgqtimers-pdt  
Makefile.tau-papi-mpi-pdt-openmp-opari  
Makefile.tau-papi-mpi-pdt-openmp-opari-scorep  
Makefile.tau-papi-mpi-pdt-scorep
```

Scaling Your Science on Mira

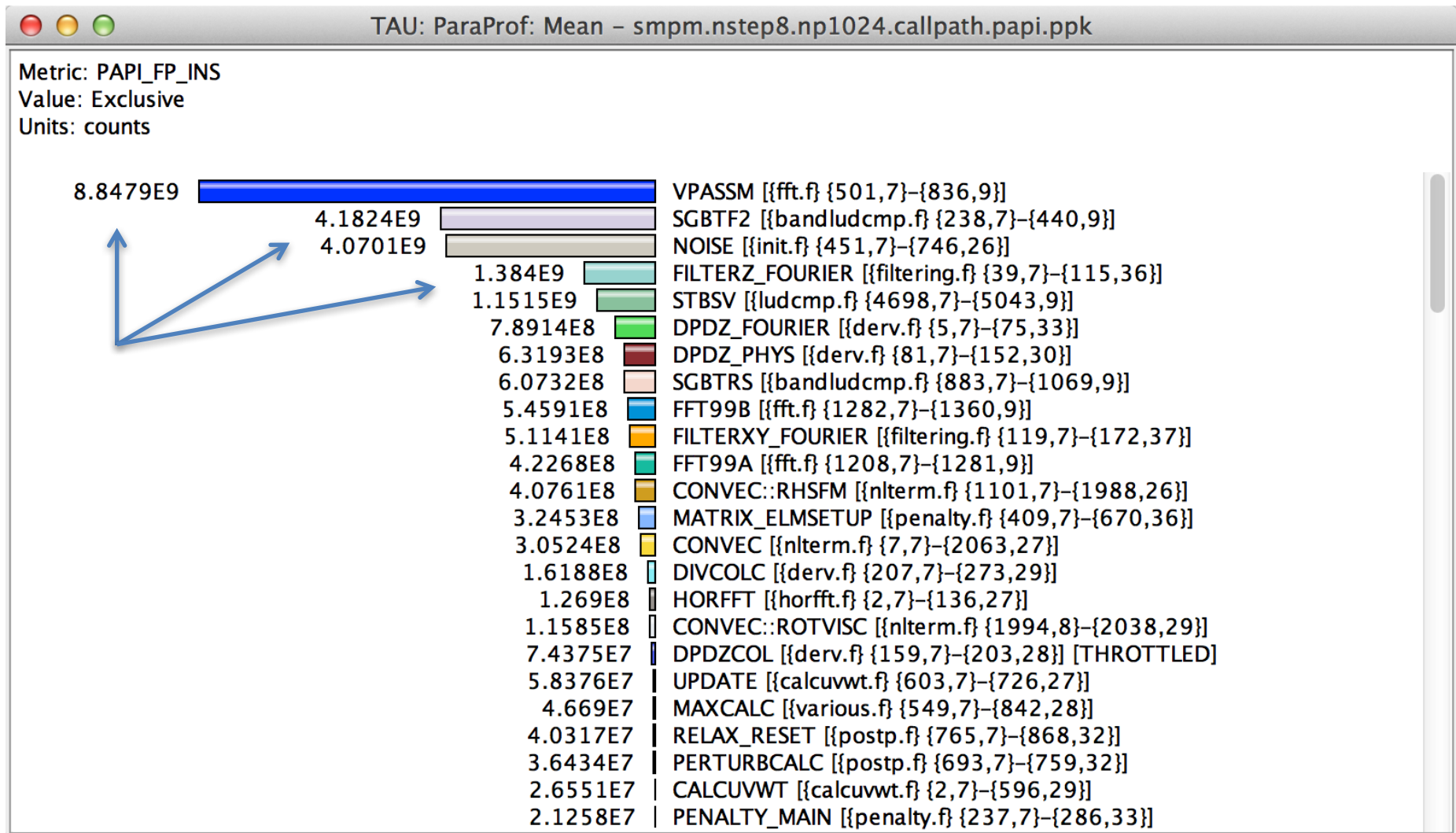
PERFORMANCE DATA ANALYSIS

How Much Time per Code Region?



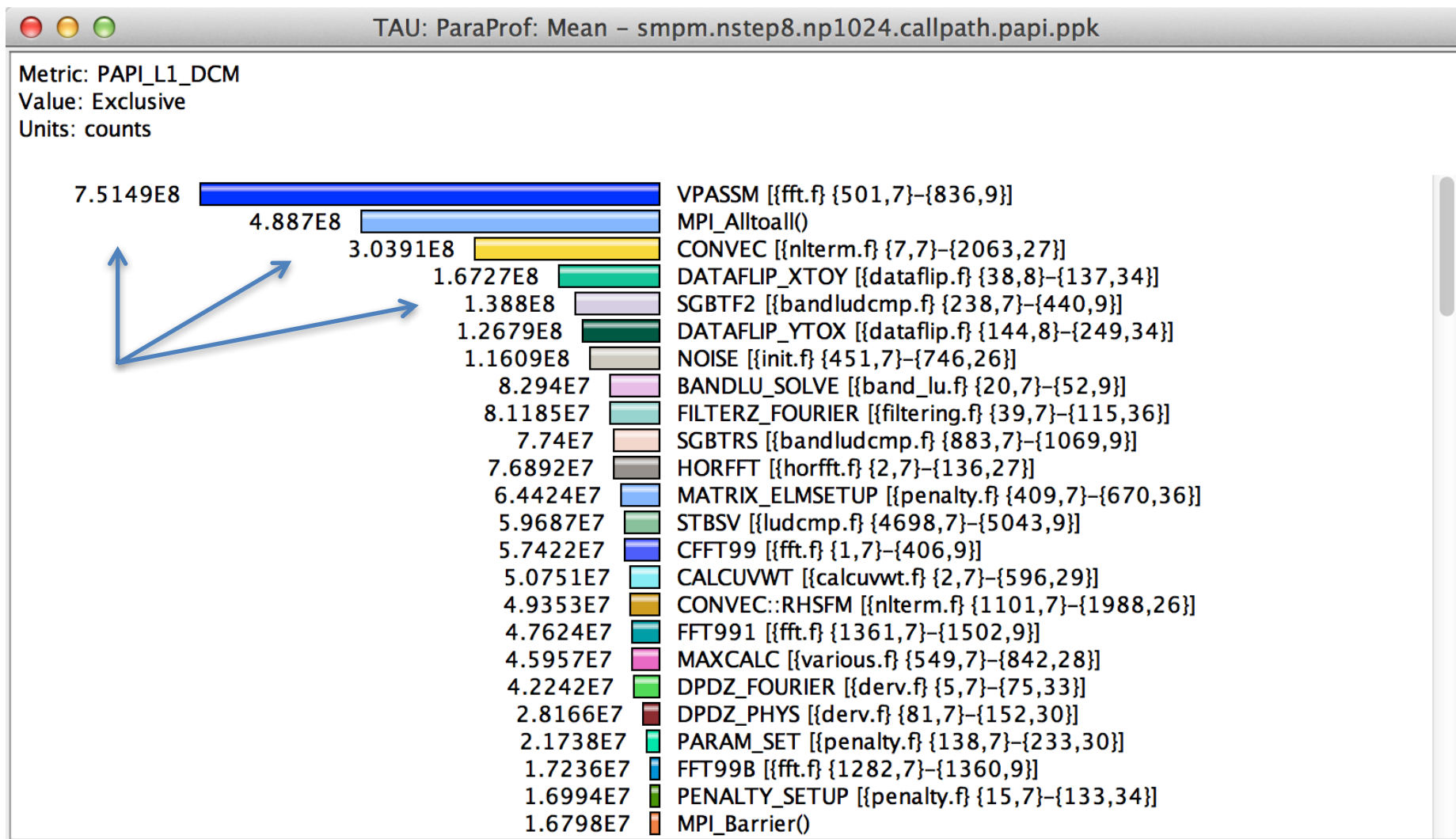
% **paraprof** (Click on label, e.g. "Mean" or "node 0")

How Many Instructions per Code Region?



% paraprof (Options → Select Metric... → Exclusive... → PAPI_FP_INS)

How Many L1 or L2 Cache Misses?



% paraprof (Options → Select Metric... → Exclusive... → PAPI_L1_DCM)

How Much Memory Does the Code Use?

TAU: ParaProf: Mean Context Events – sphere_np32_nsteps5_mem.ppk

Name Δ	Total	NumSamples	MaxValue	MinValue	MeanValue	Std. Dev.
▼ .TAU application						
free size (bytes)	14,236,992.16	27,169.781	49,152	1	524.001	2,013.103
malloc size (bytes)	13,132,932	23,292	262,144	1	563.839	4,492.057
▶ MPI_Finalize()						
▼ OurMain()						
free size (bytes)	1,298,918.679	1,495.125	461,766.25	4	868.769	16,928.073
malloc size (bytes)	48,150	20	36,032	11	2,407.5	7,911.992
▼ OurMain						
free size (bytes)	3,465	9	769	32	385	260.2
malloc size (bytes)	4,314	12	769	32	359.5	240.981
▼ <module>						
free size (bytes)	293,088	449	32,564	32	652.757	1,526.875
malloc size (bytes)	311,966	493	32,564	32	632.791	1,460.941
▶ staticCFD						
▶ __init__						
▶ <module>						
Memory Utilization (heap, in KB)		849,270.344	192,825.168	0.078	147,832.141	62,621.576
Message size for all-gather	4,096	1	4,096	4,096	4,096	0
Message size for all-reduce	23,340	843	320	4	27.687	64.653
Message size for all-to-all	104	26	4	4	4	0
Message size for broadcast	24,923	206	8,788	4	120.985	860.992
Message size for reduce	8,912	8	8,788	4	1,114	2,900.511
free size (bytes)	27,417,881,391.51	413,600.719	24,025,667	1	66,290.701	199,538.234
malloc size (bytes)	27,468,709,355.914	435,669.625	24,025,667	0	63,049.402	195,561.193

High-water mark

% **paraprof** (Right-click label [e.g “node 0”] → Show Context Event Window)

How Much Memory Does the Code Use?

TAU: ParaProf: Mean Context Events – sphere_np32_nsteps5_mem.ppk

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malloc size (bytes)	27,468,709,355.914	435,669.625	24,025,667	0	63,049.402	195,561.193

Total allocated/deallocated

% **paraprof** (Right-click label [e.g “node 0”] → Show Context Event Window)

Where is Memory Allocated / Deallocated?

TAU: ParaProf: Mean Context Events – sphere_np32_nsteps5_mem.ppk

Name Δ	Total	NumSamples	MaxValue	MinValue	MeanValue	Std. Dev.
▼ .TAU application						
free size (bytes)	14,236,992.16	27,169.781	49,152	1	524.001	2,013.103
malloc size (bytes)	13,132,932	23,292	262,144	1	563.839	4,492.057
▶ MPI_Finalize()						
▼ OurMain()						
free size (bytes)	1,298,918.679	1,495.125	461,766.25	4	868.769	16,928.073
malloc size (bytes)	48,150	20	36,032	11	2,407.5	7,911.992
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Message size for all-gather	4,096	1	4,096	4,096	4,096	0
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free size (bytes)	27,417,881,391.51	413,600.719	24,025,667	1	66,290.701	199,538.234
malloc size (bytes)	27,468,709,355.914	435,669.625	24,025,667	0	63,049.402	195,561.193

Allocation / Deallocation Events

% **paraprof** (Right-click label [e.g “node 0”] → Show Context Event Window)


What are the I/O Characteristics?


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

Name	Total	MeanValue	NumSamples	MinValue	MaxValue	Std. Dev.
▼ .TAU application						
▶ read()						
▶ fopen64()						
▶ fclose()						
▼ OurMain()						
malloc size	25,235	1,097.174	23	11	12,032	2,851.143
free size	22,707	1,746.692	13	11	12,032	3,660.642
▼ OurMain [{{wrapper.py}}{3}]						
▶ read()						
malloc size	3,877	323.083	12	32	981	252.72
free size	1,536	219.429	7	32	464	148.122
▶ fopen64()						
▶ fclose()						
▼ <module> [{{obe.py}}{8}]						
▼ writeRestartData [{{samarcInterface.py}}{145}]						
▼ samarcWriteRestartData						
▼ write()						
WRITE Bandwidth (MB/s) <file="samarc/restore.00002/nodes.00004/proc.00001">		74.565	117	0	2,156.889	246.386
WRITE Bandwidth (MB/s) <file="samarc/restore.00001/nodes.00004/proc.00001">		77.594	117	0	1,941.2	228.366
WRITE Bandwidth (MB/s)		76.08	234	0	2,156.889	237.551
Bytes Written <file="samarc/restore.00002/nodes.00004/proc.00001">	2,097,552	17,927.795	117	1	1,048,576	133,362.946
Bytes Written <file="samarc/restore.00001/nodes.00004/proc.00001">	2,097,552	17,927.795	117	1	1,048,576	133,362.946
Bytes Written	4,195,104	17,927.795	234	1	1,048,576	133,362.946
▶ open64()						

⌘ paraprof (Right-click label [e.g "node 0"] → Show Context Event Window)

What are the I/O Characteristics?

Name 	Total	NumSamples	MaxValue	MinValue	MeanValue	Std. Dev.
▶ Incl						
▶ Initialize						
▶ LoadBodyEuler						
▶ LoadMesh						
MPI-IO Bytes Written	4,328,712	144	893,152	0	30,060.5	128,042.696
MPI-IO Write Bandwidth (MB/s)		144	196.86	0	3.421	16.87
▶ MPI_Allgatherv()						
▶ MPI_Bcast()						
▶ MPI_Comm_create()						
▶ MPI_File_close()						
▶ MPI_File_open()						
▶ MPI_File_write_all()						
▶ MPI_File_write_at()						
▶ MPI_Finalize()						
▶ MPI_Gather()						
▶ MPI_Gatherv()						



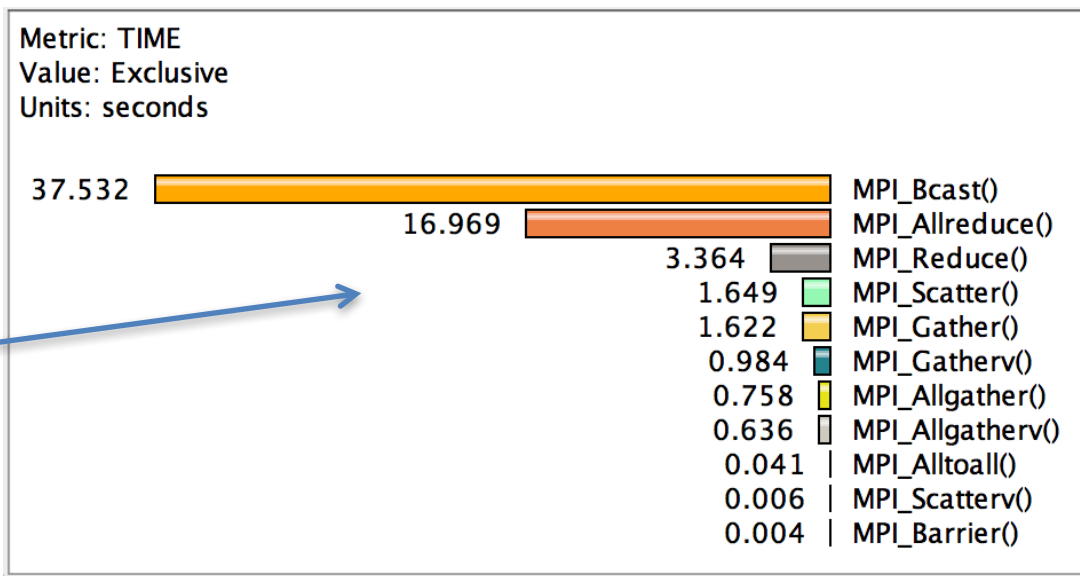
⌘ **paraprof** (Right-click label [e.g “node 0”] → Show Context Event Window)

How Much Time is spent in Collectives?

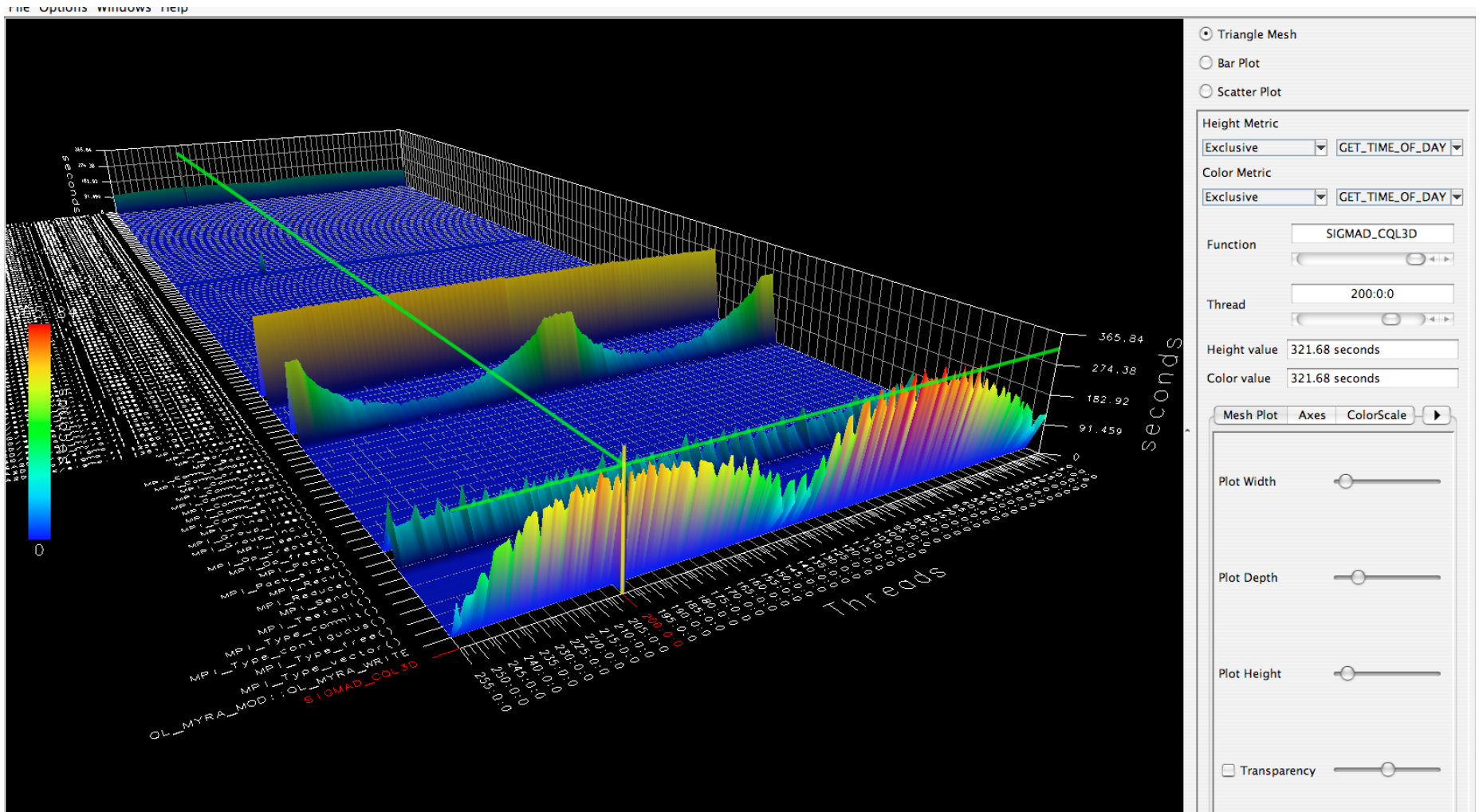
Name △	Total	Num...	MaxValue	MinValue	MeanValue	Std. Dev.
▶ MPI_Wait()						
▶ MPI_Waitall()						
Message size for all-gather	305,753,268	72	172,215,296	4	4,246,573.167	22,551,605.859
Message size for all-reduce	163,308	632	21,908	4	258.399	897.725
Message size for all-to-all	112	14	8	8	8	0
Message size for broadcast	692,208,045.5	3,346	18,117,620	0	206,876.284	1,284,673.036
Message size for gather	6,901,452.378	15.312	1,387,306.625	4	450,707.094	483,216.499
Message size for reduce	66,812	1,520	56	4	43.955	21.598
Message size for scatter	63,147.906	146	62,567.906	4	432.52	5,160.063

Message sizes

Time spent in collectives

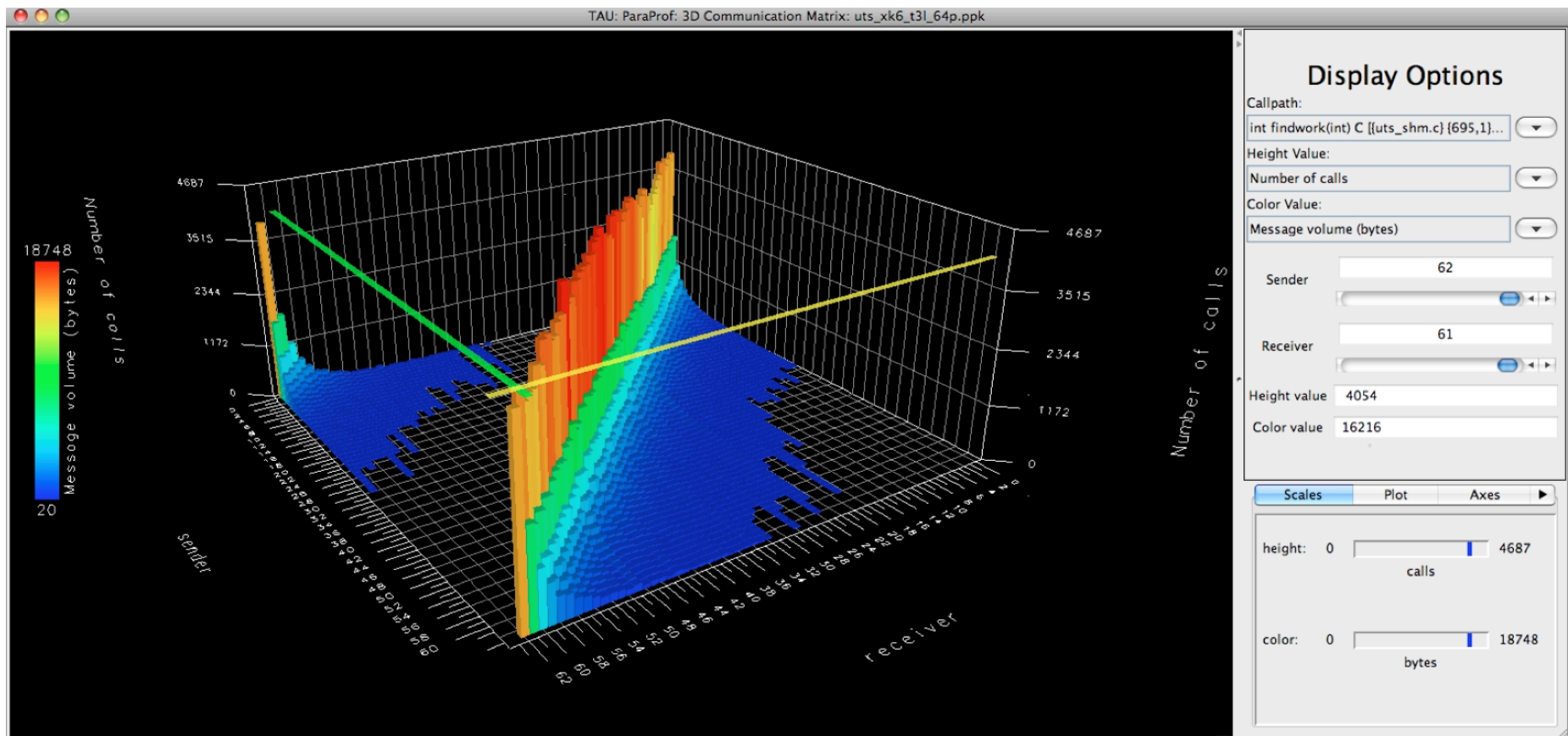


3D Profile Visualization



% paraprof (Windows → 3D Visualization)

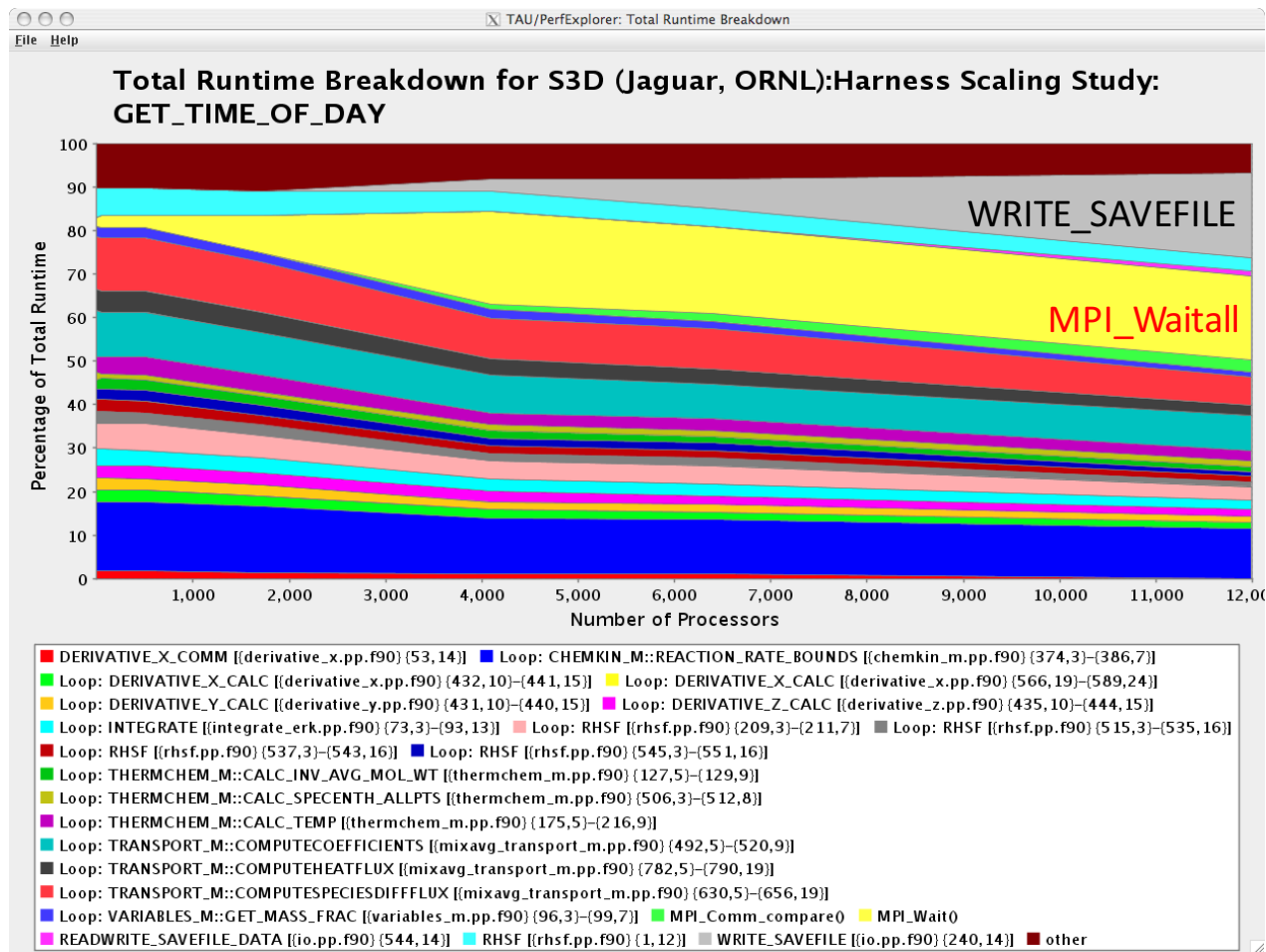
3D Communication Visualization



```
% qsub -env TAU_COMM_MATRIX=1 ...
```

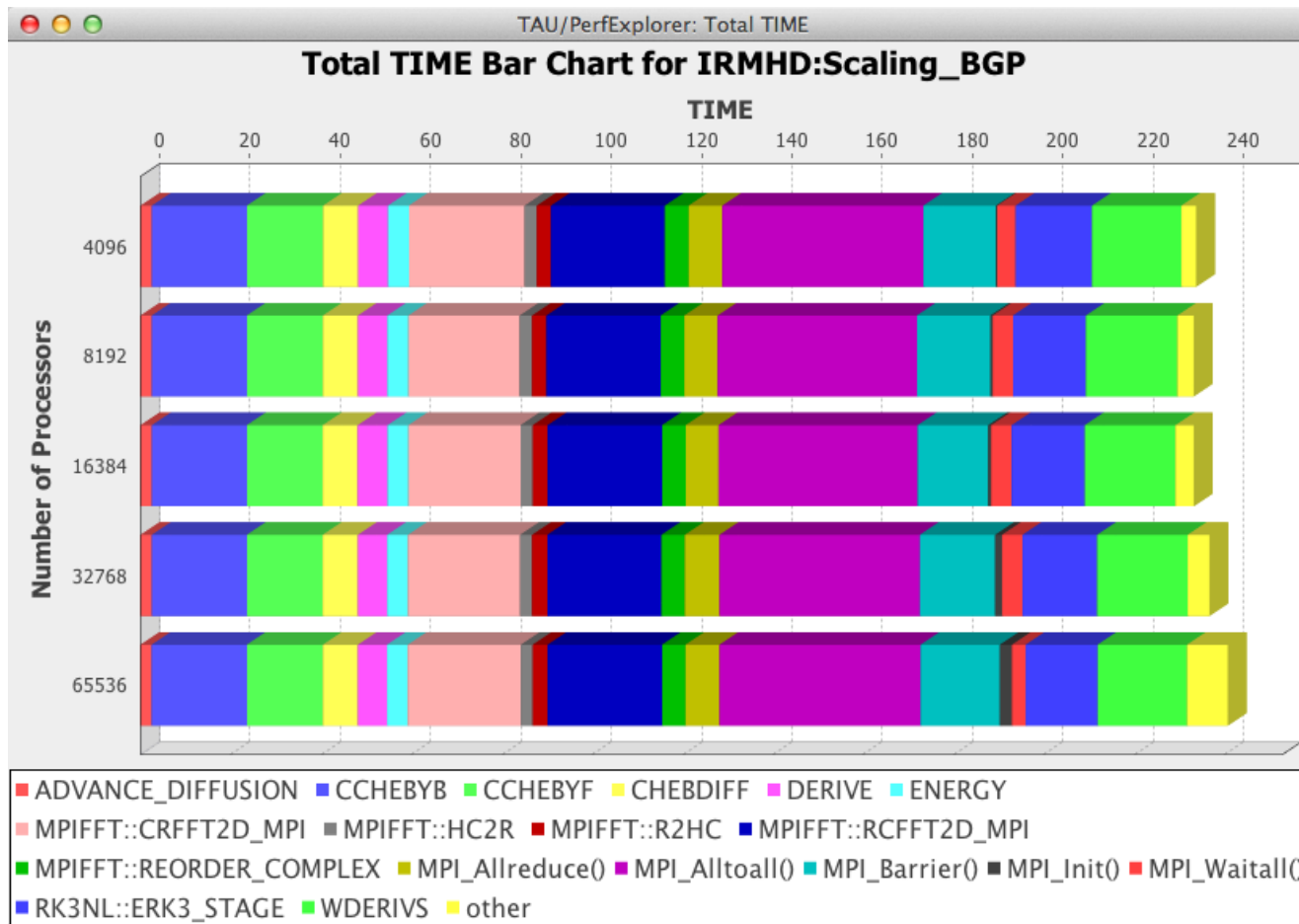
```
% paraprof (Windows → 3D Communication Matrix)
```

How Does Each Routine Scale?



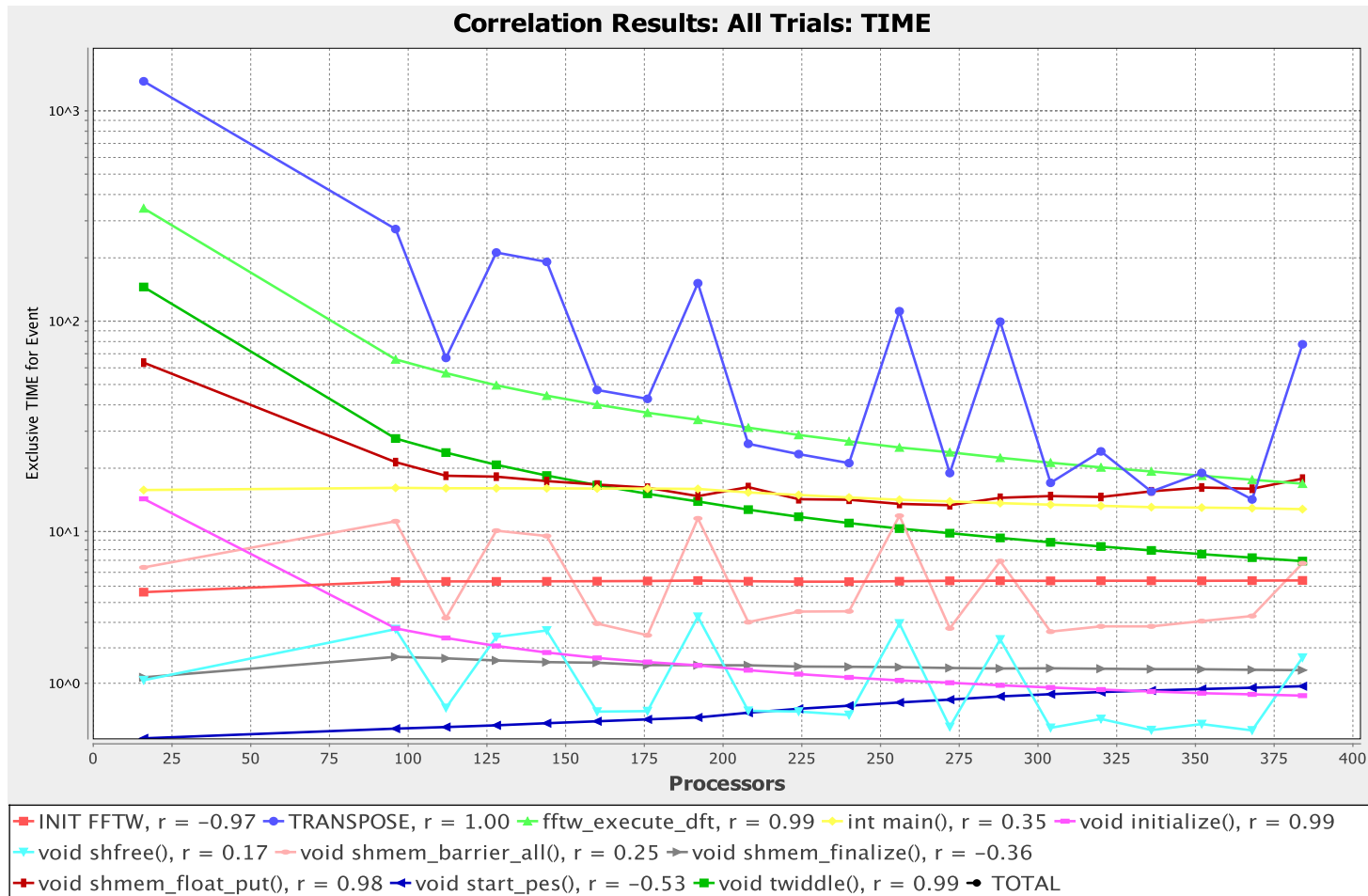
% perfexplorer (Charts → Runtime Breakdown)

How Does Each Routine Scale?



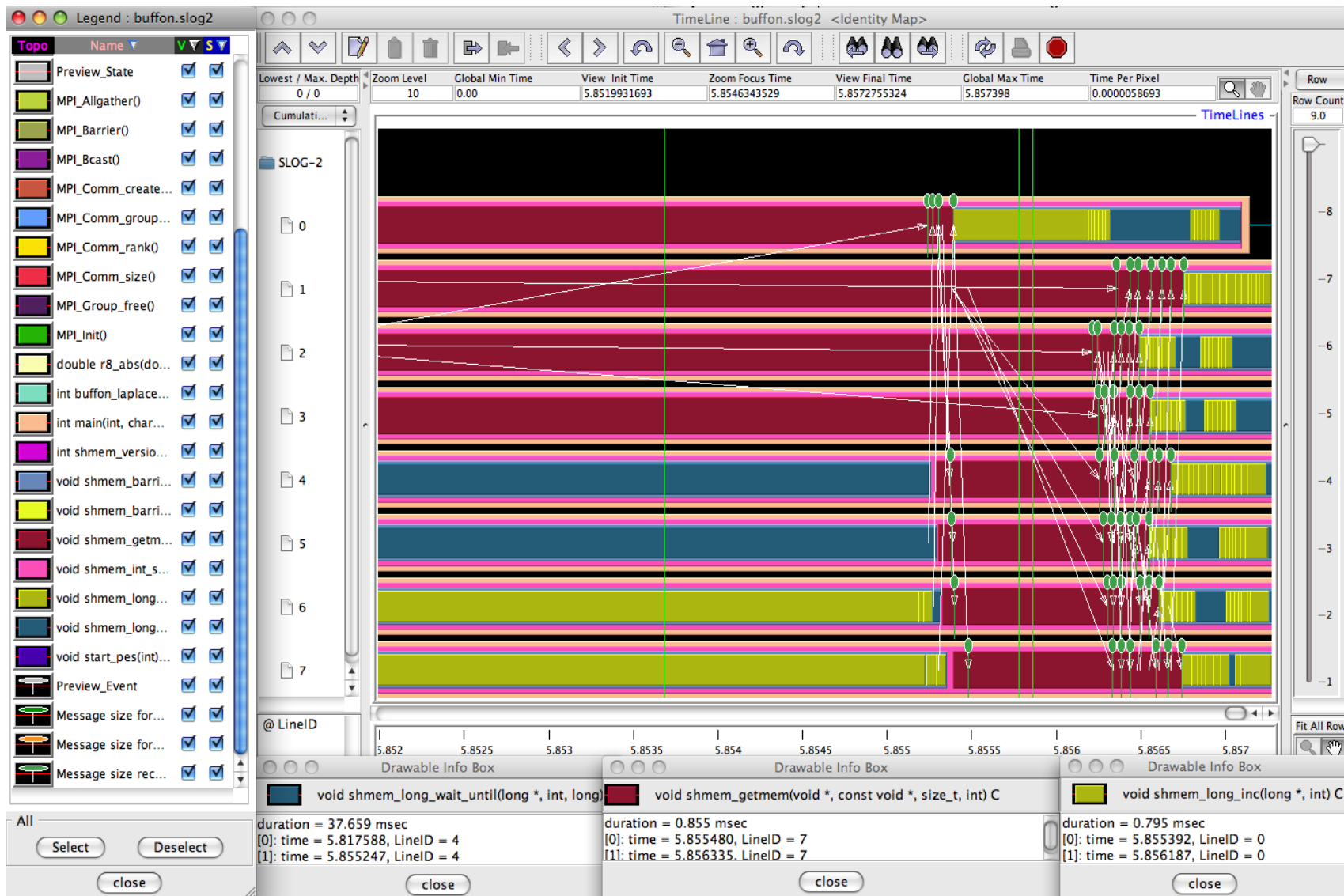
% **perfexplorer** (Charts → Stacked Bar Chart)

Which Events Correlate with Runtime?



% **perfexplorer** (Charts → Correlate Events with Total Runtime)

When do Events Occur?



When do Events Occur?

To generate a trace and visualize it in Jumpshot:

```
% qsub -env TAU_TRACE=1 ...  
% tau_treemerge.pl  
% tau2slog2 tau.trc tau.edf -o app.slog2  
% jumpshot app.slog2
```

Intuitive Performance Engineering

TAU COMMANDER (COMING THIS AUGUST)

How do we Improve Productivity?

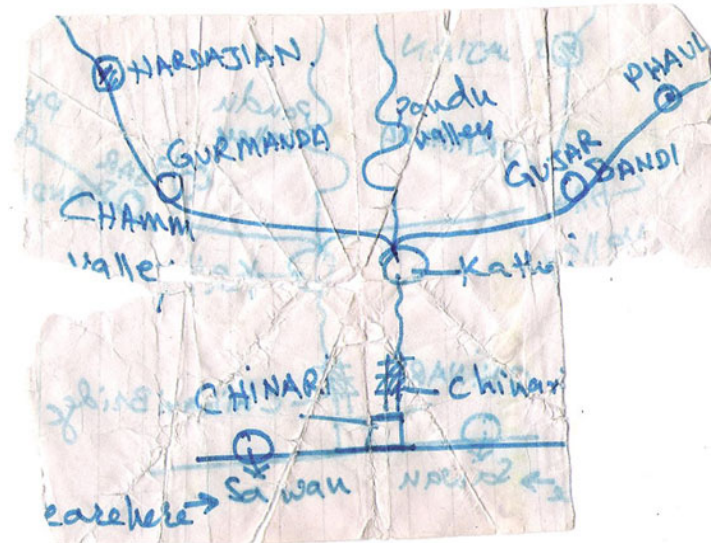


The TAU Commander Approach

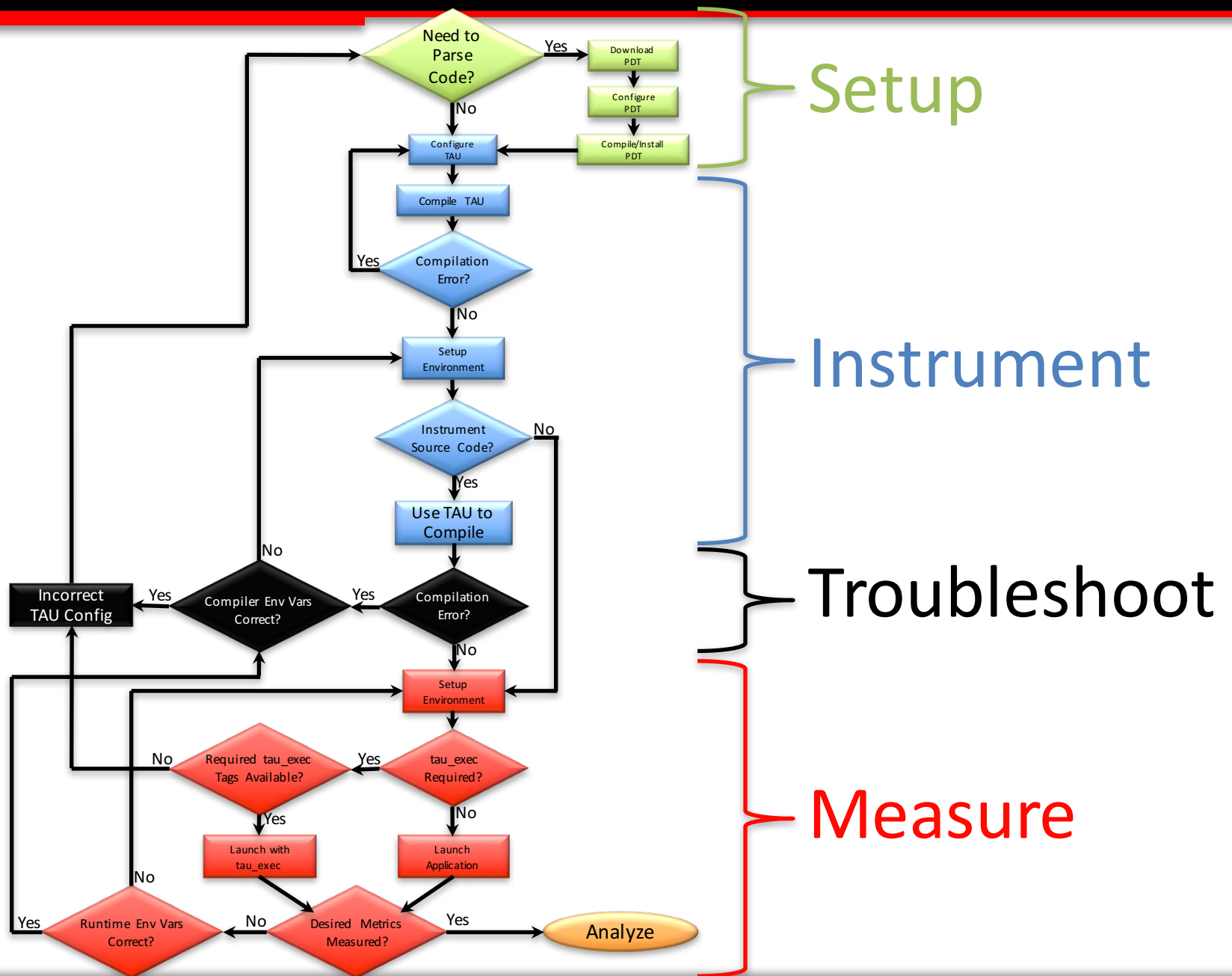
- Say where you're going, not how to get there
- **TAU Projects** give context to the user's actions
 - Defines desired metrics and measurement approach
 - Defines operating environment
 - Establishes a baseline for error checking



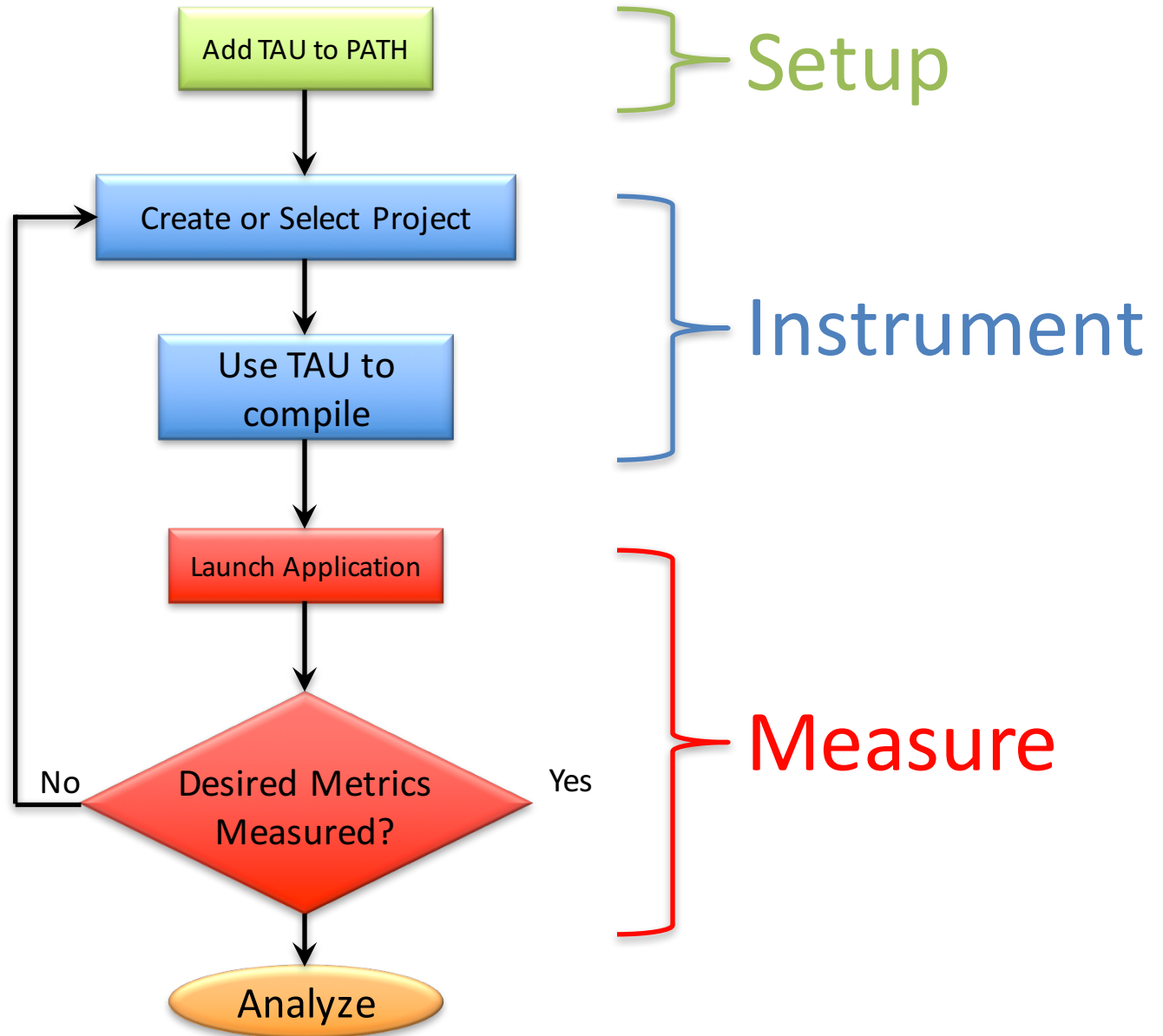
VS.



TAU Workflow



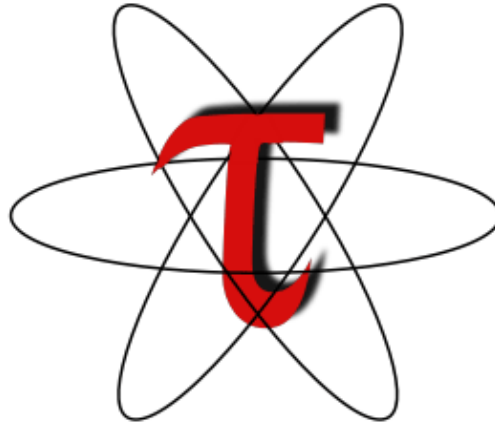
TAU Commander Workflow



Intuitive Performance Engineering

CONCLUSION

Downloads



<http://tau.uoregon.edu>

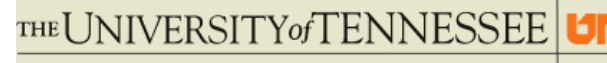
<http://github.com/ParaToolsInc/taucmdr>

<http://www.hpclinux.com>

Free download, open source, BSD license

Acknowledgements

- Department of Energy
 - Office of Science
 - Argonne National Laboratory
 - Oak Ridge National Laboratory
 - NNSA/ASC Trilabs (SNL, LLNL, LANL)
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- National Science Foundation
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- University of Tennessee
- University of New Hampshire
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- University of Oregon
 - Allen D. Malony, Sameer Shende
 - Kevin Huck, Wyatt Spear
- TU Dresden
 - Holger Brunst, Andreas Knupfer
 - Wolfgang Nagel
- Research Centre Jülich
 - Bernd Mohr
 - Felix Wolf



UNIVERSITY OF OREGON



Intuitive Performance Engineering

CASE STUDIES



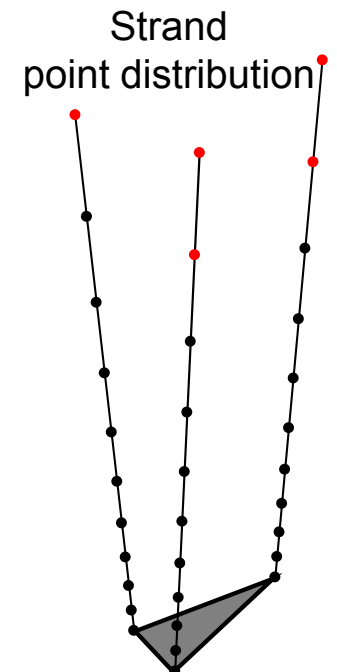
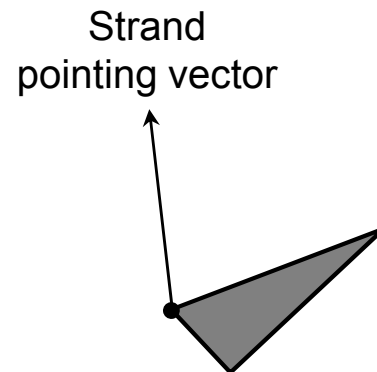
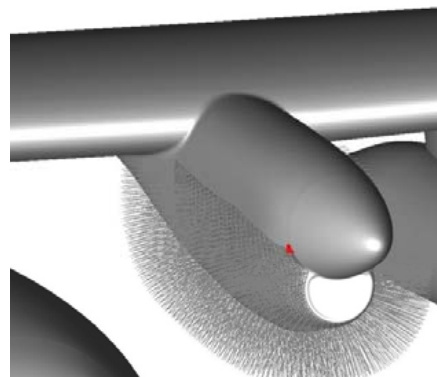
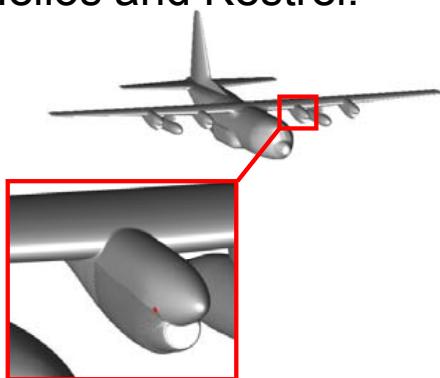
Strand Technology

Technology Drivers

- Timeliness (automation of mesh generation)
- Timeliness (automation and scalability of domain connectivity)
- Timeliness/Physical accuracy (computational efficiency and scalability of aerodynamic solvers)
- Processor architecture (small memory footprint maps well to hierarchical memory architectures, e.g., multi-core, GPU)

CREATE-AV Example

This is a new meshing paradigm introduced in 2007 by current members of the CREATE-AV technical staff. The technology is being matured in the Helios product and will be deployed through both Helios and Kestrel.

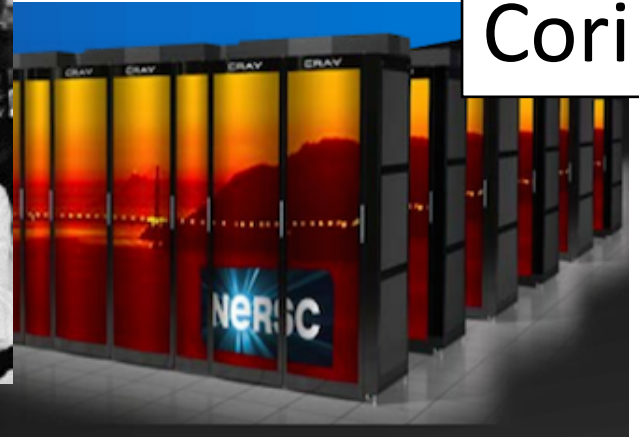


Target Platforms

Armstrong [XC30]



Cori



Haise [iDataPlex]



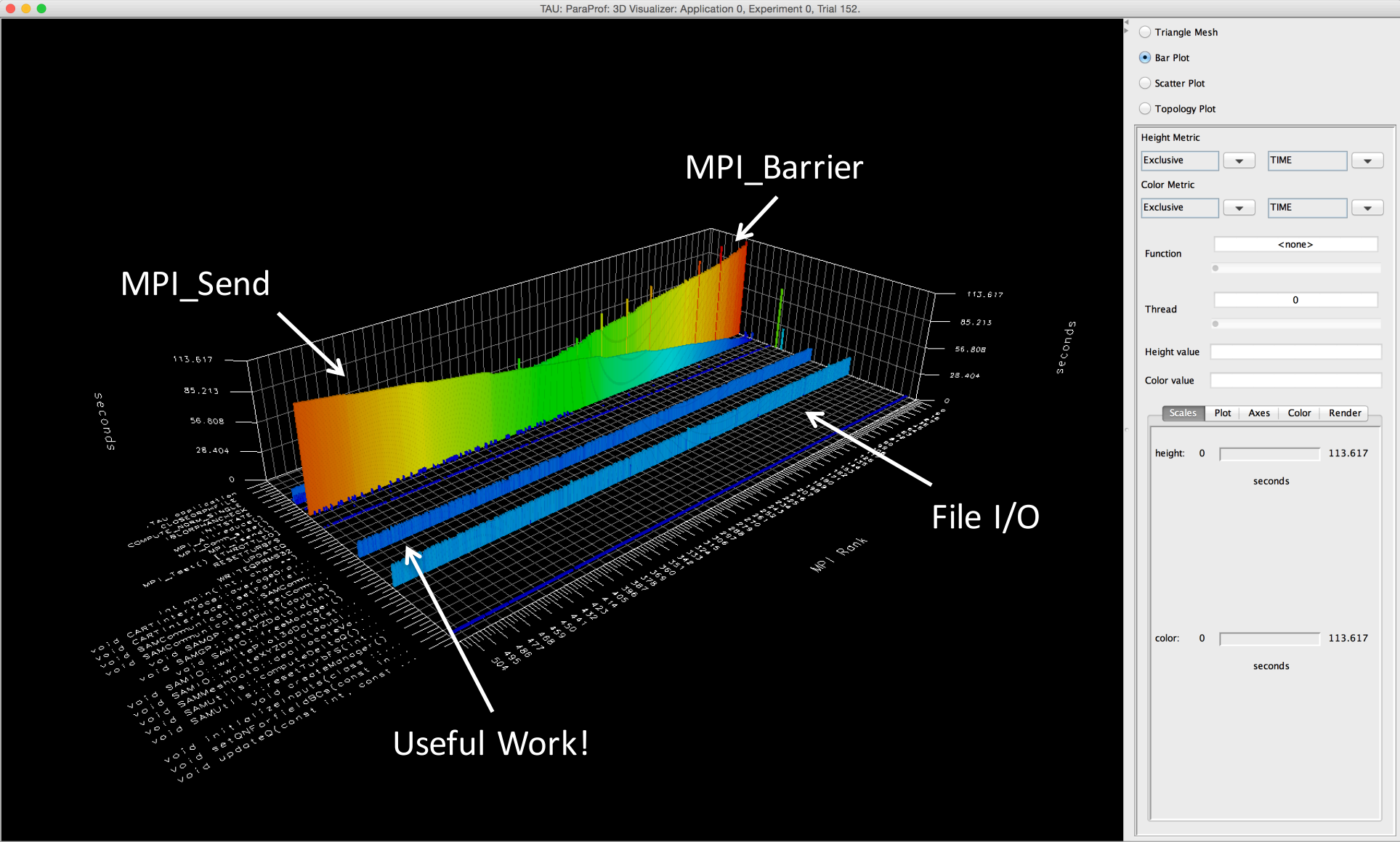
Lightning [XC30]



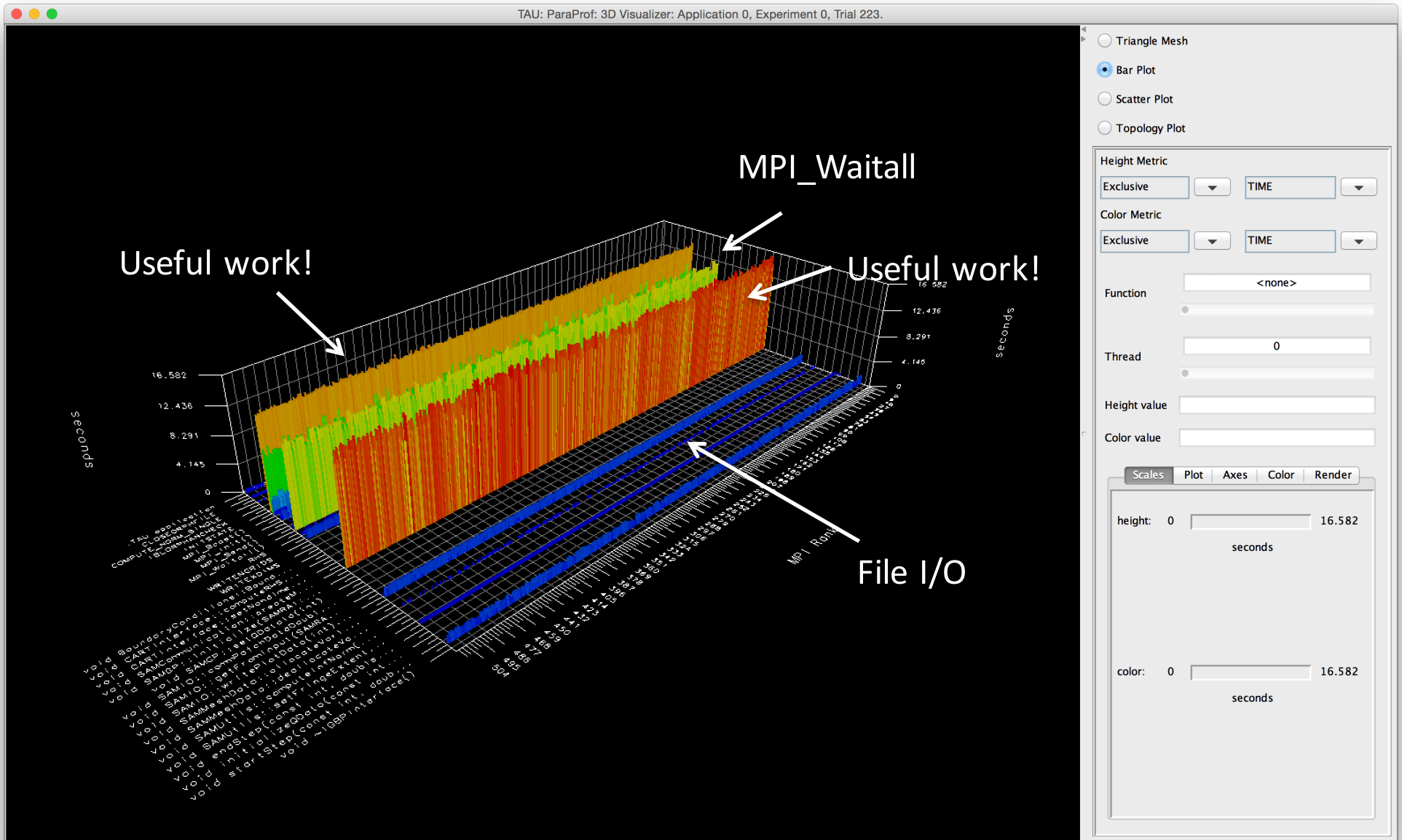
Kilrain [iDataPlex]



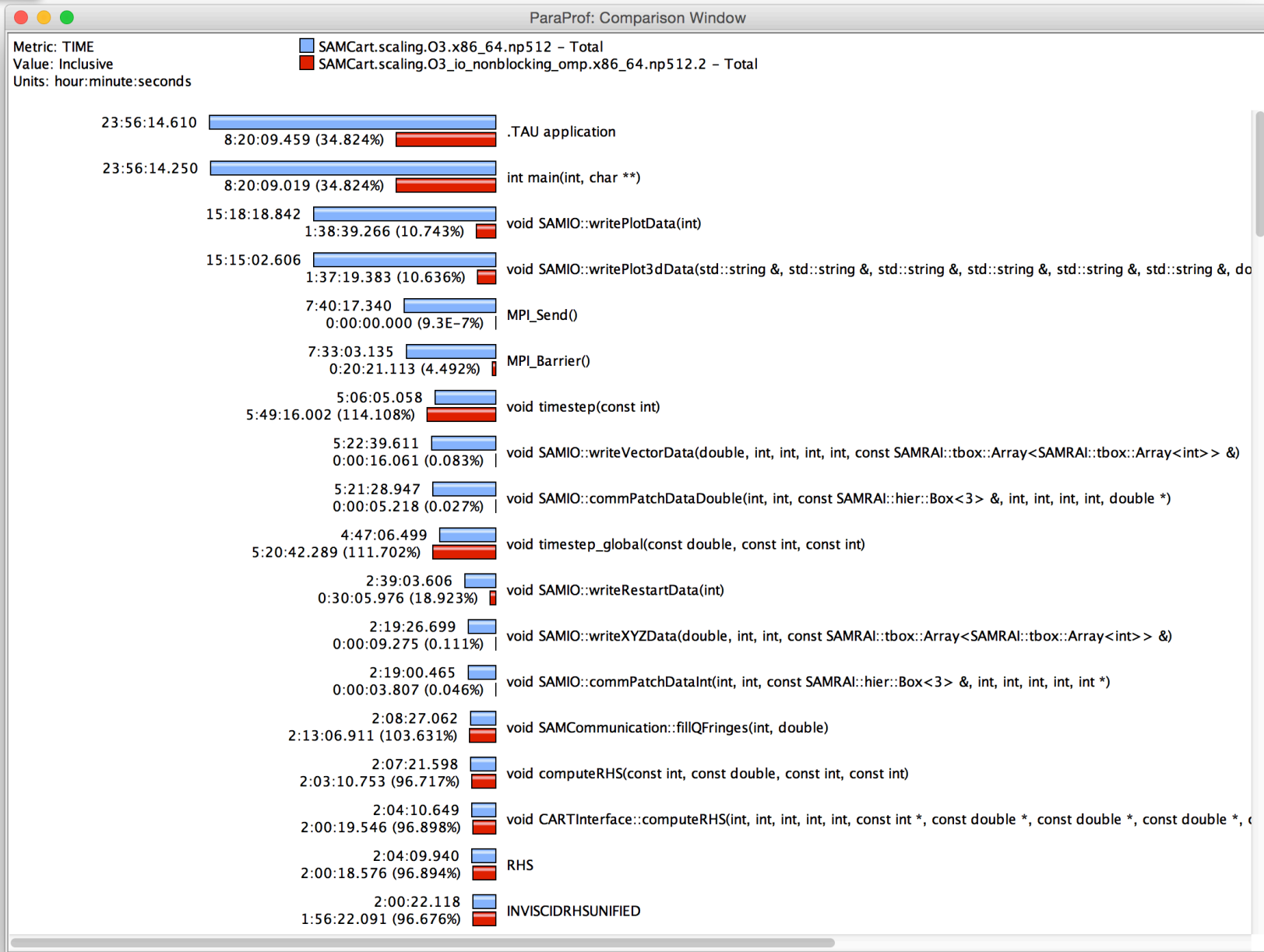
Initial Profile on Babbage



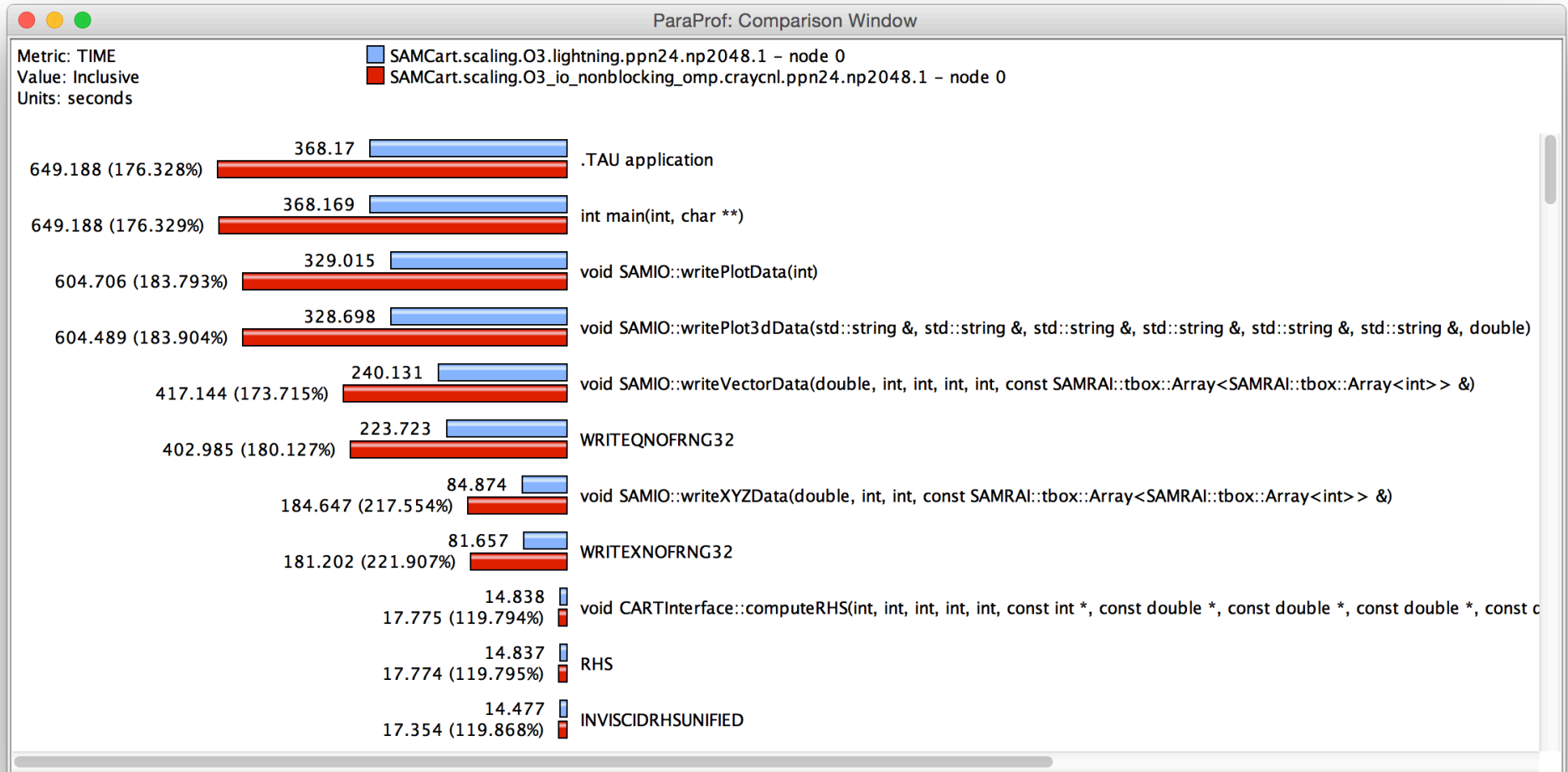
Hot Spot Optimization



65% Runtime Reduction (~2x faster)

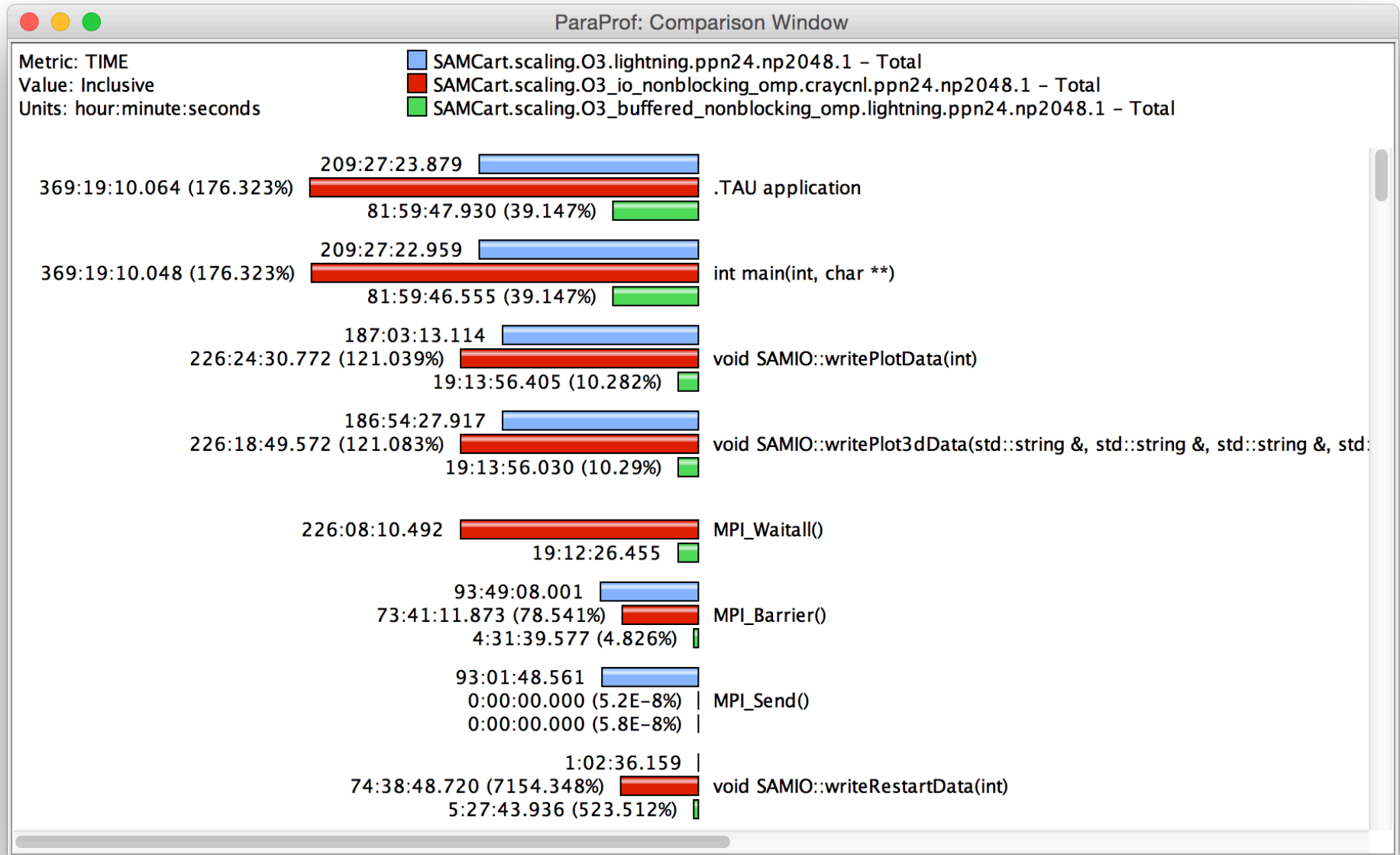


Cray XC30



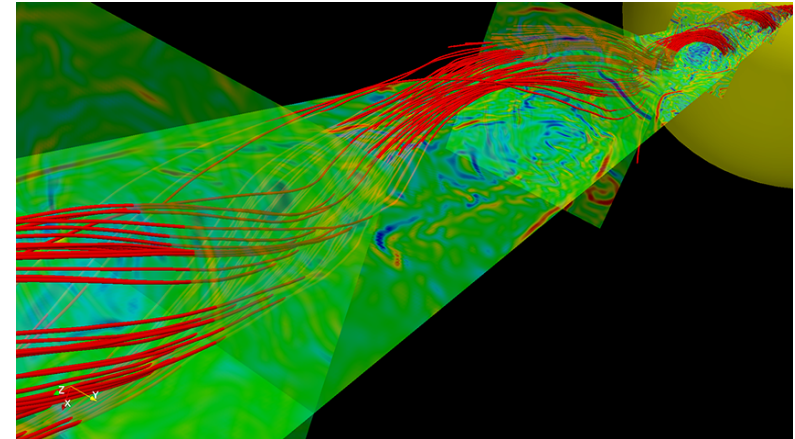
Slower! What happened???

No worries, I fix it



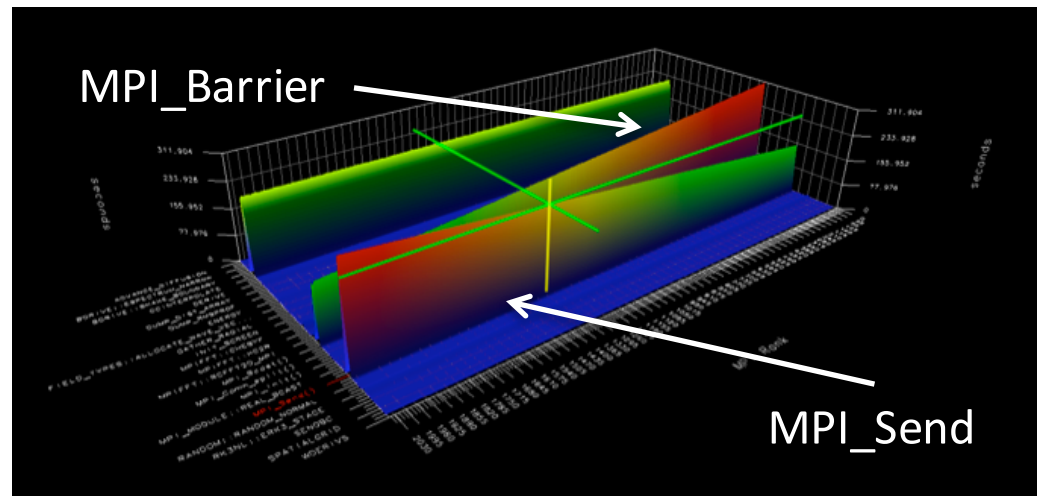
IRMHD on Intrepid and Mira

- INCITE magnetohydrodynamic simulation to understand solar winds and coronal heating
 - First direct numerical simulations of Alfvén wave (AW) turbulence in extended solar atmosphere accounting for inhomogeneities
 - Team
 - University of New Hampshire (Jean Perez and Benjamin Chandran)
 - ALCF (Tim Williams)
 - University of Oregon (Sameer Shende)
- IRMHD (Inhomogeneous Reduced Magnetohydrodynamics)
 - Fortran 90 and MPI
 - Excellent weak and strong scaling properties
 - Tested and benchmarked on Intrepid and Mira
- HPC Source article and ALCF news
<https://www.alcf.anl.gov/articles/furthering-understanding-coronal-heating-and-solar-wind-origin>



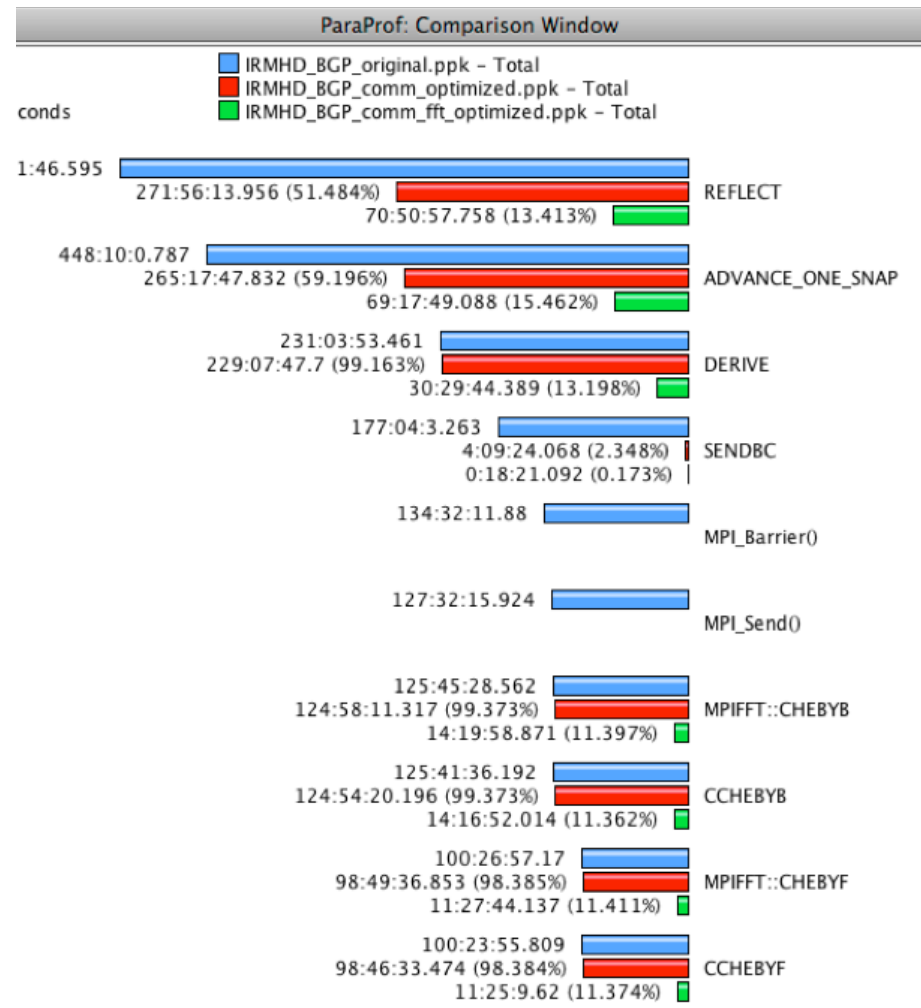
IRMHD Communication Analysis

- Source-based (direct) instrumentation
- MPI instrumentation and volume measurement
- IRMHD exhibited significant synchronous communication bottlenecks
- On 2,408 cores of BG/P:
 - **MPI_Send** and **MPI_Bcast** take significant time
 - Opportunities for communication/computation overlap
 - Identified possible targets for computation improvements



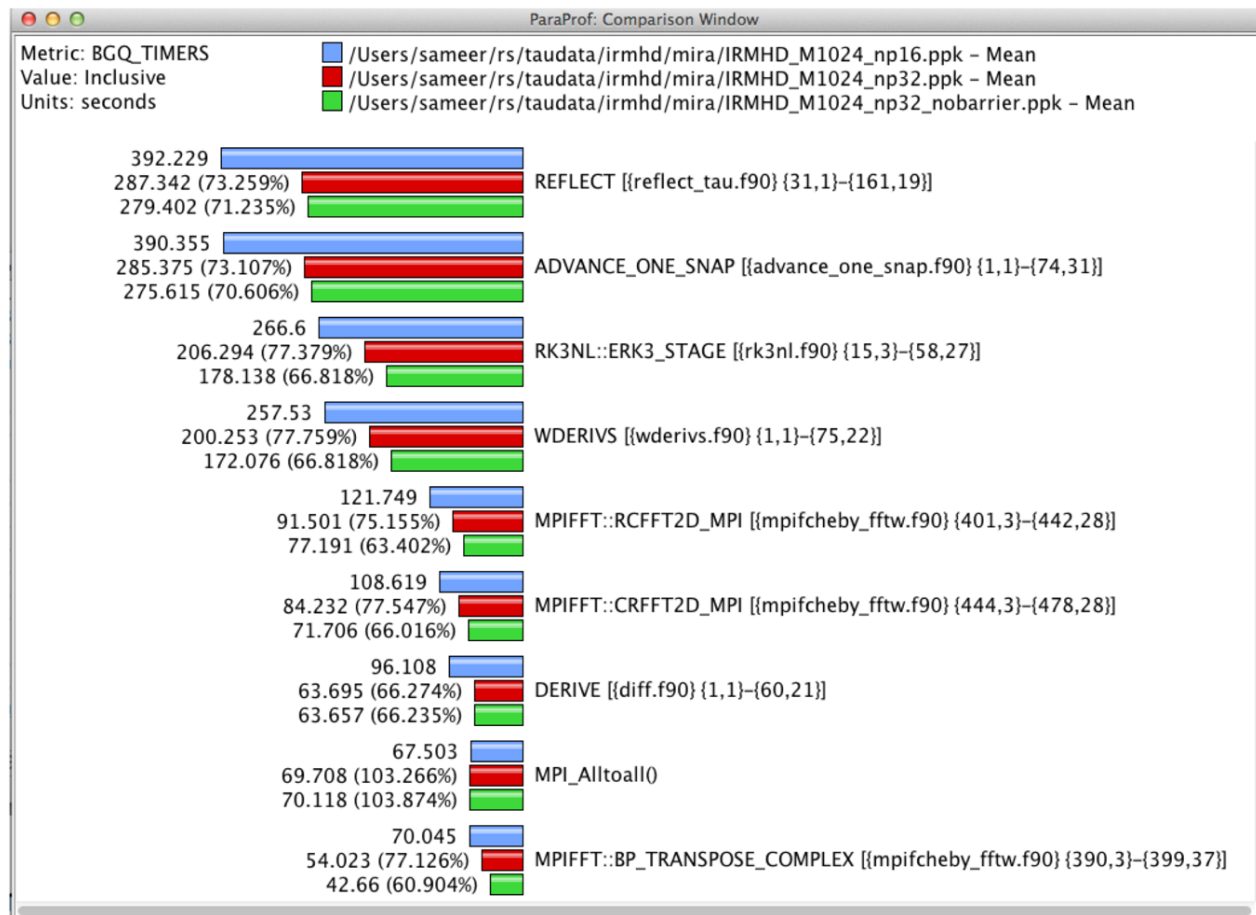
IRMHD Optimization on Intrepid (BG/P)

- On 2,408 cores, overall execution time reduced from 528.18 core hours to 70.8 core hours (**>7x improvement**)
- Non-blocking communication substrate
- More efficient implementation of underlying FFT



IRMHD Optimization on MIRA (BG/Q)

- Oversubscribe nodes: 32k ranks vs. 16k per node
- Overall time improvement: 71.23% of original



Intuitive Performance Engineering

REFERENCE

Online References

- PAPI:
 - PAPI documentation is available from the PAPI website:
<http://icl.cs.utk.edu/papi/>
- TAU:
 - TAU Users Guide and papers available from the TAU website:
<http://tau.uoregon.edu/>
- VAMPIR:
 - VAMPIR website:
<http://www.vampir.eu/>
- Scalasca:
 - Scalasca documentation page:
<http://www.scalasca.org/>
- Eclipse PTP:
 - Documentation available from the Eclipse PTP website:
<http://www.eclipse.org/ptp/>

Compiling Fortran Codes with TAU

- **If your Fortran code uses free format in .f files (fixed is default for .f):**
`% export TAU_OPTIONS='-optPdtF95Opts="-R free" -optVerbose'`
- **To use the compiler based instrumentation instead of PDT (source-based):**
`% export TAU_OPTIONS='-optComplnst -optVerbose'`
- **If your Fortran code uses C preprocessor directives (#include, #ifdef, #endif):**
`% export TAU_OPTIONS='-optPreProcess -optVerbose'`
- **To use an instrumentation specification file:**
`% export TAU_OPTIONS=
'-optTauSelectFile=select.tau -optVerbose -optPreProcess'`

Example select.tau file

```
BEGIN_INSTRUMENT_SECTION  
loops file="*" routine="#"  
memory file="foo.f90" routine="#"  
io file="abc.f90" routine="FOO"  
END_INSTRUMENT_SECTION
```

Generate a PAPI profile with 2 or more counters

```
% export TAU_MAKEFILE=$TAU/Makefile.tau-bgqtimers-papi-mpi-pdt
% export TAU_OPTIONS='-optTauSelectFile=select.tau -optVerbose'
% cat select.tau
BEGIN_INSTRUMENT_SECTION
loops routine="#"
END_INSTRUMENT_SECTION

% export PATH=$TAU_ROOT/bin:$PATH
% make F90=tau_f90.sh
(Or edit Makefile and change F90=tau_f90.sh)
%
% qsub --env TAU_METRICS=TIME:PAPI_FP_INS:PAPI_L1_DCM -n 4 -t 15 ./a.out
% paraprof --pack app.ppk
  Move the app.ppk file to your desktop.
% paraprof app.ppk
  Choose Options -> Show Derived Metrics Panel -> "PAPI_FP_INS", click "/", "TIME", click
  "Apply" and choose the derived metric.
```

Tracking I/O in static binaries

```
% export TAU_MAKEFILE=$TAU/Makefile.tau-bgqtimers-papi-mpi-pdt
% export PATH=$TAU_ROOT/bin:$PATH
% export TAU_OPTIONS='-optTrackIO -optVerbose'
% make CC=tau_cc.sh CXX=tau_cxx.sh F90=tau_f90.sh
% mpirun -n 4 ./a.out
% paraprof -pack ioprofile.ppk
% export TAU_TRACK_IO_PARAMS 1
% mpirun -n 4 ./a.out (to track parameters used in POSIX I/O calls as
  context events)
```

Installing and Configuring TAU

•Installing PDT:

- `wget http://tau.uoregon.edu/pdt.tgz`
- `./configure --prefix=<dir>; make ; make install`

•Installing TAU:

- `wget http://tau.uoregon.edu/tau.tgz`
- `./configure -bfd=download -pdt=<dir> -papi=<dir> ...`
- `make install`

•Using TAU:

- `export TAU_MAKEFILE=<taudir>/<arch>/lib/Makefile.tau-<TAGS>`
- `make CC=tau_cc.sh CXX=tau_cxx.sh F90=tau_f90.sh`

Compile-Time Options (TAU_OPTIONS)

% 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
-optMemDbg	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 <i>tau_instrumentor</i>
-optTauWrapFile=" <file>"	Specify path to <i>link_options.tau</i> generated by <i>tau_gen_wrapper</i>
-optHeaderInst	Enable Instrumentation of headers
-optTrackUPCR	Track UPC runtime layer routines (used with tau_upc.sh)
-optPdtF95Opts=""	Add options for Fortran parser in PDT (f95parse/gfparse) ...

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_LEAKS	0	Setting to 1 turns on leak detection (for use with <code>-optMemDbg</code> or <code>tau_exec</code>)
TAU_MEMDBG_PROTECT_ABOVE	0	Setting to 1 turns on bounds checking for dynamically allocated arrays. (Use with <code>-optMemDbg</code> or <code>tau_exec -memory_debug</code>).
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_TRACK_IO_PARAMS	0	Setting to 1 with <code>-optTrackIO</code> or <code>tau_exec -io</code> captures arguments of I/O calls
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. Enabled by default to remove 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_COMPENSATE	0	Setting to 1 enables runtime compensation of instrumentation overhead
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., TIME:P_VIRTUAL_TIME:PAPI_FP_INS:PAPI_NATIVE_<event>\\:<subevent>)