Performance Engineering of Parallel Applications

Philip Blood, Raghu Reddy

Pittsburgh Supercomputing Center

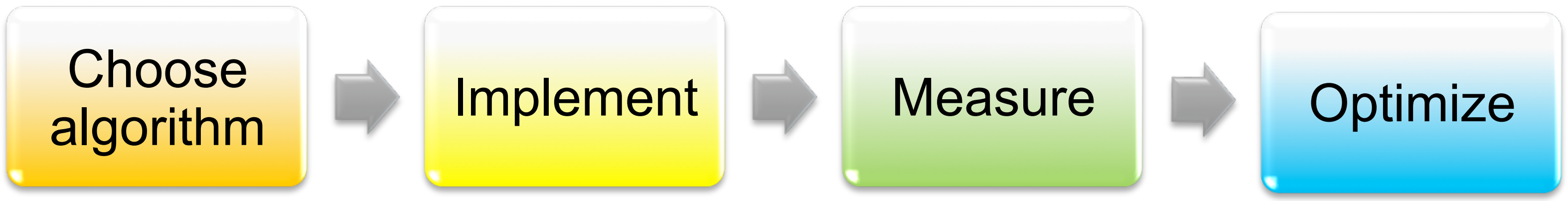
POINT Project

- “High-Productivity Performance Engineering (Tools, Methods, Training) for NSF HPC Applications”
  - NSF SDCI, Software Improvement and Support
  - University of Oregon, University of Tennessee, National Center for Supercomputing Applications, Pittsburgh Supercomputing Center
- POINT project
  - Petascale Productivity from Open, Integrated Tools
  - http://www.nic.uoregon.edu/point

Parallel Performance Technology

- PAPI
  - University of Tennessee, Knoxville
- PerfSuite
  - National Center for Supercomputing Applications
- TAU Performance System
  - University of Oregon
- Kojak / Scalasca
  - Research Centre Juelich

Code Development and Optimization Process



- Choice of algorithm most important consideration (serial and parallel)
- Measurement may reveal need for new algorithm or completely different implementation rather than optimization
- Focus of this lecture: using tools to assess parallel performance

A little background...

Hardware Counters

- Counters: set of registers that count processor events, like floating point operations, or cycles (Opteron has 4 registers, so 4 events can be monitored simultaneously)
- **PAPI: P**erformance **API**
- Standard API for accessing hardware performance counters
- Enable mapping of code to underlying architecture
- Facilitates compiler optimizations and hand tuning
- Seeks to guide compiler improvements and architecture development to relieve common bottlenecks

Features of PAPI

- Portable: uses same routines to access counters across all architectures
- High-level interface
  - Using predefined standard events the same source code can access similar counters across various architectures without modification.
  - papi_avail
- Low-level interface
  - Provides access to all machine specific counters (requires source code modification)
  - Increased efficiency and flexibility
  - papi_native_avail
- Third-party tools
  - TAU, Perfsuite, IPM

Example: High-level interface

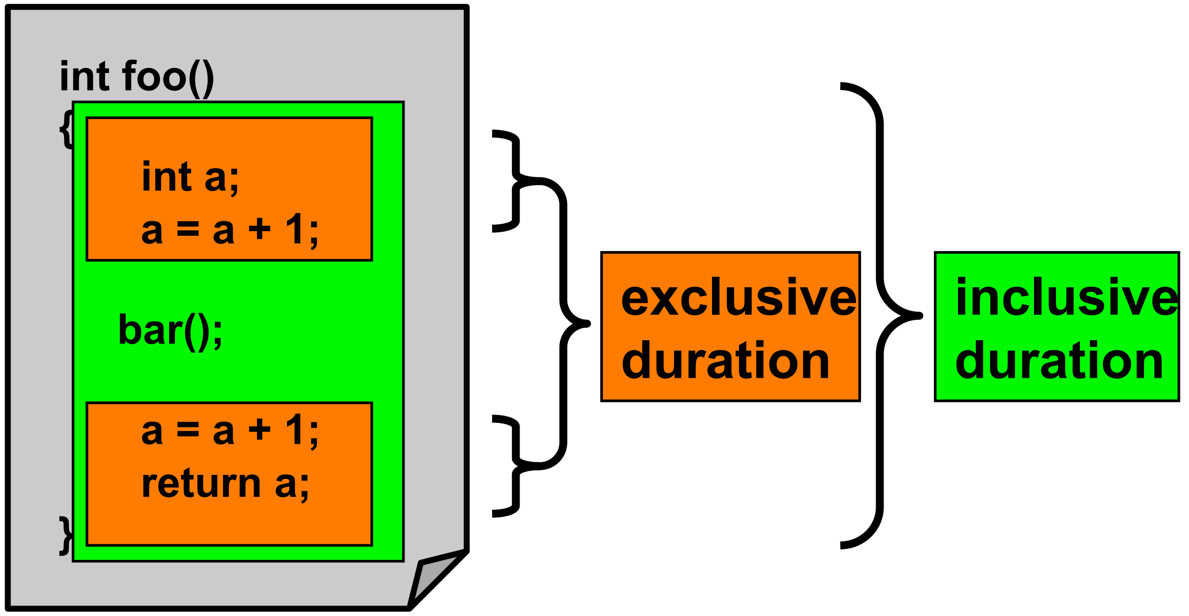
```
#include <papi.h>
#define NUM_EVENTS 2
main()
{
int Events[NUM_EVENTS] = {PAPI_TOT_INS, PAPI_TOT_CYC};
long_long values[NUM_EVENTS];
/* Start counting events */
if (PAPI_start_counters(Events, NUM_EVENTS) != PAPI_OK)
handle_error(1);
/* Do some computation here*/
/* Read the counters */
if (PAPI_read_counters(values, NUM_EVENTS) != PAPI_OK)
handle_error(1);
/* Do some computation here */
/* Stop counting events */
if (PAPI_stop_counters(values, NUM_EVENTS) != PAPI_OK)
handle_error(1);
}
```

Measurement Techniques

- When is measurement triggered?
  - Sampling (indirect, external, low overhead)
    - interrupts, hardware counter overflow, …
  - Instrumentation (direct, internal, high overhead)
    - through code modification
- How are measurements made?
  - Profiling
    - summarizes performance data during execution
    - per process / thread and organized with respect to context
  - Tracing
    - trace record with performance data and timestamp
    - per process / thread

Inclusive and Exclusive Profiles

- Performance with respect to code regions
- Exclusive measurements for region only
- Inclusive measurements includes child regions



Performance Engineering: Procedure

- Serial
  - Assess overall serial performance (percent of peak)
  - Identify functions where code spends most time
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  - Identify inefficient regions of source code and cause of inefficiencies
- Parallel
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Is There a Performance Problem?

- My code takes 3 hrs to run each time!
  - Does that mean it is performing poorly?
    - HPL on 4K cores can take a couple of hrs
    - Depends on the work being done

- Performance problems
  - Single core performance problem?
  - Scalability problem?

Detecting Performance Problems

- Fraction of Peak
  - 20% peak (overall) is usually decent; After that you decide how much effort is it worth
  - 80:20 rule
- Scalability
  - Does run time decrease by 2x when I use 2x cores?
    - Strong scalability
  - Does run time remain the same when I keep the amount of work per core the same?
    - Weak scalability

IPM

- Very good tool to get an overall picture
  - Overall MFLOP
  - Communication/Computation ratio
- Pros
  - Quick and easy!
  - Minimal overhead
- Cons
  - Needs manual work to drill down

http://ipm-hpc.sourceforge.net/

IPM Mechanics

On Ranger:

1) module load ipm

2) just before the ibrun command in the batch script add:

```
setenv LD_PRELOAD $TACC_IPM_LIB/libipm.so
```

3) run as normal

4) to generate webpage

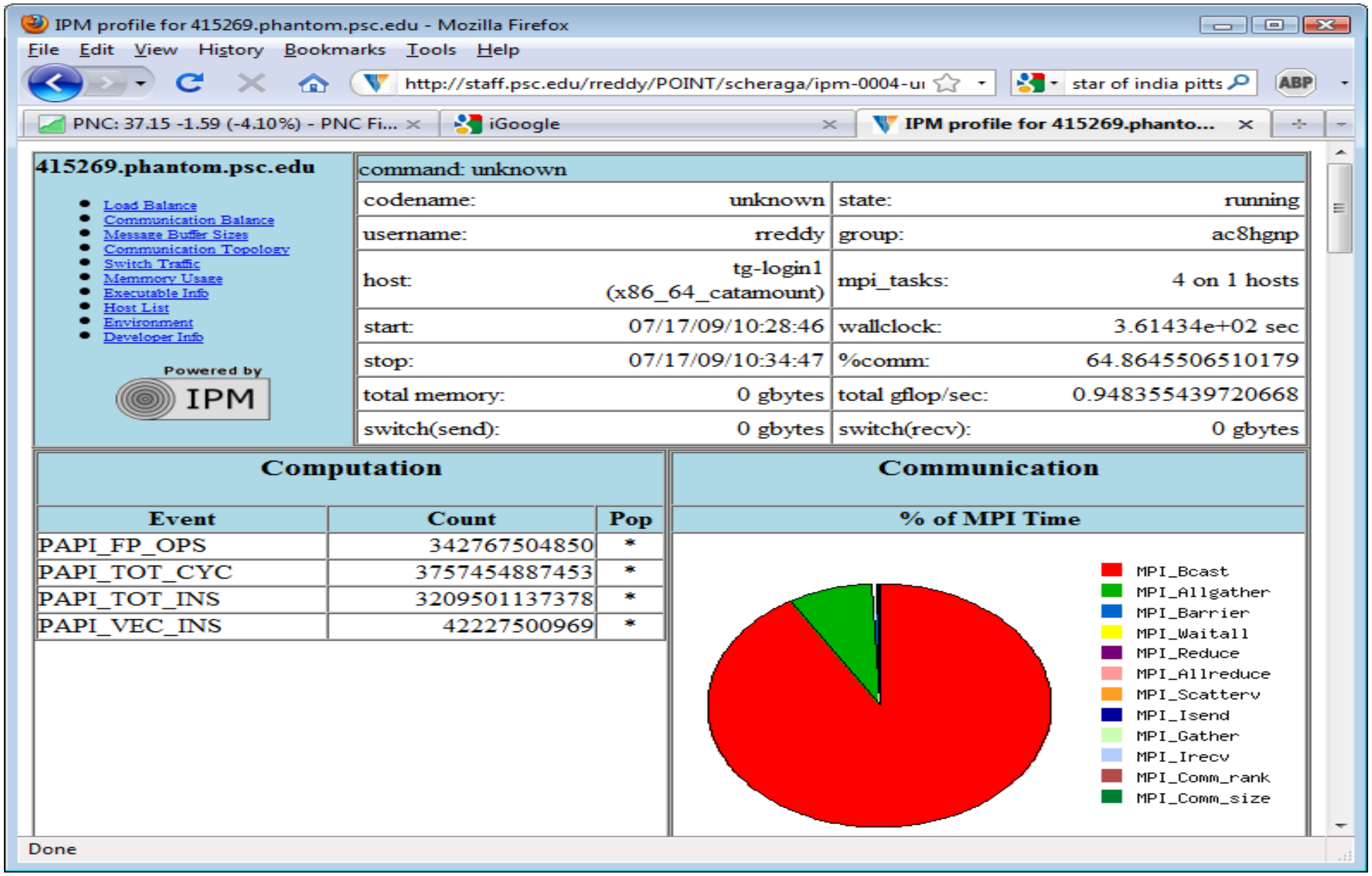
```
module load ipm (if not already)
ipm_parse -html <xml_file>
```

You should be left with a directory with the html in. Tar it up, move to to your local computer and open index.html with your browser.

IPM Overhead

- Was run with 500 MD steps (time in sec)
  - base: MD steps: 5.14637E+01
  - base-ipm: MD steps: 5.13576E+01
- Overhead is negligible

IPM Results: Overall Picture


IPM profile for 415269.phantom.psc.edu - Mozilla Firefox
File Edit View History Bookmarks Tools Help
http://staff.psc.edu/rreddy/POINT/scheraga/ipm-0004-u
star of india pitts
PNC: 37.15 -1.59 (-4.10%) - PNC Fi...
iGoogle
IPM profile for 415269.phanto...
Done

415269.phantom.psc.edu

- Load Balance
- Communication Balance
- Message Buffer Sizes
- Communication Topology
- Switch Traffic
- Memmory Usage
- Executable Info
- Host List
- Environment
- Developer Info

Powered by IPM

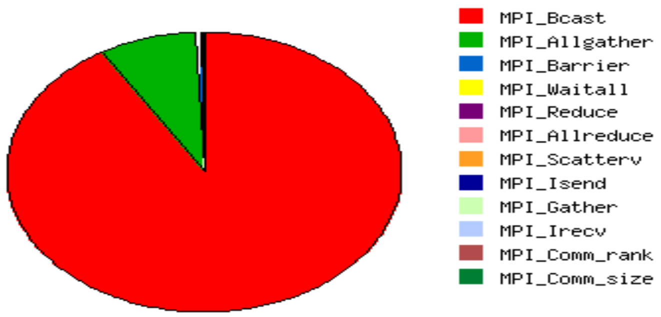
command: unknown			
codename:	unknown	state:	running
username:	rreddy	group:	ac8hgnp
host:	tg-login1 (x86_64_catamount)	mpi_tasks:	4 on 1 hosts
start:	07/17/09/10:28:46	wallclock:	3.61434e+02 sec
stop:	07/17/09/10:34:47	%comm:	64.8645506510179
total memory:	0 gbytes	total gflop/sec:	0.948355439720668
switch(send):	0 gbytes	switch(recv):	0 gbytes

Computation

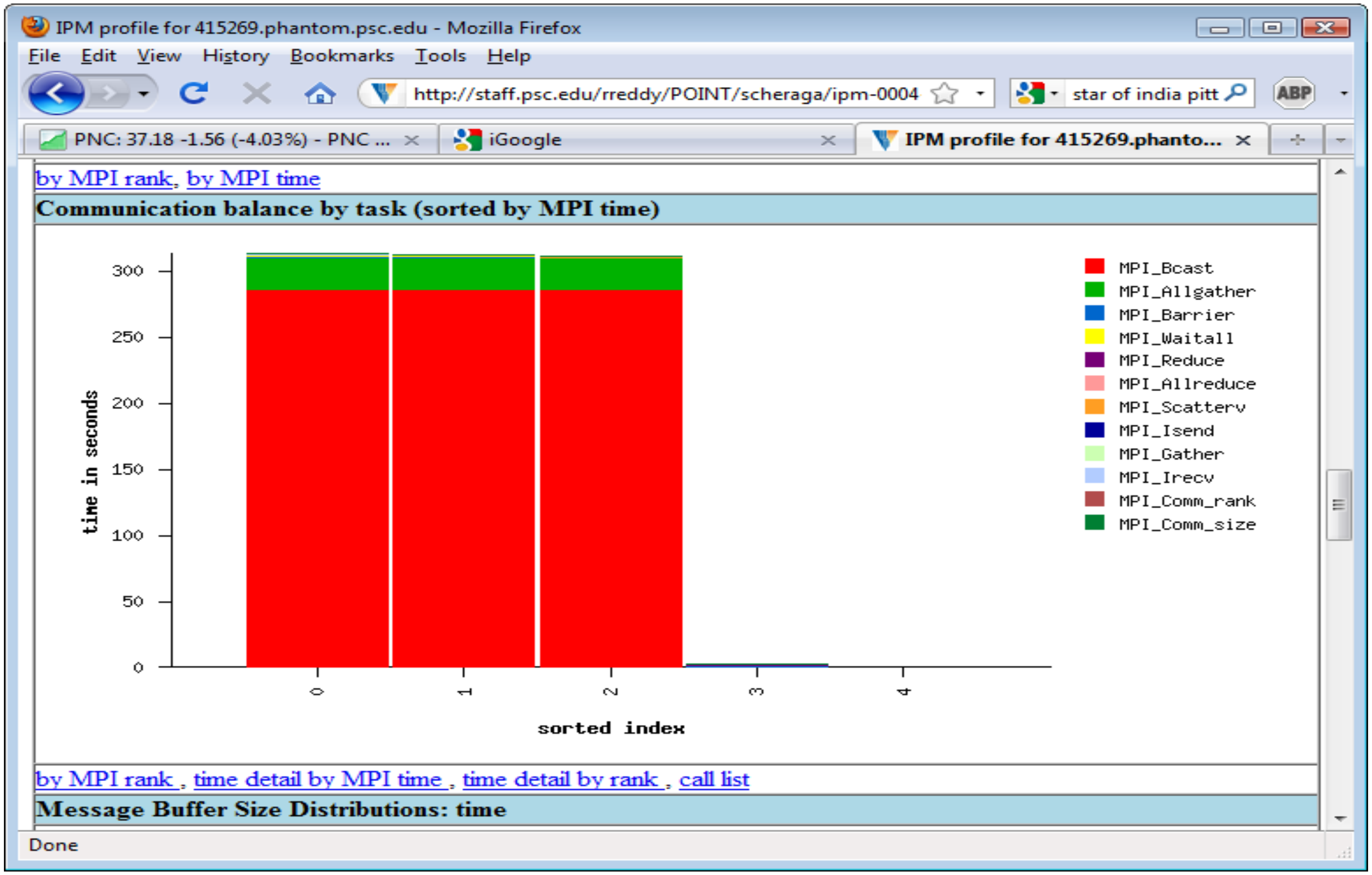
Event	Count	Pop
PAPI_FP_OPS	342767504850	*
PAPI_TOT_CYC	3757454887453	*
PAPI_TOT_INS	3209501137378	*
PAPI_VEC_INS	42227500969	*

Communication

% of MPI Time



IPM – Communication (overall)


IPM profile for 415269.phantom.psc.edu - Mozilla Firefox

http://staff.psc.edu/rreddy/POINT/scheraga/ipm-0004

by MPI rank, by MPI time

Communication balance by task (sorted by MPI time)

by MPI rank , time detail by MPI time , time detail by rank , call list

Message Buffer Size Distributions: time

Done

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Which Functions are Important?

- Usually a handful of functions account for 90% of the execution time
- Make sure you are measuring the production part of your code
- For parallel apps, measure at high core counts – insignificant functions become significant!

PerfSuite

- Similar to IPM: great for getting overall picture of application performance
- Pros
  - Easy: no need to recompile
  - Minimal overhead
  - Provides function-level information
- Cons
  - Not available on all architectures: (x86, x86-64, em64t, and ia64)

http://perfsuite.ncsa.uiuc.edu/

PerfSuite Mechanics

```
# First, be sure to set all paths properly (can do in .cshrc/.profile)

 % set PSDIR=/opt/perfsuite
 % source $PSDIR/bin/psenv.csh

 # Use psrun on your program to generate the data,
 # then use psprocess to produce an HTML file (default is plain text)

 % psrun myprog
 % psprocess --html myprog.12345.xml > myprog.html

 # Take a look at the results

 % your-web-browser myprog.html

 # Second run, but this time profiling instead of counting

 % psrun –C -c papi_profile_cycles.xml myprog
 % psprocess -e myprog myprog.67890.xml
```

First case provides hardware counter stats

```
Index Description                                    Counter Value
==================================================================
1 Conditional branch instructions mispredicted.....     4831072449
4 Floating point instructions......................    86124489172
5 Total cycles.....................................   594547754568
6 Instructions completed...........................  1049339828741

Statistics
==================================================================
Graduated instructions per cycle...................          1.765
Graduated floating point instructions per cycle....          0.145
Level 3 cache miss ratio (data)....................          0.957
Bandwidth used to level 3 cache (MB/s).............        385.087
% cycles with no instruction issue.................         10.410
% cycles stalled on memory access..................         43.139
MFLOPS (cycles)....................................        115.905
MFLOPS (wallclock).................................        114.441
```

Second case gives contributions of functions

```
Function Summary
---------------------------------------------------------------------------------
 Samples   Self %  Total %  Function

   154346   76.99%   76.99%  pc_jac2d_blk3
    14506    7.24%   84.23%  cg3_blk
    10185    5.08%   89.31%  matxvec2d_blk3
     6937    3.46%   92.77%  __kmp_x86_pause
     4711    2.35%   95.12%  __kmp_wait_sleep
     3042    1.52%   96.64%  dot_prod2d_blk3
     2366    1.18%   97.82%  add_exchange2d_blk3


Function:File:Line Summary
---------------------------------------------------------------------------------
 Samples   Self %  Total %  Function:File:Line

    39063   19.49%   19.49%  pc_jac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:20
    24134   12.04%   31.52%  pc_jac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:19
    15626    7.79%   39.32%  pc_jac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:21
    15028    7.50%   46.82%  pc_jac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:33
    13878    6.92%   53.74%  pc_jac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:24
    11880    5.93%   59.66%  pc_jac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:31
     8896    4.44%   64.10%  pc_jac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:22
     7863    3.92%   68.02%  matxvec2d_blk3:/home/rkufrin/apps/aspcg/matxvec2d_blk3.f:19
     7145    3.56%   71.59%  pc_jac2d_blk3:/home/rkufrin/apps/aspcg/pc_jac2d_blk3.f:32
```

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Instrument Key Functions

- Instrumentation: insert functions into source code to measure performance
- Pro: Gives precise information about where things happen
- Con: High overhead and perturbation of application performance
- Thus essential to only instrument important functions

TAU: Tuning and Analysis Utilities

- Useful for a more detailed analysis
  - Routine level
  - Loop level
  - Performance counters
  - Communication performance
- A more sophisticated tool
  - Performance analysis of Fortran, C, C++, Java, and Python
  - Portable: Tested on all major platforms
  - Steeper learning curve

  http://www.cs.uoregon.edu/research/tau/home.php

General Instructions for TAU

- Use a TAU Makefile stub (even if you don’t use makefiles for your compilation)
- Use TAU scripts for compiling
- Example (most basic usage):

```
module load tau

setenv TAU_MAKEFILE <path>/Makefile.tau-papi-pdt-pgi

setenv TAU_OPTIONS "-optVerbose -optKeepFiles“

tau_f90.sh -o hello hello_mpi.f90
```

- Excellent “Cheat Sheet”!
  - Everything you need to know?! (Almost)

  http://www.psc.edu/general/software/packages/tau/TAU-quickref.pdf

Using TAU with Makefiles

- Fairly simple to use with well written makefiles:

```
setenv TAU_MAKEFILE <path>/Makefile.tau-papi-mpi-pdt-pgi
setenv TAU_OPTIONS "-optVerbose –optKeepFiles –optPreProcess”
make FC=tau_f90.sh
```

  - run code as normal
  - run pprof (text) or paraprof (GUI) to get results
  - paraprof --pack file.ppk (packs all of the profile files into one file, easy to copy back to local workstation)

- Example scenarios
  - Typically you can do cut and paste from here:

  http://www.cs.uoregon.edu/research/tau/docs/scenario/index.html

Tiny Routines: High Overhead

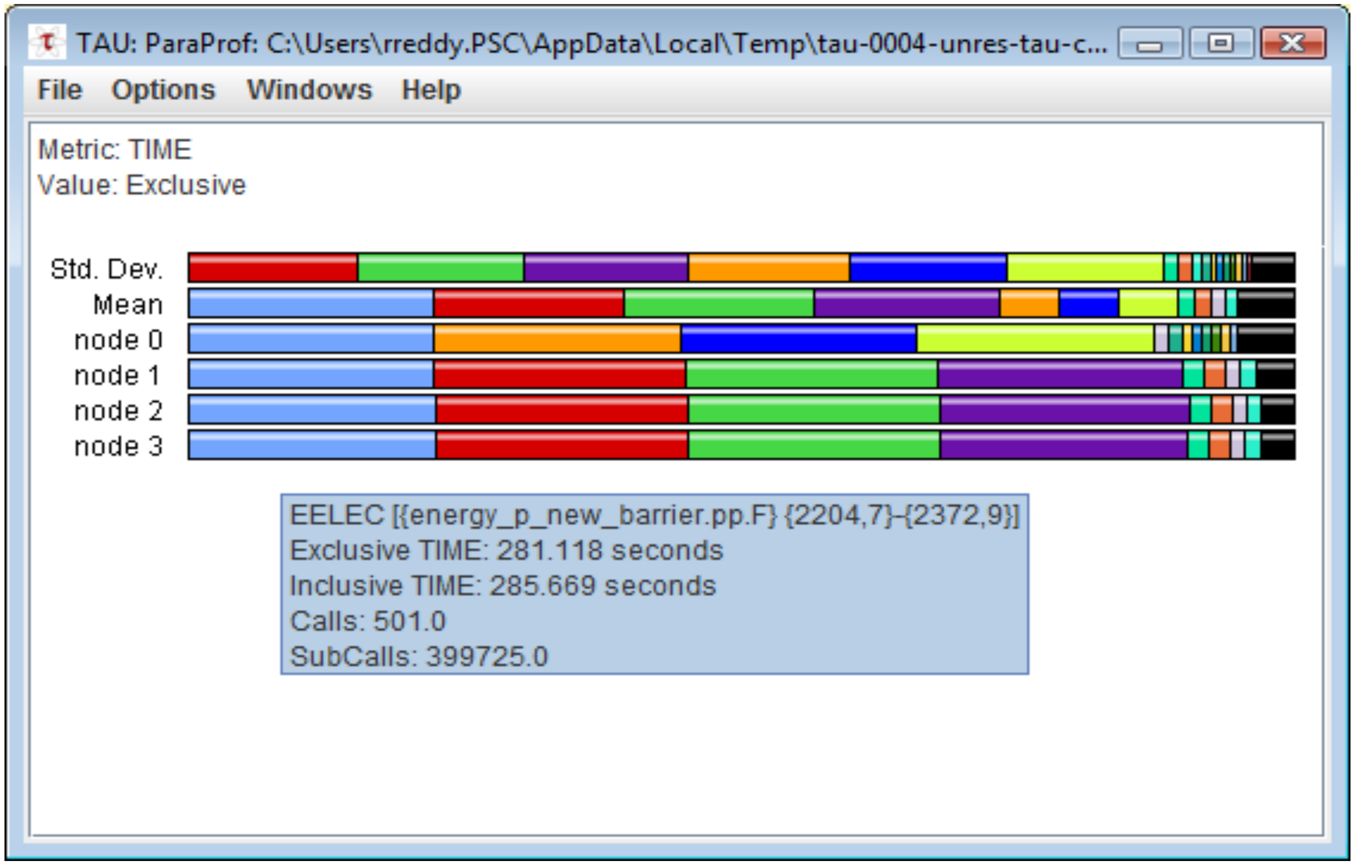
Before:

```
double precision function scalar(u,v)
double precision u(3),v(3)
      scalar=u(1)*v(1)+u(2)*v(2)+u(3)*v(3)
return
end
```

After:

```
double precision function scalar(u,v)
double precision u(3),v(3)
     call TAU_PROFILE_TIMER(profiler, 'SCALAR […]')
     call TAU_PROFILE_START(profiler)
     scalar=u(1)*v(1)+u(2)*v(2)+u(3)*v(3)
     call TAU_PROFILE_STOP(profiler)
return
     call TAU_PROFILE_STOP(profiler)
end
```

Reducing Overhead


TAU: ParaProf: C:\Users\rreddy.PSC\AppData\Local\Temp\tau-0004-unres-tau-c...
File Options Windows Help
Std. Dev.
Mean
node 0
node 1
node 2
node 3

Metric: TIME
Value: Exclusive

EELEC [{energy_p_new_barrier.pp.F} {2204,7}-{2372,9}]
Exclusive TIME: 281.118 seconds
Inclusive TIME: 285.669 seconds
Calls: 501.0
SubCalls: 399725.0

Overhead (time in sec):

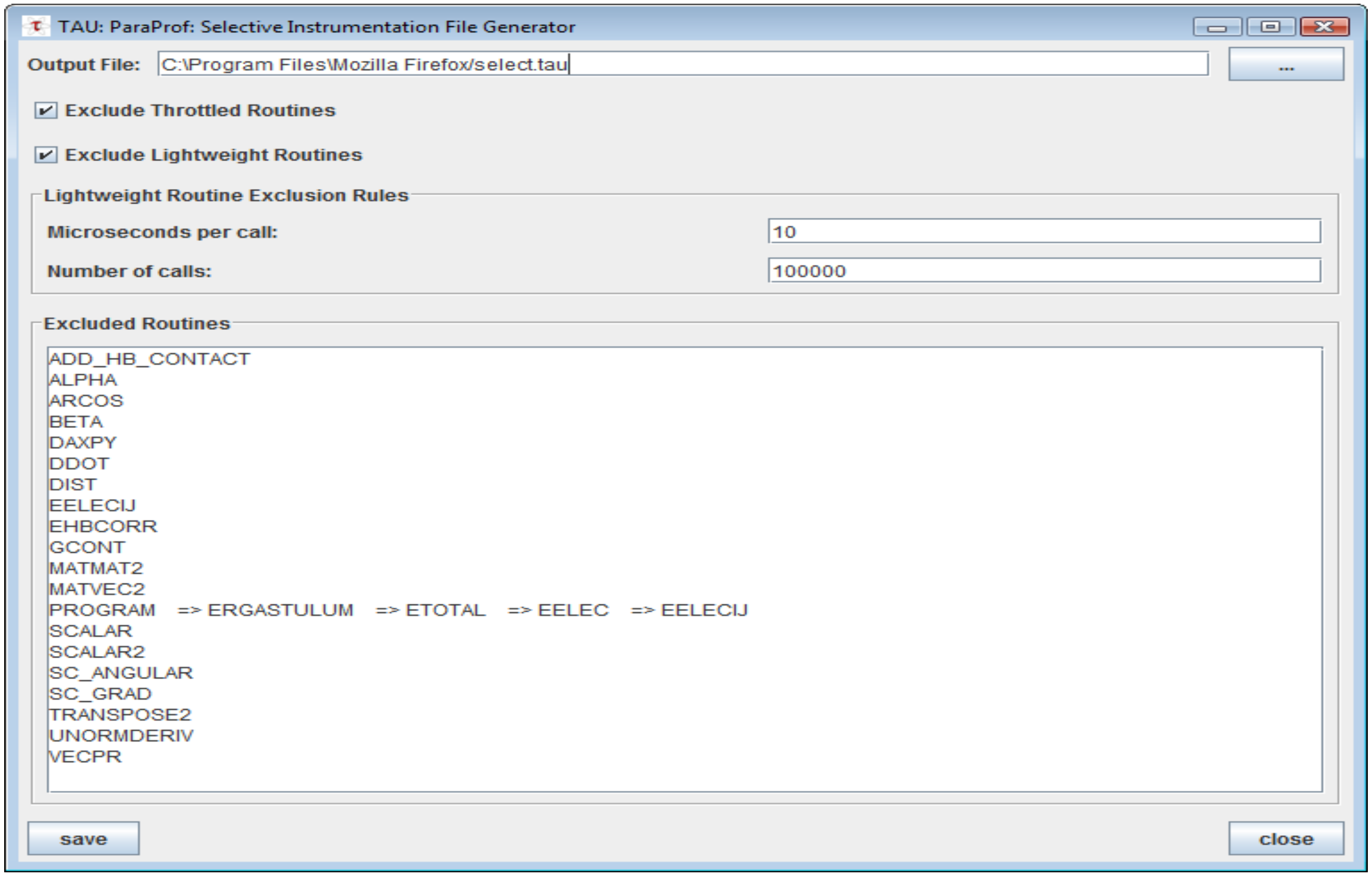
MD steps base:
5.14637E+01

MD steps base with TAU :
3.15578E+02

Must reduce overhead to get meaningful results:

- In paraprof go to "File" and select "Create Selective Instrumentation File"

Selective Instrumentation File



Output File: C:\Program Files\Mozilla Firefox/select.tau

[✓] Exclude Throttled Routines

[✓] Exclude Lightweight Routines

Lightweight Routine Exclusion Rules

Microseconds per call: 10

Number of calls: 100000

Excluded Routines

```
ADD_HB_CONTACT
ALPHA
ARCOS
BETA
DAXPY
DDOT
DIST
EELECIJ
EHBCORR
GCONT
MATMAT2
MATVEC2
PROGRAM   => ERGASTULUM   => ETOTAL   => EELEC   => EELECIJ
SCALAR
SCALAR2
SC_ANGULAR
SC_GRAD
TRANSPOSE2
UNORMDERIV
VECPR
```

Selective Instrumentation File

- Files to include/exclude
- Routines to include/exclude
- Directives for loop instrumentation
- Phase definitions
- Specify the file in TAU_OPTIONS and recompile:

```
setenv TAU_OPTIONS "-optVerbose –optKeepFiles
 –optPreProcess -optTauSelectFile=select .tau“
```

- http://www.cs.uoregon.edu/research/tau/docs/newguide/bk03ch01.html

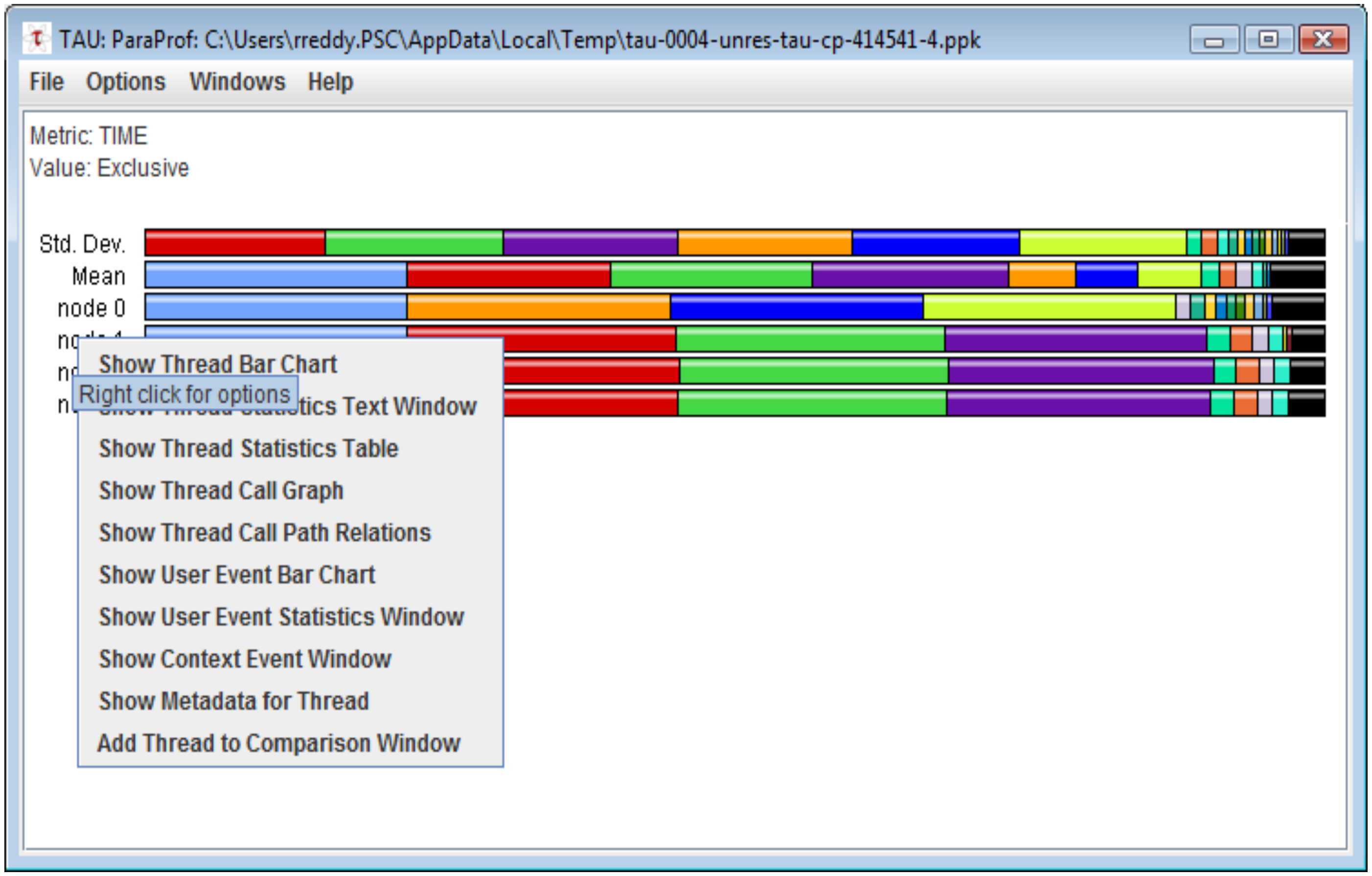
Getting a Call Path with TAU

- Why do I need this?
  - To optimize a routine, you often need to know what is above and below it
  - Helps with defining phases: stages of execution within the code that you are interested in
- To get callpath info, do the following at runtime:

  setenv TAU_CALLPATH 1 (this enables callpath)

  setenv TAU_CALLPATH_DEPTH 50 (defines depth)

Getting Call Path Information


TAU: ParaProf: C:\Users\rreddy.PSC\AppData\Local\Temp\tau-0004-unres-tau-cp-414541-4.ppk
File
Options
Windows
Help
Std. Dev.
Mean
node 0
Show Thread Bar Chart
Right click for options
Show Thread Statistics Text Window
Show Thread Statistics Table
Show Thread Call Graph
Show Thread Call Path Relations
Show User Event Bar Chart
Show User Event Statistics Window
Show Context Event Window
Show Metadata for Thread
Add Thread to Comparison Window

Metric: TIME
Value: Exclusive

Right click name of node and select "Show Thread Call Graph"

Phase Profiling: Isolate regions of code execution

- Specify a region of the code of interest: e.g. the main computational kernel
- Use call path to find where in the code that region begins and ends
- Then put something like this in selective instrumentation file:

```
static phase name="foo1_bar“ file="foo.c“ line=26 to line=27
```

- Recompile and rerun

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Hardware Counters

Hardware performance counters available on most modern microprocessors can provide insight into:

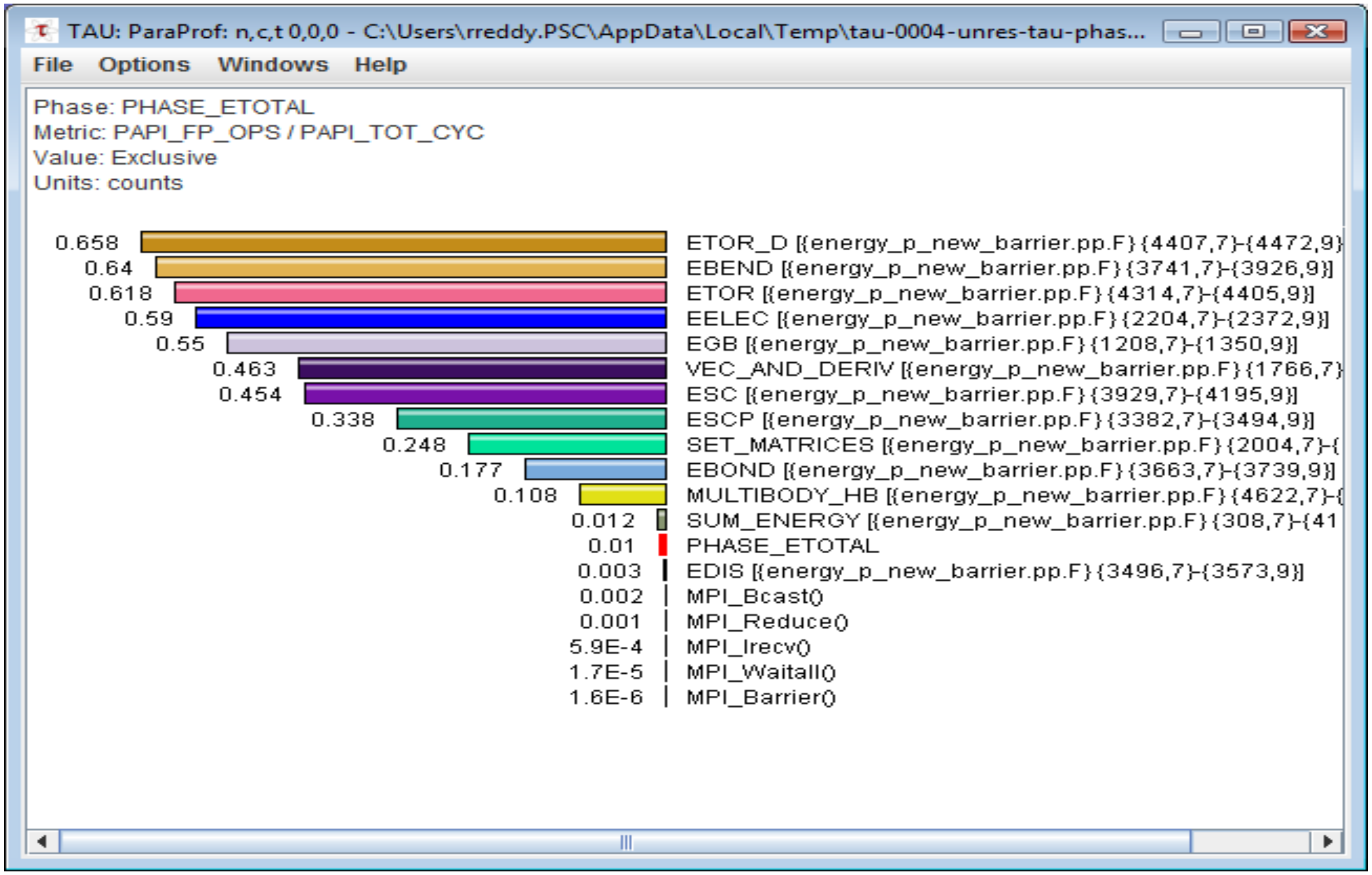
1. **Whole program timing**
2. **Cache behaviors**
3. **Branch behaviors**
4. **Memory and resource access patterns**
5. **Pipeline stalls**
6. **Floating point efficiency**
7. **Instructions per cycle**
8. **Subroutine resolution**
9. **Process or thread attribution**

Detecting Serial Performance Issues

- Identify hardware performance counters of interest
  - papi_avail
  - papi_native_avail
  - Run these commands on compute nodes! Login nodes will give you an error.
- Run TAU (perhaps with phases defined to isolate regions of interest)
- Specify PAPI hardware counters at run time:

```
setenv TAU_METRICS GET_TIME_OF_DAY:PAPI_FP_OPS:PAPI_TOT_CYC
```

Perf of EELEC (peak is 2)


TAU: ParaProf: n,c,t 0,0,0 - C:\Users\rreddy.PSC\AppData\Local\Temp\tau-0004-unres-tau-phas...
File Options Windows Help

Phase: PHASE_ETOTAL
Metric: PAPI_FP_OPS / PAPI_TOT_CYC
Value: Exclusive
Units: counts

```
0.658   ETOR_D [{energy_p_new_barrier.pp.F} {4407,7}-{4472,9}
0.64    EBEND [{energy_p_new_barrier.pp.F} {3741,7}-{3926,9}]
0.618   ETOR [{energy_p_new_barrier.pp.F} {4314,7}-{4405,9}]
0.59    EELEC [{energy_p_new_barrier.pp.F} {2204,7}-{2372,9}]
0.55    EGB [{energy_p_new_barrier.pp.F} {1208,7}-{1350,9}]
0.463   VEC_AND_DERIV [{energy_p_new_barrier.pp.F} {1766,7}
0.454   ESC [{energy_p_new_barrier.pp.F} {3929,7}-{4195,9}]
0.338   ESCP [{energy_p_new_barrier.pp.F} {3382,7}-{3494,9}]
0.248   SET_MATRICES [{energy_p_new_barrier.pp.F} {2004,7}-{
0.177   EBOND [{energy_p_new_barrier.pp.F} {3663,7}-{3739,9}]
0.108   MULTIBODY_HB [{energy_p_new_barrier.pp.F} {4622,7}-{
0.012   SUM_ENERGY [{energy_p_new_barrier.pp.F} {308,7}-{41
0.01    PHASE_ETOTAL
0.003   EDIS [{energy_p_new_barrier.pp.F} {3496,7}-{3573,9}]
0.002   MPI_Bcast()
0.001   MPI_Reduce()
5.9E-4  MPI_Irecv()
1.7E-5  MPI_Waitall()
1.6E-6  MPI_Barrier()
```

Go to: Paraprof manager Options ->"Show derived metrics panel"

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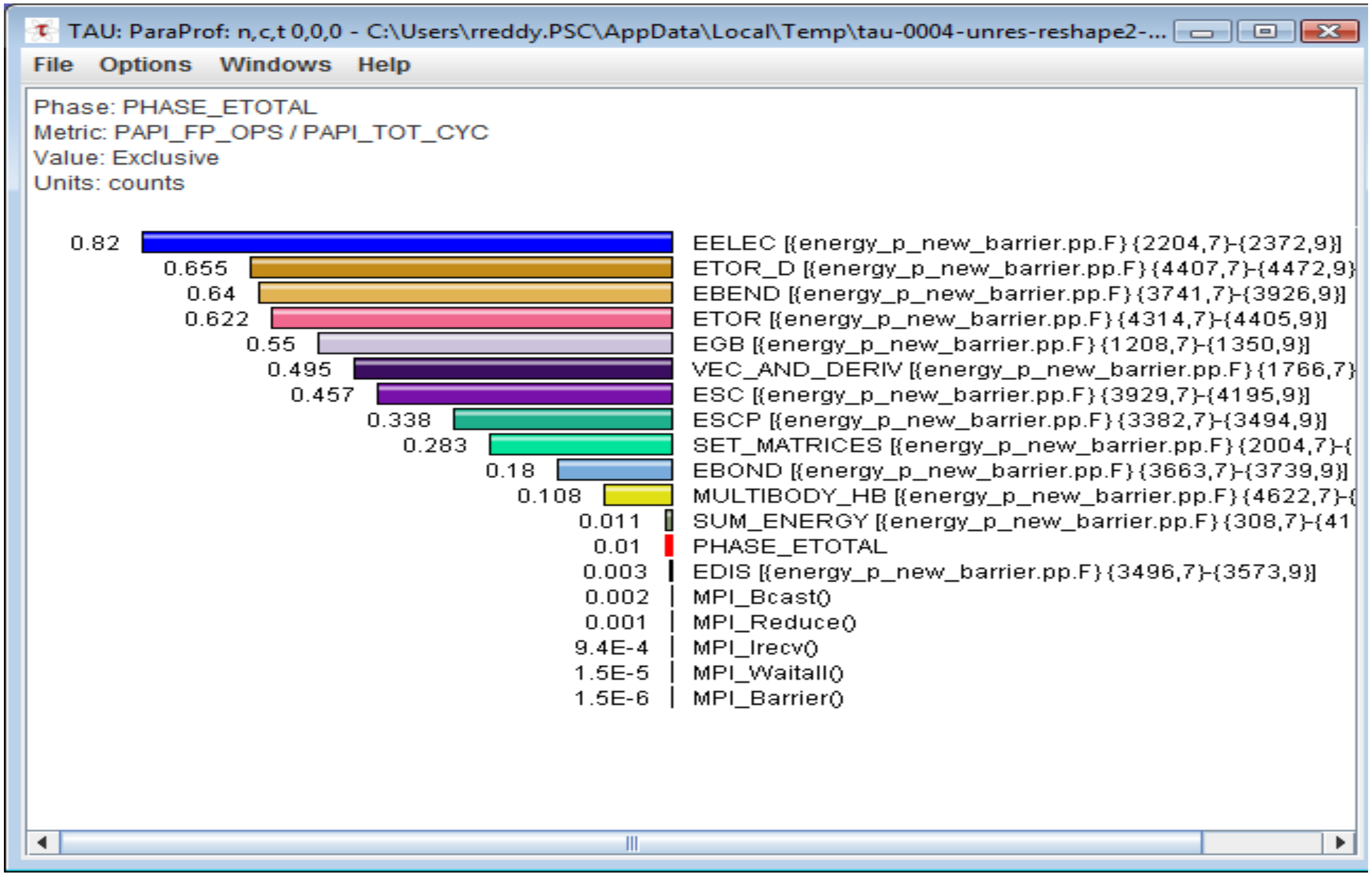
EELEC – After forcing inlining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File Options Windows Help

Phase: PHASE_ETOTAL
Metric: PAPI_FP_OPS / PAPI_TOT_CYC
Value: Exclusive
Units: counts

```
0.82    EELEC [{energy_p_new_barrier.pp.F} {2204,7}-{2372,9}]
0.655   ETOR_D [{energy_p_new_barrier.pp.F} {4407,7}-{4472,9}
0.64    EBEND [{energy_p_new_barrier.pp.F} {3741,7}-{3926,9}]
0.622   ETOR [{energy_p_new_barrier.pp.F} {4314,7}-{4405,9}]
0.55    EGB [{energy_p_new_barrier.pp.F} {1208,7}-{1350,9}]
0.495   VEC_AND_DERIV [{energy_p_new_barrier.pp.F} {1766,7}
0.457   ESC [{energy_p_new_barrier.pp.F} {3929,7}-{4195,9}]
0.338   ESCP [{energy_p_new_barrier.pp.F} {3382,7}-{3494,9}]
0.283   SET_MATRICES [{energy_p_new_barrier.pp.F} {2004,7}-{
0.18    EBOND [{energy_p_new_barrier.pp.F} {3663,7}-{3739,9}]
0.108   MULTIBODY_HB [{energy_p_new_barrier.pp.F} {4622,7}-{
0.011   SUM_ENERGY [{energy_p_new_barrier.pp.F} {308,7}-{41
0.01    PHASE_ETOTAL
0.003   EDIS [{energy_p_new_barrier.pp.F} {3496,7}-{3573,9}]
0.002   MPI_Bcast()
0.001   MPI_Reduce()
9.4E-4  MPI_Irecv()
1.5E-5  MPI_Waitall()
1.5E-6  MPI_Barrier()
```

Further Info on Serial Optimization

- Tools help you find issues – solving issues is application and hardware specific
- Good resource on techniques for serial optimization:

  “Performance Optimization of Numerically Intensive Codes” Stefan Goedecker, Adolfy Hoisie, SIAM, 2001.

Performance Engineering: Procedure

- Serial
  - Assess overall serial performance (percent of peak)
  - Identify functions where code spends most time
  - Instrument those functions
  - Measure code performance using hardware counters
  - Identify inefficient regions of source code and cause of inefficiencies
- Parallel
  - Assess overall parallel performance (scaling)
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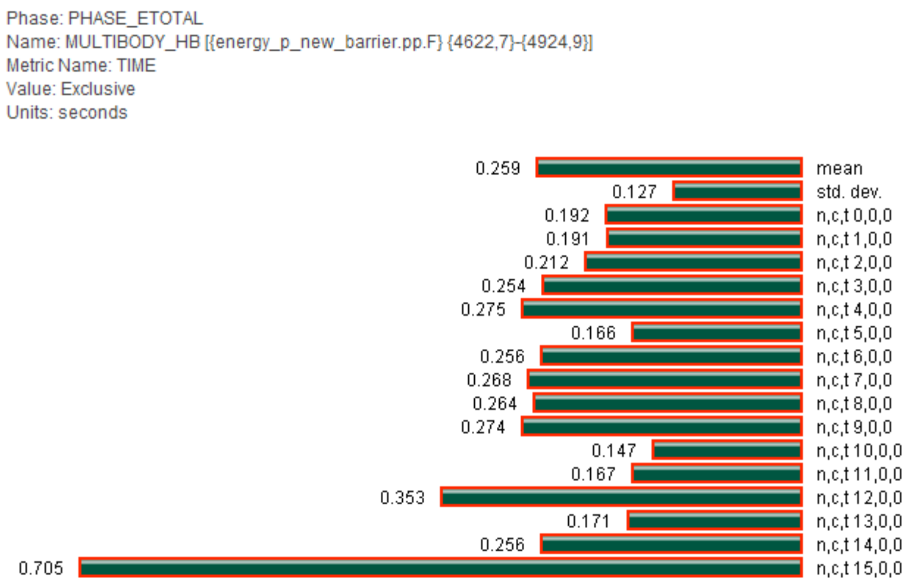
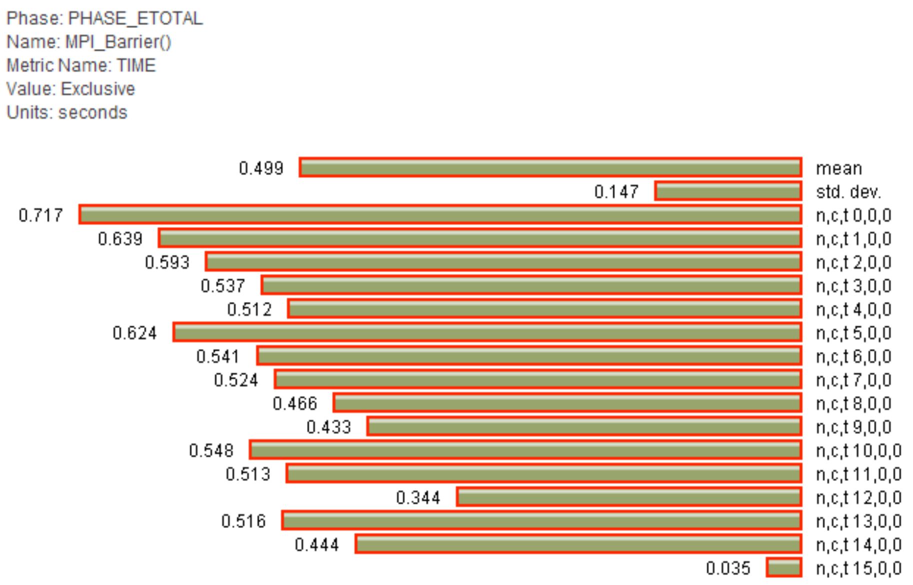
  - Identify load balancing issues, serial regions
  - Identify communication bottlenecks--use tracing to help identify cause and effect

Detecting Parallel Performance Issues: Load Imbalance

- Examine timings of functions in your region of interest
- To look at load imbalance:
  - If you defined a phase, from paraprof window, right-click on phase name and select: “Show profile for this phase”
  - Left-click on function name to look at timings across all processors

Load Imbalance





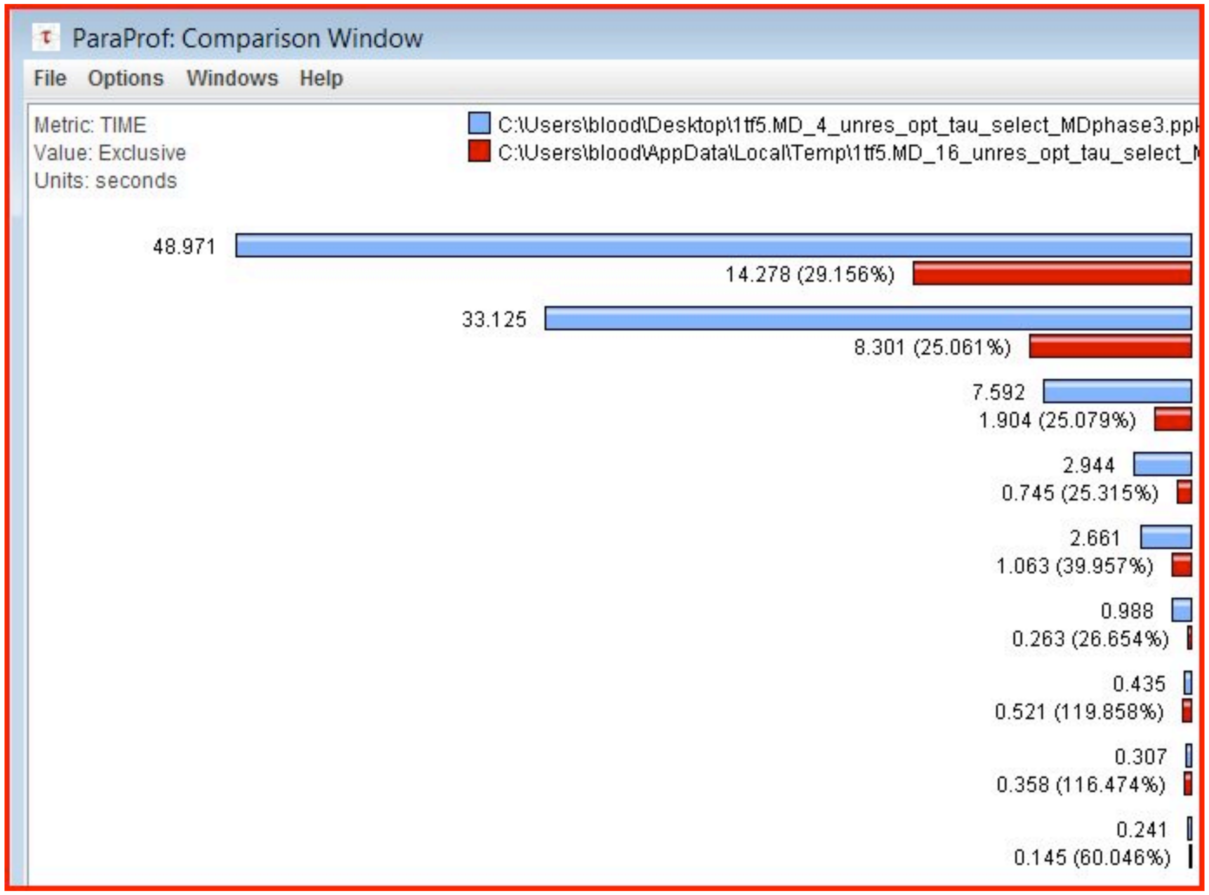
Load imbalance on one processor causing other processors to idle in MPI_Barrier

May need to change how data is distributed, or even change underlying algorithm.

Detecting Parallel Performance Issues: Serial Bottlenecks

- To identify scaling bottlenecks (including serial regions), do the following for each run in a scaling study (e.g. 2-64 cores):
  - In Paraprof manager right-click “Default Exp” and select “Add Trial”. Find packed profile file and add it.
  - If you defined a phase, from main paraprof window select: Windows -> Function Legend-> Filter->Advanced Filtering
  - Type in the name of the phase you defined, and click ‘OK’
  - Return to Paraprof manager, right-click the name of the trial, and select “Add to Mean Comparison Window”
- Compare functions across increasing core counts

Function Scaling and Serial Bottlenecks



Metric: TIME
Value: Exclusive
Units: seconds

🟦 C:\Users\blood\Desktop\1tf5.MD_4_unres_opt_tau_select_MDphase3.ppk
🟥 C:\Users\blood\AppData\Local\Temp\1tf5.MD_16_unres_opt_tau_select_M

```
48.971
14.278 (29.156%)
33.125
8.301 (25.061%)
7.592
1.904 (25.079%)
2.944
0.745 (25.315%)
2.661
1.063 (39.957%)
0.988
0.263 (26.654%)
0.435
0.521 (119.858%)
0.307
0.358 (116.474%)
0.241
0.145 (60.046%)
```

Identify which functions need to scale better, or be parallelized, in order to increase overall scalability.

Find which communication routines are starting to dominate runtimes.

Use call path information to find where those communication routines are being called

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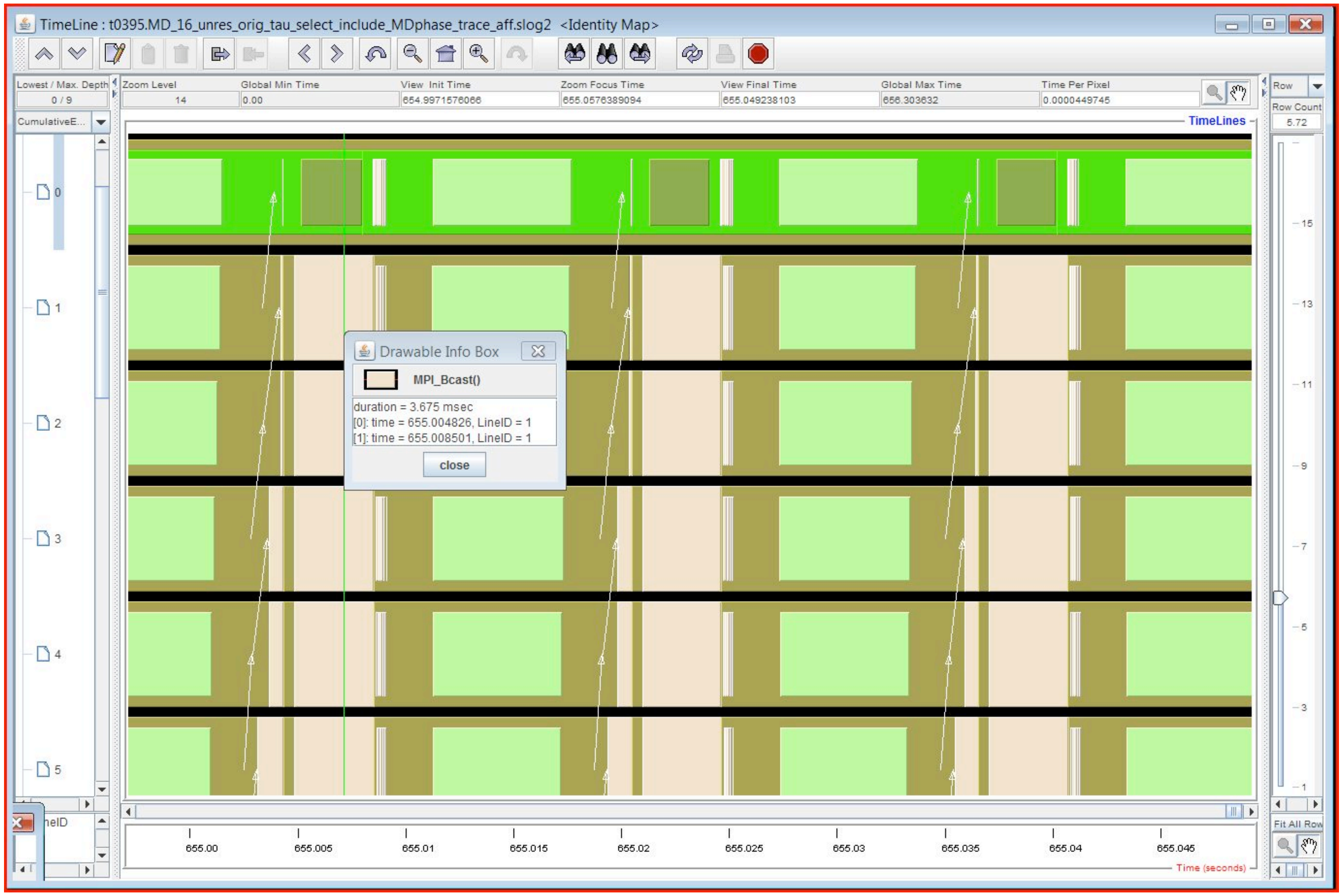
Generating a Trace

- At runtime: setenv TAU_TRACE 1
- Follow directions here to analyze:

http://www.psc.edu/general/software/packages/tau/TAU-quickref.pdf

- Insight into causes of communication bottlenecks
  - Duration of individual MPI calls
  - Use of blocking calls
  - Posting MPI calls too early or too late
  - Opportunities to overlap computation and communication

TAU Trace in Jumpshot



TimeLine : t0395.MD_16_unres_orig_tau_select_include_MDphase_trace_aff.slog2 <Identity Map>

Lowest / Max. Depth	Zoom Level	Global Min Time	View Init Time	Zoom Focus Time	View Final Time	Global Max Time	Time Per Pixel	Row Count
0 / 9	14	0.00	654.9971576066	655.0576389094	655.049238103	656.303632	0.0000449745	5.72

```
Drawable Info Box
MPI_Bcast()
duration = 3.675 msec
[0]: time = 655.004826, LineID = 1
[1]: time = 655.008501, LineID = 1
close
```

Issues with Tracing

- At high processor counts the amount of data becomes overwhelming
- Very selective instrumentation is critical to manage data
- Also need to isolate the computational kernel and trace for minimum number of iterations to see patterns
- Complexity of manually analyzing traces on thousands of processors is an issue
- SCALASCA attempts to do automated analysis of traces to determine communication problems
- Vampir, Intel Trace Analyzer: cutting-edge trace analyzers (but not free)

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Hands-On

- Find parallel performance issues in a production scientific application using TAU
- Feel free to experiment with your own application
- Document posted on Google groups:

  Performance_Profiling_Exercise.pdf