

# HPC Software – Debugger and Performance Tools

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- Local module setup
- Compilers
- Libraries

## **Debugger:**

- TotalView / DDT
- MUST
- Intel Inspector

Make it work,  
make it right,  
make it fast.

*Kent Beck*

## **Performance Tools:**

- Score-P
- Scalasca
- Vampir
- Intel Vtune Amplifier
- Intel Advisor
- Performance Reports
- TAU
- NVIDIA Visual Profiler
- Darshan
- PAPI

# Module setup & compiler

- Tools are available through “modules”
  - Allows to **easily manage** different versions of programs
  - Works by **dynamic** modification of a user's environment
- Module setup based on **EasyBuild** and **Imod**
  - Staged, hierarchical setup
  - Automatically manages dependencies via toolchains
- Consistent setup on JURECA (cluster & booster) and JEWELS

# Most Important Module Commands

module

- spider # show all products
- spider *product* # show product details
- avail # show all available products
- list # list loaded products
  
- load *product(s)* # setup access to product
- unload *product(s)* # release access
- swap *product1 product2* # replace v1 of product with v2
  
- whatis *product(s)* # print short description
- help *product(s)* # print longer description
- show *product(s)* # show what “settings” are performed

- Compiler
  - Intel C/C++ and Fortran compiler
  - GNU C/C++ and Fortran compiler
  - PGI C/C++ and Fortran compiler
  - Clang C/C++ compiler
  - NVIDIA CUDA compiler
- MPI libraries
  - Intel MPI
  - Parastation MPI
  - MVAPICH MPI (CUDA aware)

# Debuggers

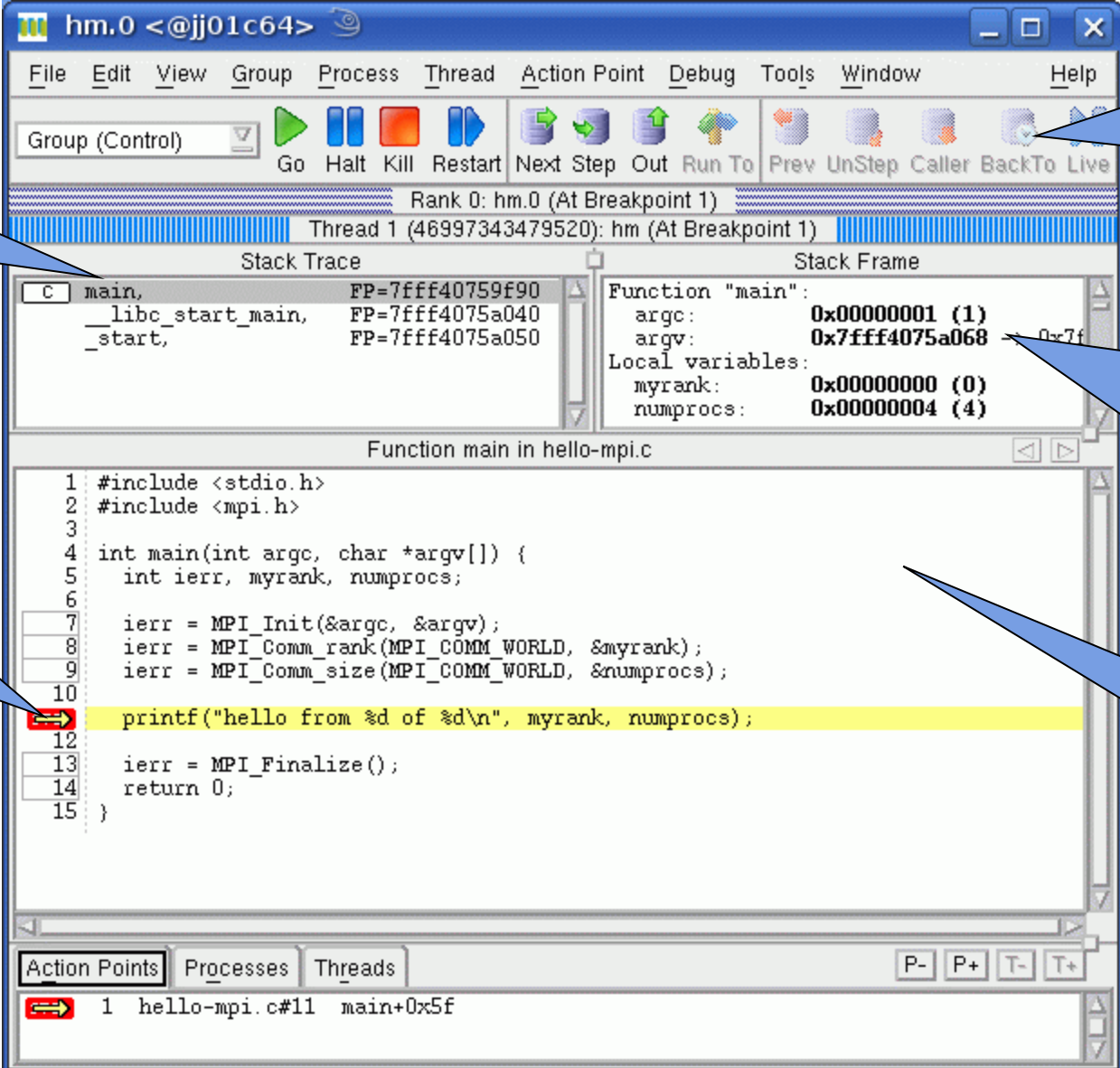
# Debugging Tools (**status: May 2018**)

- TotalView
- DDT
- MUST
- Intel Inspector



- UNIX Symbolic Debugger  
for C, C++, F77, F90, PGI HPF, assembler programs
- “Standard” debugger
- Special, non-traditional features
  - Multi-process and multi-threaded
  - C++ support (templates, inheritance, inline functions)
  - F90 support (user types, pointers, modules)
  - 1D + 2D Array Data visualization
  - Support for parallel debugging (MPI: automatic attach, message queues, OpenMP, pthreads)
  - Scripting and batch debugging
  - Memory Debugging
  - CUDA and OpenACC support
- <http://www.roguewave.com>
- **NOTE:** License limited to 2048 processes (shared between all users)

# TotalView: Main Window



The screenshot shows the TotalView debugger interface. At the top is a menu bar (File, Edit, View, Group, Process, Thread, Action Point, Debug, Tools, Window, Help) and a toolbar with icons for Go, Halt, Kill, Restart, Next Step, Out, Run To, Prev, UnStep, Caller, BackTo, and Live. Below the toolbar is a status bar showing 'Rank 0: hm.0 (At Breakpoint 1)' and 'Thread 1 (46997343479520): hm (At Breakpoint 1)'. The main window is divided into several panes. The 'Stack Trace' pane on the left shows a list of frames: 'C main, FP=7fff40759f90', '\_libc\_start\_main, FP=7fff4075a040', and '\_start, FP=7fff4075a050'. The 'Stack Frame' pane on the right shows details for the 'main' function, including arguments 'argc: 0x00000001 (1)' and 'argv: 0x7fff4075a068', and local variables 'myrank: 0x00000000 (0)' and 'numprocs: 0x00000004 (4)'. The 'Source code' pane at the bottom shows the code for 'Function main in hello-mpi.c', with a breakpoint set at line 11: 'printf("hello from %d of %d\n", myrank, numprocs);'. The 'Breakpoints' pane at the bottom left shows a list of breakpoints, with one active at '1 hello-mpi.c#11 main+0x5f'. Callouts point to the 'Stack trace' pane, the 'Break points' pane, the 'Toolbar for common options', the 'Local variables for selected stack frame' pane, and the 'Source code window'.

Stack trace

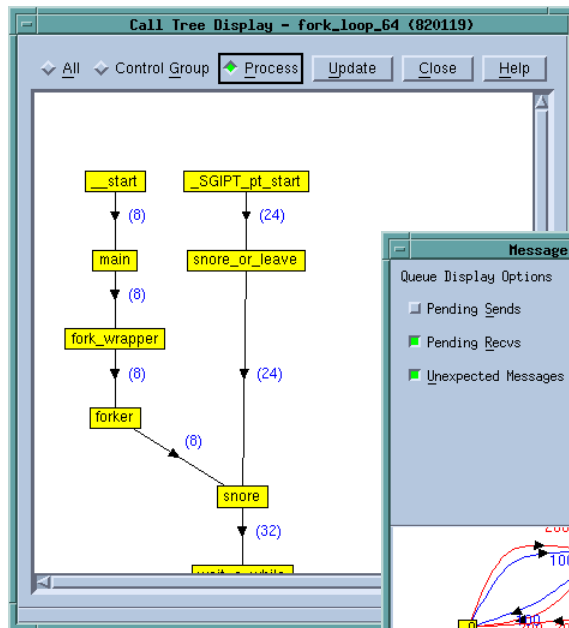
Break points

Toolbar for common options

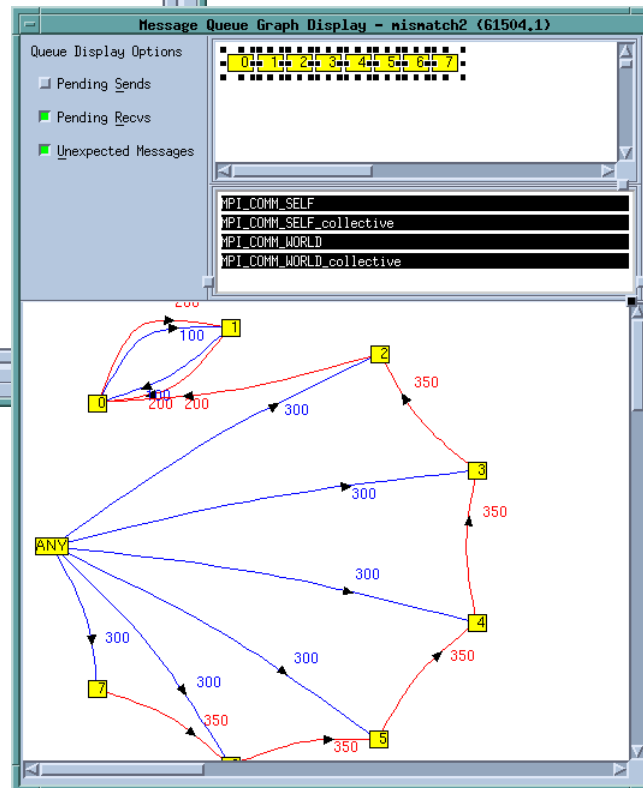
Local variables for selected stack frame

Source code window

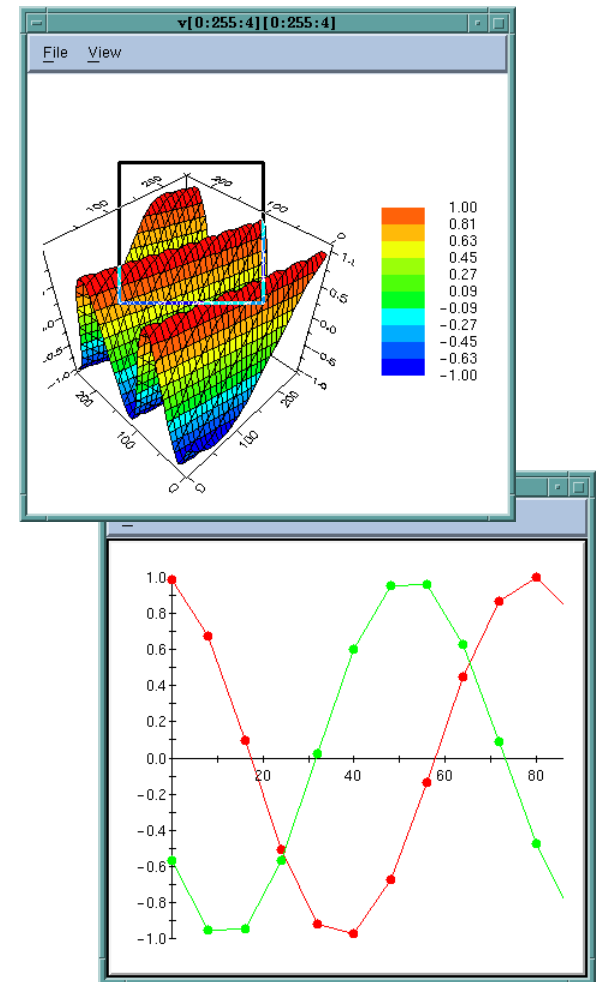
- Call Graph



- Message queue graph

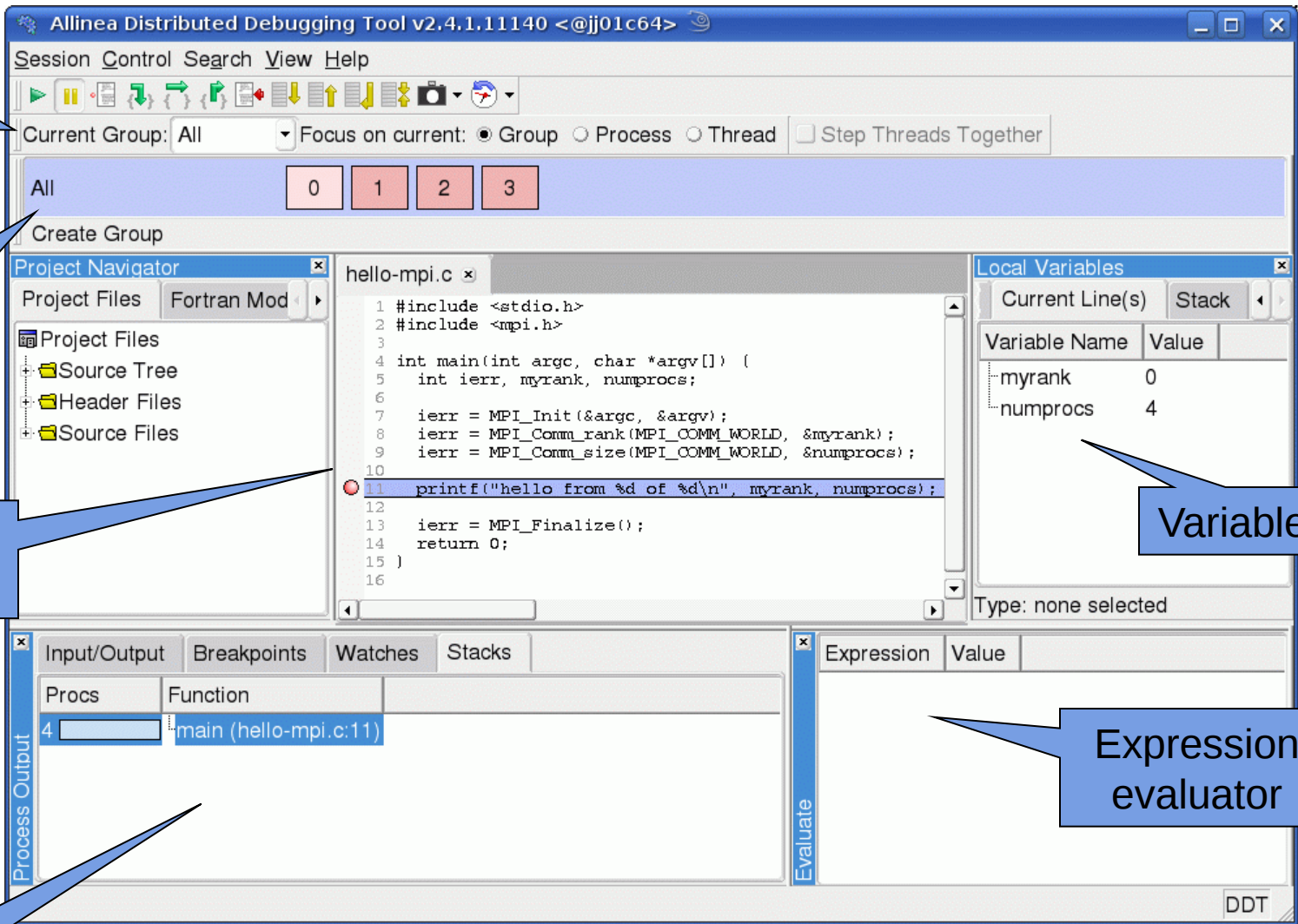


- Data visualization



- UNIX Graphical Debugger for C, C++, F77, F90 programs
- Modern, easy-to-use debugger
- Special, non-traditional features
  - Multi-process and multi-threaded
  - 1D + 2D array data visualization
  - Support for MPI parallel debugging (automatic attach, message queues)
  - Support for OpenMP (Version 2.x and later)
  - Support for CUDA and OpenACC
  - Job submission from within debugger
- <http://www.allinea.com>
- **NOTE:** License limited to 64 processes (shared between all users)

# DDT: Main Window



Process controls

Process groups

Source code

Variables

Expression evaluator

Stack trace

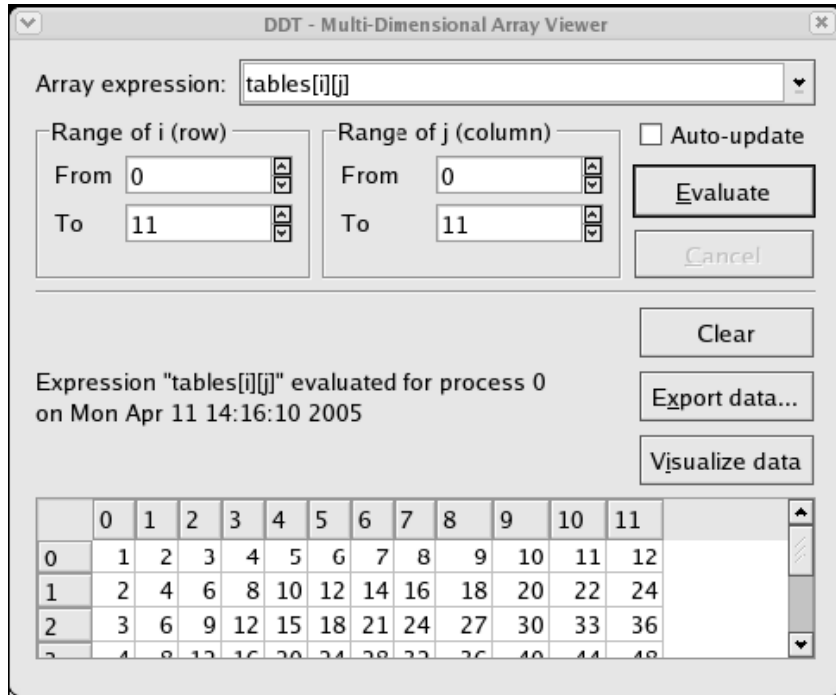
```
1 #include <stdio.h>
2 #include <mpi.h>
3
4 int main(int argc, char *argv[]) {
5     int ierr, myrank, numprocs;
6
7     ierr = MPI_Init(&argc, &argv);
8     ierr = MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
9     ierr = MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
10    printf("hello from %d of %d\n", myrank, numprocs);
11
12    ierr = MPI_Finalize();
13    return 0;
14 }
15
16
```

| Variable Name | Value |
|---------------|-------|
| myrank        | 0     |
| numprocs      | 4     |

| Procs | Function              |
|-------|-----------------------|
| 4     | main (hello-mpi.c:11) |

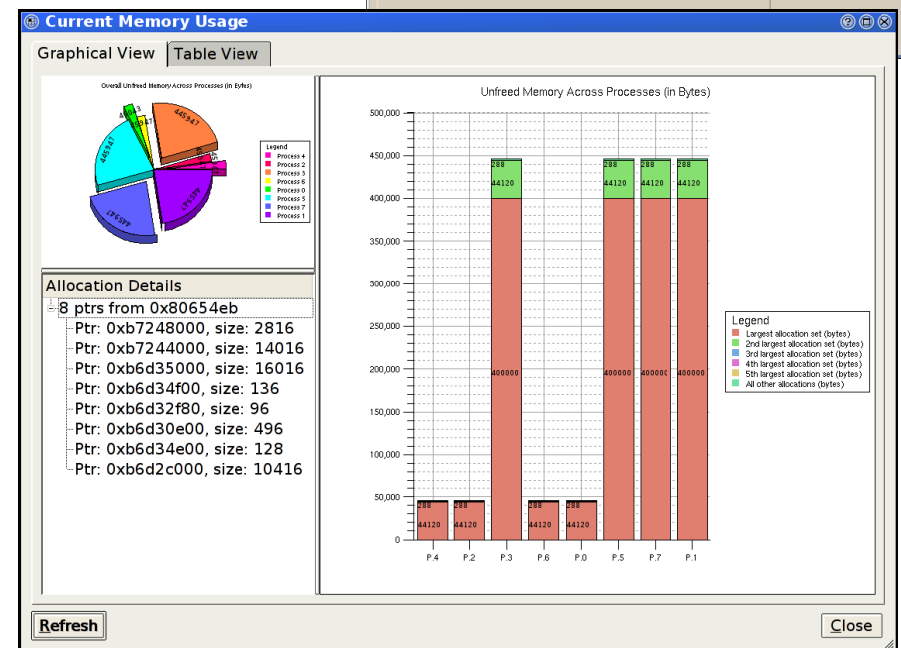
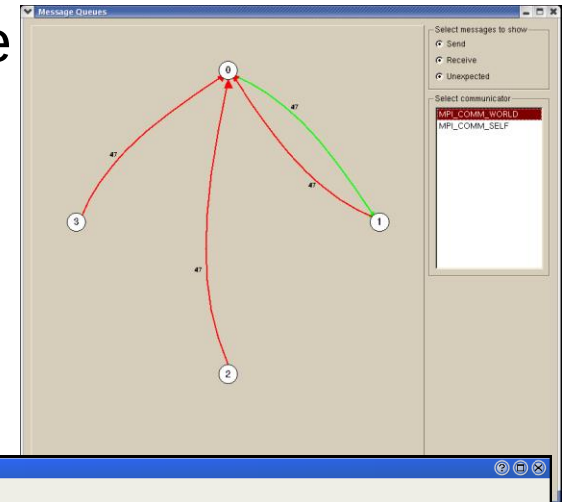
| Expression | Value |
|------------|-------|
|------------|-------|

# DDT: Non-standard Features



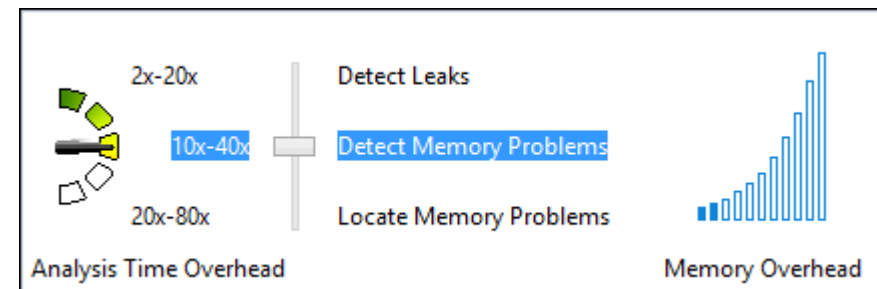
- Multi-Dimensional Array Viewer

- Message queue graph



- Memory Usage

- Detects memory and threading errors
  - Memory leaks, corruption and illegal accesses
  - Data races and deadlocks
- Dynamic instrumentation requiring no recompilation
- Supports C/C++ and Fortran as well as third party libraries
- Multi-level analysis to adjust overhead and analysis capabilities
- API to limit analysis range to eliminate false positives and speed-up analysis



**Intel Inspector**  
Detect Deadlocks and Data Races

Target Analysis Type Collection Log Summary

| ID | Type      | Sources                                                  | Modules                           | State |
|----|-----------|----------------------------------------------------------|-----------------------------------|-------|
| P1 | Data race | find_and_fix_threading_errors.cpp; task_scheduler_init.h | find_and_fix_threading_errors.exe | New   |
| P2 | Data race | blocked_range.h; parallel_for.h; partitioner.h; task.h   | find_and_fix_threading_errors.exe | New   |
| P3 | Data race | winvideo.h                                               | find_and_fix_threading_errors.exe | New   |

Filters: Severity (Error: 3 item(s)), Type (Data race: 3 item(s)), Source (blocked\_range.h, find\_and\_fix\_threading\_errors.c..., parallel\_for.h, partitioner.h, task.h, task\_scheduler\_init.h, winvideo.h), Module (Find\_and\_fix\_threading\_errors.exe: 3 item(s)).

Code Locations: Data race

| Description                                                     | Source                                                  | Function            | Module                            | Variable |
|-----------------------------------------------------------------|---------------------------------------------------------|---------------------|-----------------------------------|----------|
| Write                                                           | find_and_fix_threading_errors.cpp:105                   | render_one_pixel    | find_and_fix_threading_errors.exe | col:r    |
| 103                                                             | primary.scene = ascene;                                 |                     |                                   |          |
| 104                                                             |                                                         |                     |                                   |          |
| 105                                                             | col=trec(a(primary)); //Threading Error: col is a globe |                     |                                   |          |
| 106                                                             | //2 ways to fix this threading error                    |                     |                                   |          |
| 107                                                             | // 1) Make col a local variable                         |                     |                                   |          |
| Write                                                           | find_and_fix_threading_errors.cpp:105                   | render_one_pixel    | find_and_fix_threading_errors.exe | col:r    |
| 103                                                             | primary.scene = ascene;                                 |                     |                                   |          |
| 104                                                             |                                                         |                     |                                   |          |
| 105                                                             | col=trec(a(primary)); //Threading Error: col is a globe |                     |                                   |          |
| 106                                                             | //2 ways to fix this threading error                    |                     |                                   |          |
| 107                                                             | // 1) Make col a local variable                         |                     |                                   |          |
| HINT: Synchronization allocation site task_scheduler_init.h:104 |                                                         | task_scheduler_init | find_and_fix_threading_errors.exe |          |
| 104                                                             | thread_stack_size  = TBB_USE_CAPTURED_EXCEPTION ? p     |                     |                                   |          |

Timeline: thread video (2108)

**Intel Inspector XE 2015**  
Detect Memory Problems

Target Analysis Type Collection Log Summary

| ID | Type                               | Sources                       | State     |
|----|------------------------------------|-------------------------------|-----------|
| P1 | Mismatched allocation/deallocation | find_and_fix_memory_errors... | New       |
| P2 | Invalid memory access              | find_and_fix_memory_errors... | New       |
| P3 | Memory growth                      | [Unknown]; find_and_fix_me... | Not fixed |
| P4 | Memory growth                      | [Unknown]; find_and_fix_me... | Confirmed |

Code Locations: Invalid memory access

| Description | Source                             | Function   | Module                         | Object Size | Offset |
|-------------|------------------------------------|------------|--------------------------------|-------------|--------|
| Write       | find_and_fix_memory_error...       | operator() | find_and_fix_memory_error...   |             |        |
| 164         |                                    |            | find_and_fix_memory_errors.exe |             |        |
| 165         | for (unsigned int i=0;i<=(mboxsize |            | find_and_fix_memory_errors.exe |             |        |
| 166         | local_mbox[i]=0; //Memory Err      |            | find_and_fix_memory_errors.exe |             |        |
| 167         |                                    |            | find_and_fix_memory_errors.exe |             |        |
| 168         | for (int y = r.begin(); y != r.end |            | tbb_debug.dll!local_wait_for_a |             |        |

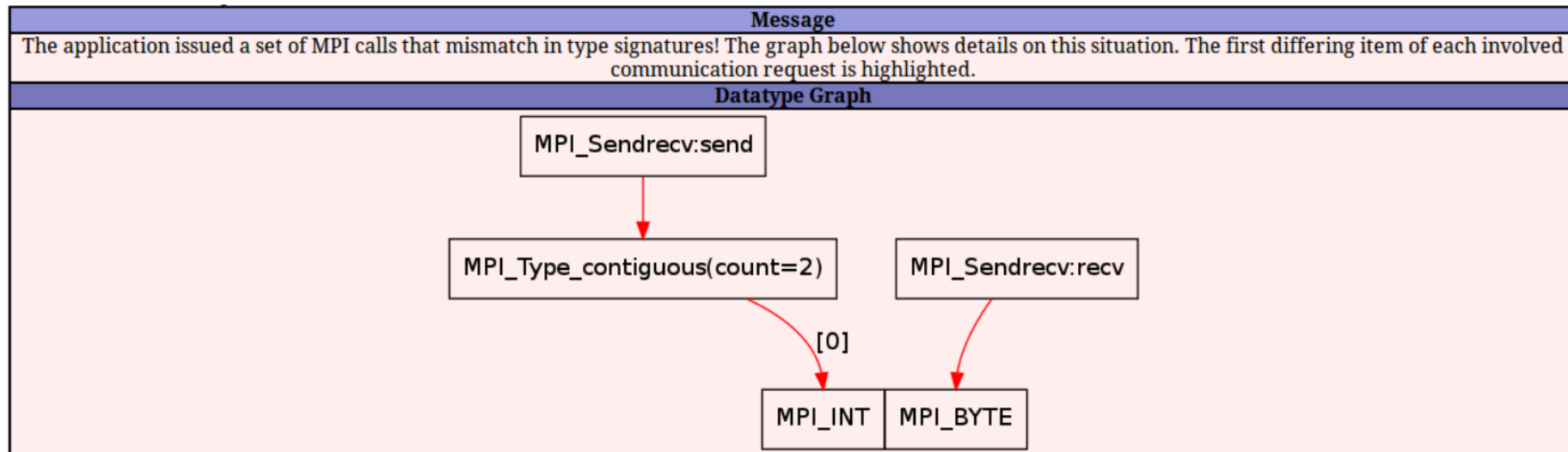
- Next generation MPI correctness and portability checker
- <http://doc.itc.rwth-aachen.de/display/CCP/Project+MUST>



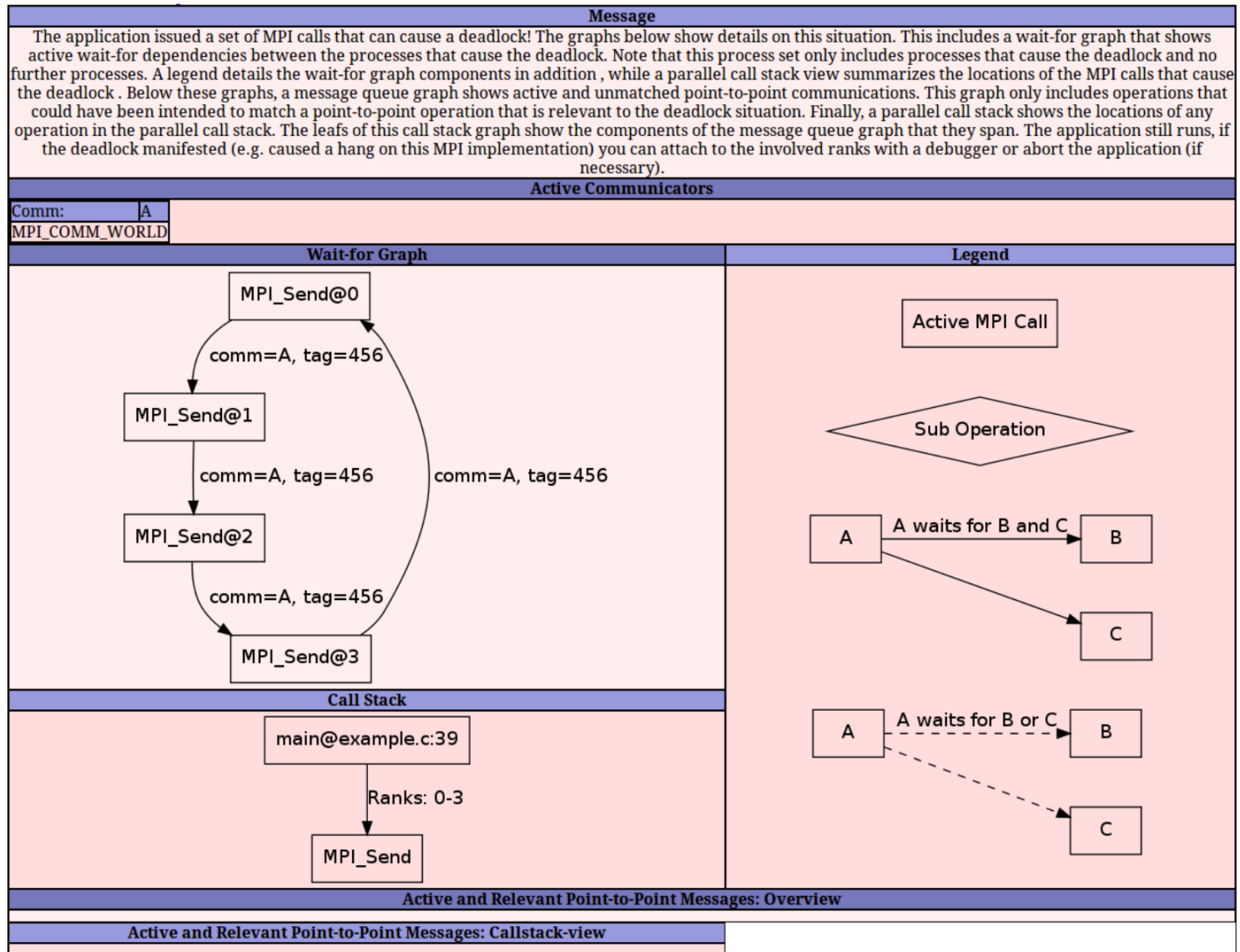
- MUST reports
  - Errors: violations of the MPI-standard
  - Warnings: unusual behavior or possible problems
  - Notes: harmless but remarkable behavior
  - Further: potential deadlock detection
- Usage
  - Relink application with `mustc`, `mustcxx`, `mustf90`, ...
  - Run application under the control of `mustrun` (requires one additional MPI process)
  - See `MUST_Output.html` report

# MUST Datatype Mismatch

| Rank | Type  | Message                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | From                                                                     | References                                                                                                                                                                                                                                                                                                                                                                                    |
|------|-------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 0    | Error | <p>A send and a receive operation use datatypes that do not match! Mismatch occurs at (contiguous) [0](MPI_INT) in the send type and at (MPI_BYTE) in the receive type (consult the MUST manual for a detailed description of datatype positions). A graphical representation of this situation is available in a <a href="#">detailed type mismatch view (MUST Output-files/MUST_Typemismatch_0.html)</a>. The send operation was started at reference 1, the receive operation was started at reference 2. (Information on communicator: MPI_COMM_WORLD) (Information on send of count 1 with type:Datatype created at reference 3 is for C, committed at reference 4, based on the following type(s): { MPI_INT}Typemap = {(MPI_INT, 0), (MPI_INT, 4)}) (Information on receive of count 8 with type:MPI_BYTE)</p> | <p><b>MPI_Sendrecv</b><br/>called from:<br/>#0<br/>main@example.c:33</p> | <p>reference 1 rank 0:<br/><b>MPI_Sendrecv</b> called<br/>from:<br/>#0 main@example.c:33</p> <p>reference 2 rank 1:<br/><b>MPI_Sendrecv</b> called<br/>from:<br/>#0 main@example.c:33</p> <p>reference 3 rank 0:<br/><b>MPI_Type_contiguous</b><br/>called from:<br/>#0 main@example.c:29</p> <p>reference 4 rank 0:<br/><b>MPI_Type_commit</b> called<br/>from:<br/>#0 main@example.c:30</p> |



# MUST Deadlock Detection



# Performance Analysis Tools

- Do I have a performance problem at all?
  - Time / speedup / scalability measurements
- **What** is the key bottleneck (computation / communication)?
  - MPI / OpenMP / flat profiling
- **Where** is the key bottleneck?
  - Call-path profiling, detailed basic block profiling
- **Why** is it there?
  - Hardware counter analysis
  - Trace selected parts (to keep trace size manageable)
- Does the code have scalability problems?
  - Load imbalance analysis, compare profiles at various sizes function-by-function, performance modeling

# Remark: No Single Solution is Sufficient!



☞ *A combination of different methods, tools and techniques is typically needed!*

- Analysis
  - Statistics, visualization, automatic analysis, data mining, ...
- Measurement
  - Sampling / instrumentation, profiling / tracing, ...
- Instrumentation
  - Source code / binary, manual / automatic, ...

- Accuracy
  - Intrusion overhead
    - Measurement itself needs time and thus lowers performance
  - Perturbation
    - Measurement alters program behavior, e.g., memory access pattern
    - Might prevent compiler optimization, e.g. function inlining
  - Accuracy of timers & counters
- Granularity
  - How many measurements?
  - How much information / processing during each measurement?

☞ *Tradeoff: Accuracy vs. Expressiveness of data*

- Score-P
- Scalasca 2
- Vampir[Server]
- HPCToolkit
- Alinea Performance Reports
- Darshan
- NVIDIA Visual Profiler
- TAU
- Intel VTune Amplifier XE
- Intel Advisor
- mpiP\*
- Extrae/Paraver\*
- PAPI\*



- Community instrumentation and measurement infrastructure
  - Developed by a consortium of performance tool groups



UNIVERSITY OF OREGON

- Next generation measurement system of
  - Scalasca 2.x
  - Vampir
  - TAU
  - Periscope
- Common data formats improve tool interoperability
- <http://www.score-p.org>

- Collection of trace-based performance analysis tools
  - Specifically designed for large-scale systems
  - Unique features:
    - Scalable, automated search for event patterns representing inefficient behavior
    - Scalable identification of the critical execution path
    - Delay / root-cause analysis
- Based on Score-P for instrumentation and measurement
  - Includes convenience / post-processing commands providing added value
- <http://www.scalasca.org>

# What is the Key Bottleneck?

- Generate **flat MPI profile** using Score-P/Scalasca
  - Only requires re-linking
  - Low runtime overhead
- Provides detailed information on MPI usage
  - How much time is spent in which operation?
  - How often is each operation called?
  - How much data was transferred?
- Limitations:
  - Computation on non-master threads and outside of MPI\_Init/MPI\_Finalize scope ignored

# Flat MPI Profile: Recipe

1. Prefix your *link command* with  
“scorep --nocompiler”
2. Prefix your MPI *launch command* with  
“scalasca -analyze”
3. After execution, examine analysis results using  
“scalasca -examine scorep\_<title>”

# Flat MPI Profile: Example

```
% module load Toolchain Score-P Scalasca
% mpif90 -O3 -c foo.f90
% mpif90 -O3 -c bar.f90
% scorep --nocompiler \
    mpif90 -O3 -o myprog foo.o bar.o
```

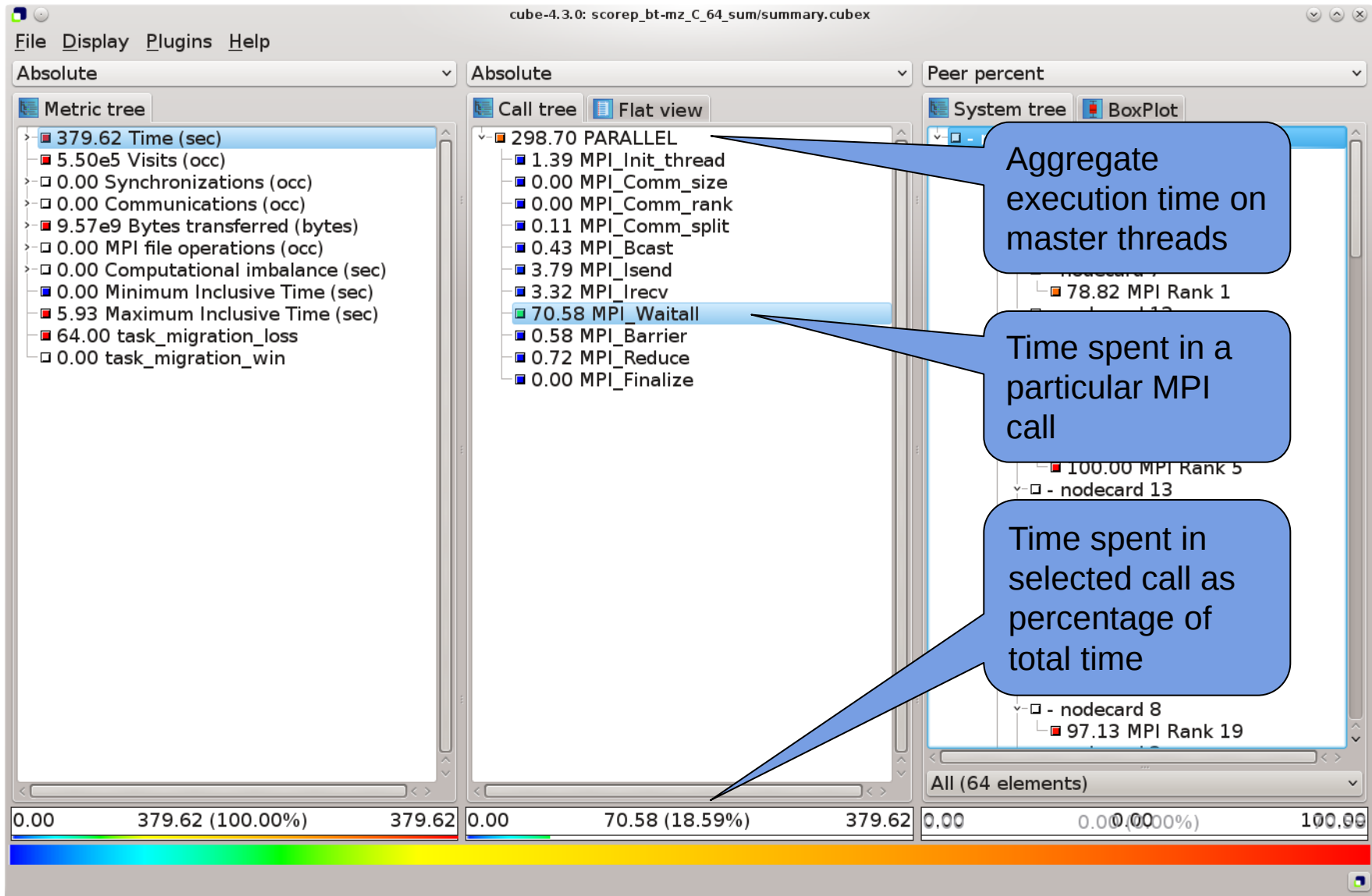
```
#####
##  In the job script:  ##
#####
```

```
module load Toolchain Scalasca
scalasca -analyze \
    srun --tasks-per-node  $P$  --ntasks  $n$  [...] --exe ./myprog
```

```
#####
## After job finished: ##
#####
```

```
% scalasca -examine scorep_myprog_ $P$  $n$  $x$  $t$ _sum
```

# Flat MPI Profile: Example (cont.)



Aggregate execution time on master threads

Time spent in a particular MPI call

Time spent in selected call as percentage of total time

# Where is the Key Bottleneck?

- Generate **call-path profile** using Score-P/Scalasca
  - Requires re-compilation
  - Runtime overhead depends on application characteristics
  - Typically needs some care setting up a good measurement configuration
    - Filtering
    - Selective instrumentation
- Option 1 (recommended):  
Automatic compiler-based instrumentation
- Option 2:  
Manual instrumentation of interesting phases, routines, loops

1. Prefix your *compile & link commands* with  
“scorep”
2. Prefix your MPI *launch command* with  
“scalasca -analyze”
3. After execution, compare overall runtime with uninstrumented run to determine overhead
4. If overhead is too high
  1. Score measurement using  
“scalasca -examine -s scorep\_<title>”
  2. Prepare filter file
  3. Re-run measurement with filter applied using prefix  
“scalasca -analyze -f <filter\_file>”
5. After execution, examine analysis results using  
“scalasca -examine scorep\_<title>”

# Call-path Profile: Example

```
% module load Toolchain Score-P Scalasca
% scorep mpif90 -O3 -c foo.f90
% scorep mpif90 -O3 -c bar.f90
% scorep \
    mpif90 -O3 -o myprog foo.o bar.o
```

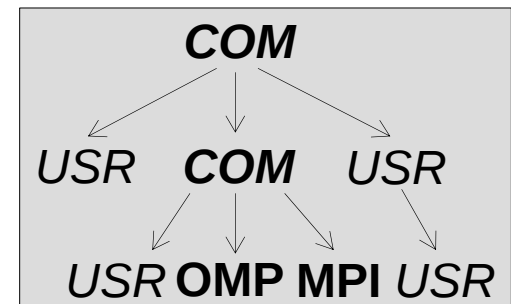
```
#####
##  In the job script:  ##
#####
```

```
module load Toolchain Scalasca
scalasca -analyze \
    srun --tasks-per-node  $P$  --ntasks  $n$  [...] --exe ./myprog
```

# Call-path Profile: Example (cont.)

```
% scalasca -examine -s epik_myprog_Ppnext_sum  
scorep-score -r ./epik_myprog_Ppnext_sum/profile.cubex  
INFO: Score report written to ./scorep_myprog_Ppnext_sum/scorep.score
```

- Estimates trace buffer requirements
- Allows to identify candidate functions for filtering
  - ☞ Computational routines with high visit count and low time-per-visit ratio
- Region/call-path classification
  - MPI (pure MPI library functions)
  - OMP (pure OpenMP functions/regions)
  - USR (user-level source local computation)
  - COM (“combined” USR + OpeMP/MPI)
  - ANY/ALL (aggregate of all region types)



# Call-path Profile: Example (cont.)

```
% less scorep_myprog_Ppnext_sum/scorep.score
```

```
Estimated aggregate size of event trace:          162GB
Estimated requirements for largest trace buffer (max_buf): 2758MB
Estimated memory requirements (SCOREP_TOTAL_MEMORY): 2822MB
(hint: When tracing set SCOREP_TOTAL_MEMORY=2822MB to avoid
intermediate flushes or reduce requirements using USR regions
filters.)
```

| flt type | max_buf[B]    | visits        | time[s]  | time[%] | time/<br>visit[us] | region          |
|----------|---------------|---------------|----------|---------|--------------------|-----------------|
| ALL      | 2,891,417,902 | 6,662,521,083 | 36581.51 | 100.0   | 5.49               | ALL             |
| USR      | 2,858,189,854 | 6,574,882,113 | 13618.14 | 37.2    | 2.07               | USR             |
| OMP      | 54,327,600    | 86,353,920    | 22719.78 | 62.1    | 263.10             | OMP             |
| MPI      | 676,342       | 550,010       | 208.98   | 0.6     | 379.96             | MPI             |
| COM      | 371,930       | 735,040       | 34.61    | 0.1     | 47.09              | COM             |
| USR      | 921,918,660   | 2,110,313,472 | 3290.11  | 9.0     | 1.56               | matmul_sub      |
| USR      | 921,918,660   | 2,110,313,472 | 5914.98  | 16.2    | 2.80               | binvrhs         |
| USR      | 921,918,660   | 2,110,313,472 | 3822.64  | 10.4    | 1.81               | matvec_sub      |
| USR      | 41,071,134    | 87,475,200    | 358.56   | 1.0     | 4.10               | lhsinit         |
| USR      | 41,071,134    | 87,475,200    | 145.42   | 0.4     | 1.66               | binvrhs         |
| USR      | 29,194,256    | 68,892,672    | 86.15    | 0.2     | 1.25               | exact_solution  |
| OMP      | 3,280,320     | 3,293,184     | 15.81    | 0.0     | 4.80               | !\$omp parallel |
| [...]    |               |               |          |         |                    |                 |

- In this example, the 6 most frequently called routines are of type USR
  - These routines contribute around 35% of total time
    - However, much of that is most likely measurement overhead
      - Frequently executed
      - Time-per-visit ratio in the order of a few microseconds
- ➡ Avoid measurements to reduce the overhead
- ➡ List routines to be filtered in simple text file

```
% cat filter.txt
SCOREP_REGION_NAMES_BEGIN
    EXCLUDE
        binvcrhs
        matmul_sub
        matvec_sub
        binvrhs
        lhsinit
        exact_solution
SCOREP_REGION_NAMES_END
```

- Score-P filtering files support
  - Wildcards (shell globs)
  - Blacklisting
  - Whitelisting
  - Filtering based on filenames

# Call-path Profile: Example (cont.)

```
## To verify effect of filter:

% scalasca -examine -s -f filter.txt \
  scorep_myprog_Pp n x t_sum

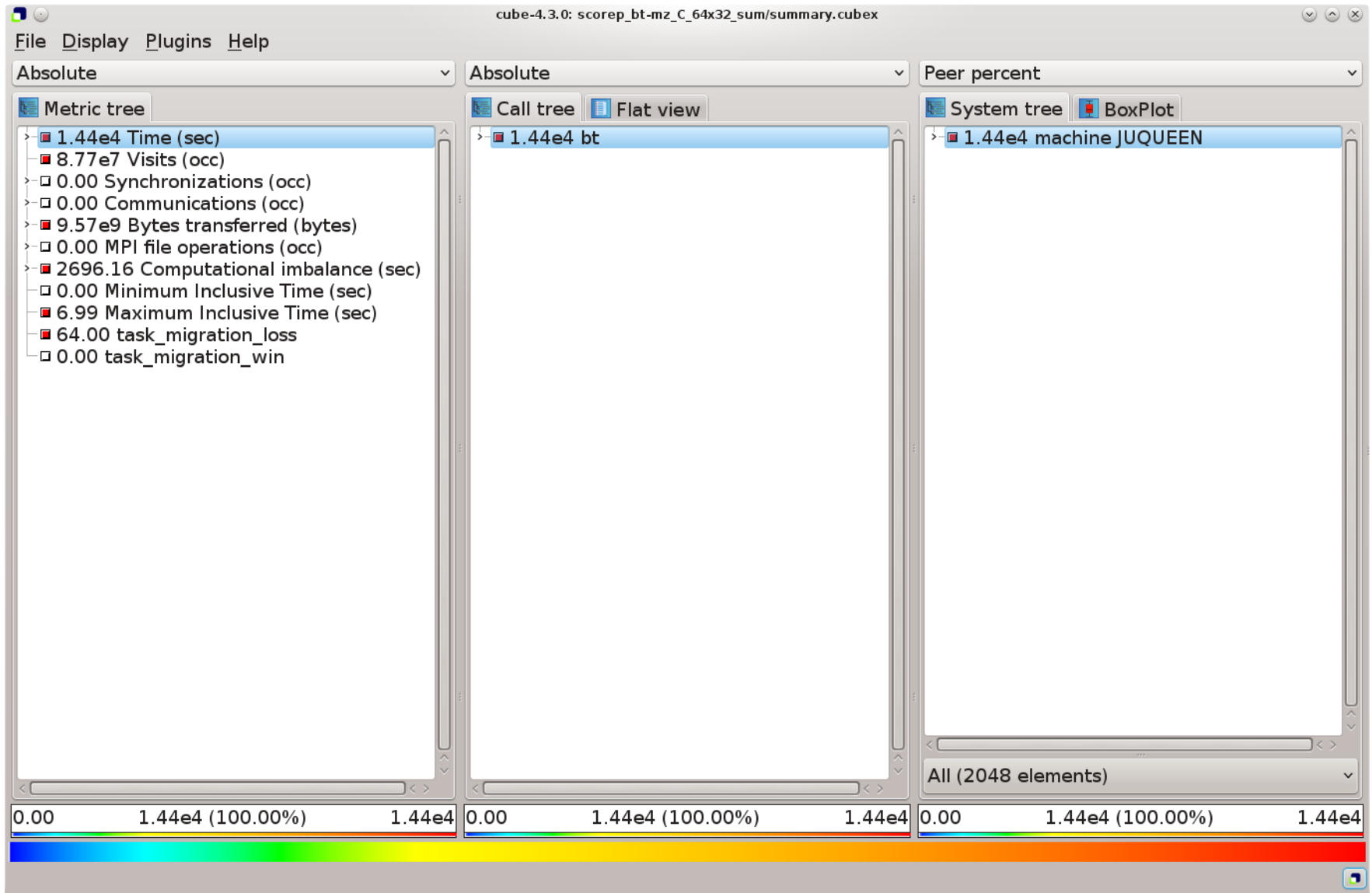
#####
## In the job script: ##
#####

module load UNITE scalasca
scalasca -analyze -f filter.txt \
  runjob --ranks-per-node P --np n [...] --exe ./myprog

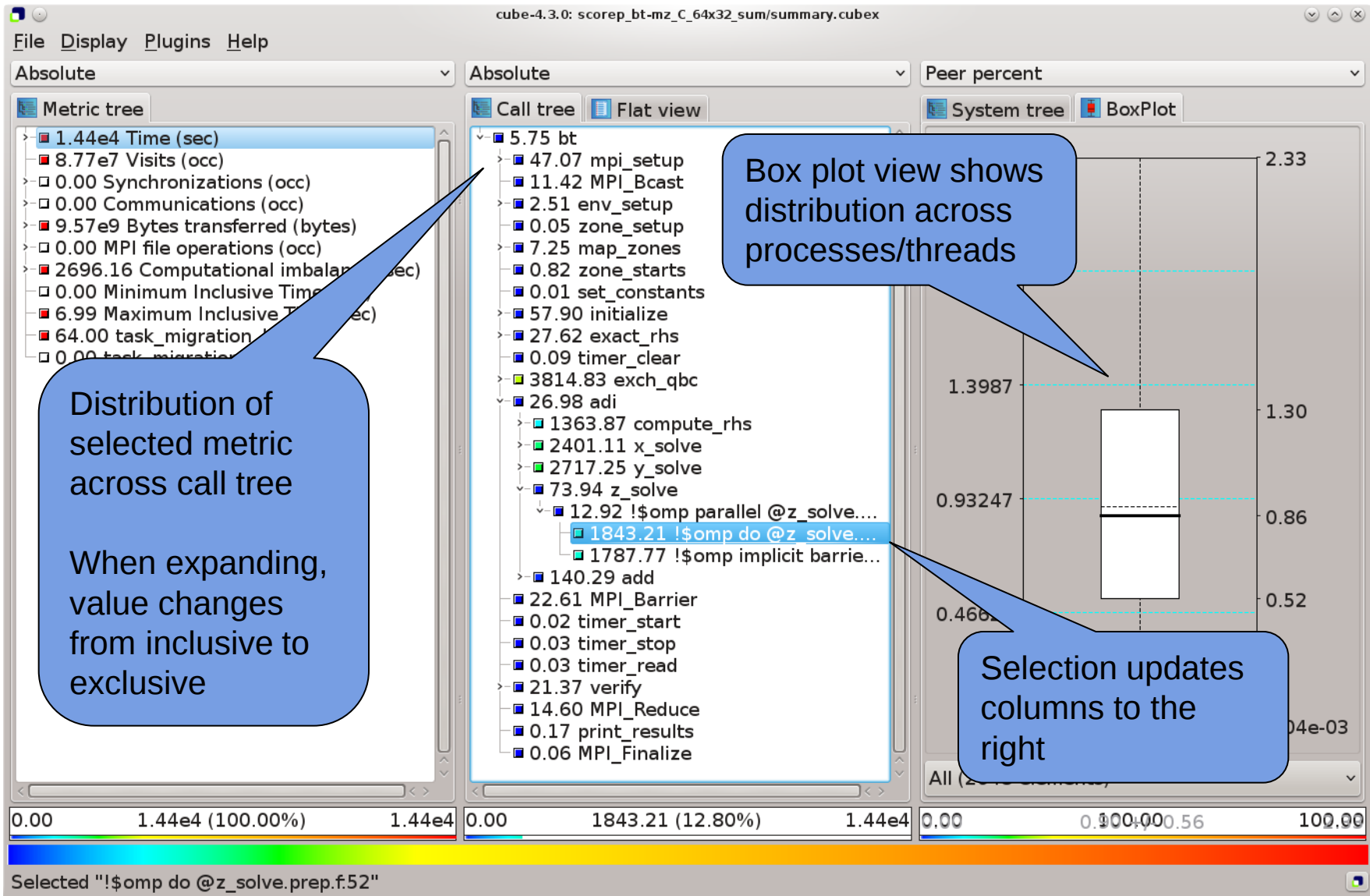
#####
## After job finished: ##
#####

% scalasca -examine scorep_myprog_Pp n x t_sum
```

# Call-path Profile: Example (cont.)



# Call-path Profile: Example (cont.)





- Sampling support
  - x86 only
- Measurement can be extensively configured via environment variables
  - Check output of “scorep-info config-vars” for details
- Allows for targeted measurements:
  - Selective recording
  - Phase profiling
  - Parameter-based profiling
  - ...
- Please ask us or see the user manual for details

- Record CUDA events using the CUPTI interface

```
% export SCOREP_CUDA_ENABLE=gpu,kernel,idle
```

- Important record types:
  - runtime      CUDA runtime API
  - driver      CUDA driver API
  - gpu      GPU activities
  - kernel      CUDA kernels
  - Idle      GPU compute idle time
  - memcpy      CUDA memory copy
- For all record types consult the Score-P user guide

# Why is the Bottleneck There?

- This is **highly** application dependent!
- Might require additional measurements
  - Hardware-counter analysis
    - CPU utilization
    - Cache behavior
  - Selective instrumentation
  - Manual/automatic event trace analysis

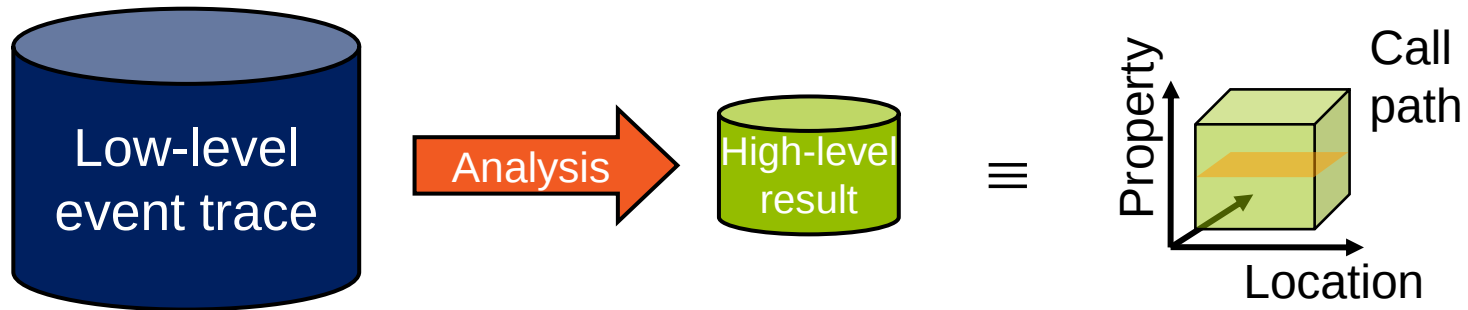
- Score-P supports both PAPI preset and native counters
- Available counters: `papi_avail` or `papi_native_avail`

```
% module load PAPI
```

- Specify using “SCOREP\_METRIC\_PAPI” environment variable

```
#####  
## In the job script: ##  
#####  
  
module load UNITE scalasca  
export SCOREP_METRIC_PAPI="PAPI_FP_OPS,PAPI_TOT_CYC"  
scalasca -analyze -f filter.txt \  
runjob --ranks-per-node P --np n [...] --exe ./myprog
```

- Idea: Automatic search for patterns of inefficient behavior
  - Identification of wait states and their root causes
  - Classification of behavior & quantification of significance
  - Scalable identification of the critical execution path



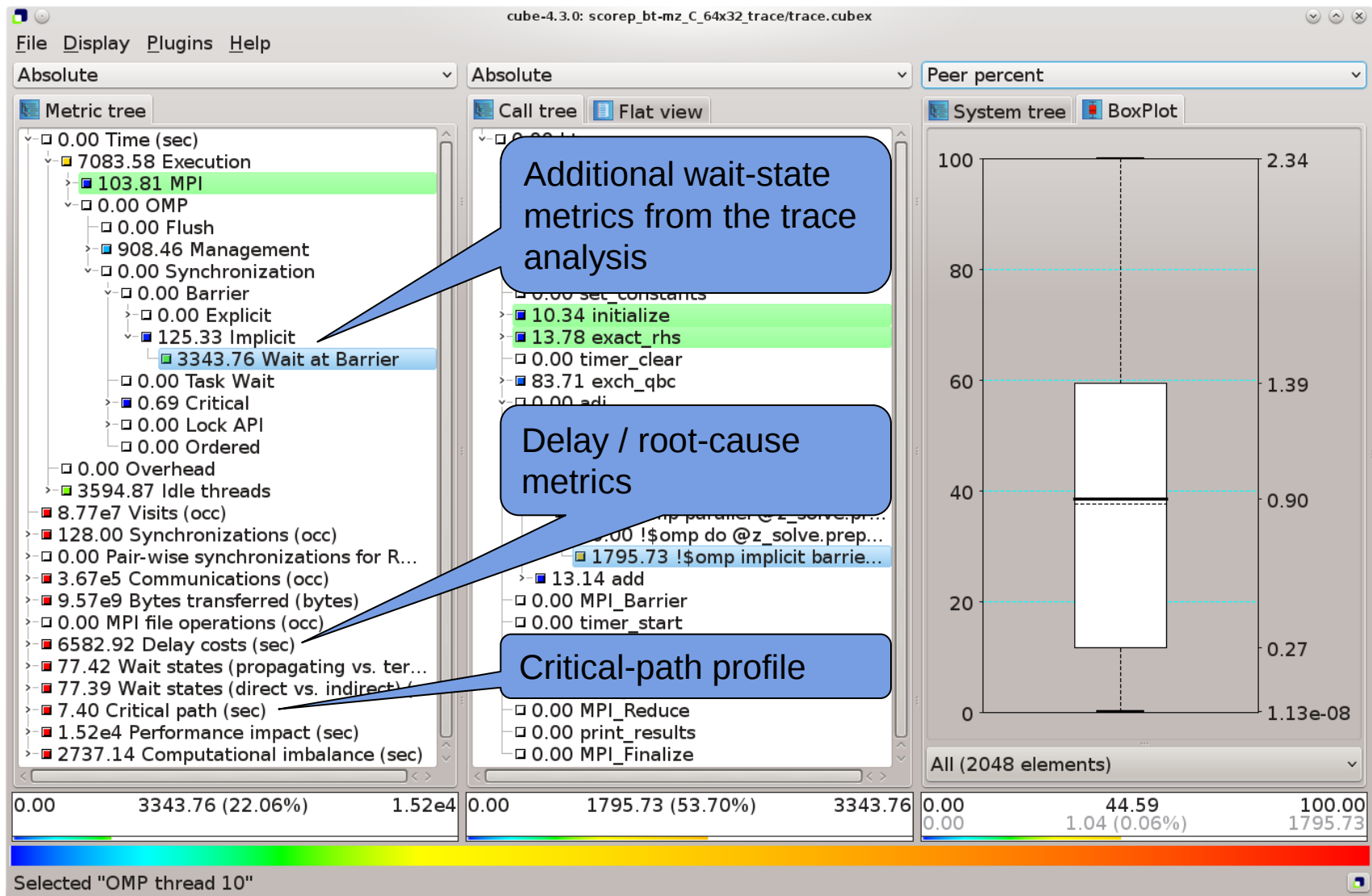
- Advantages
  - Guaranteed to cover the entire event trace
  - Quicker than manual/visual trace analysis
  - Helps to identify hot-spots for in-depth manual analysis

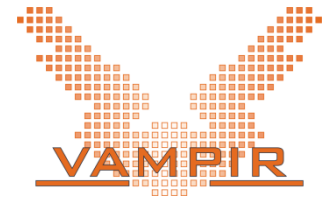
- Enable trace collection & analysis using “-t” option of “scalasca -analyze”:

```
#####  
##  In the job script:  ##  
#####  
  
module load Toolchain Scalasca  
export SCOREP_TOTAL_MEMORY=120MB    # Consult score report  
scalasca -analyze -f filter.txt -t \  
  srun --tasks-per-node P --ntasks n [...] --exe ./myprog
```

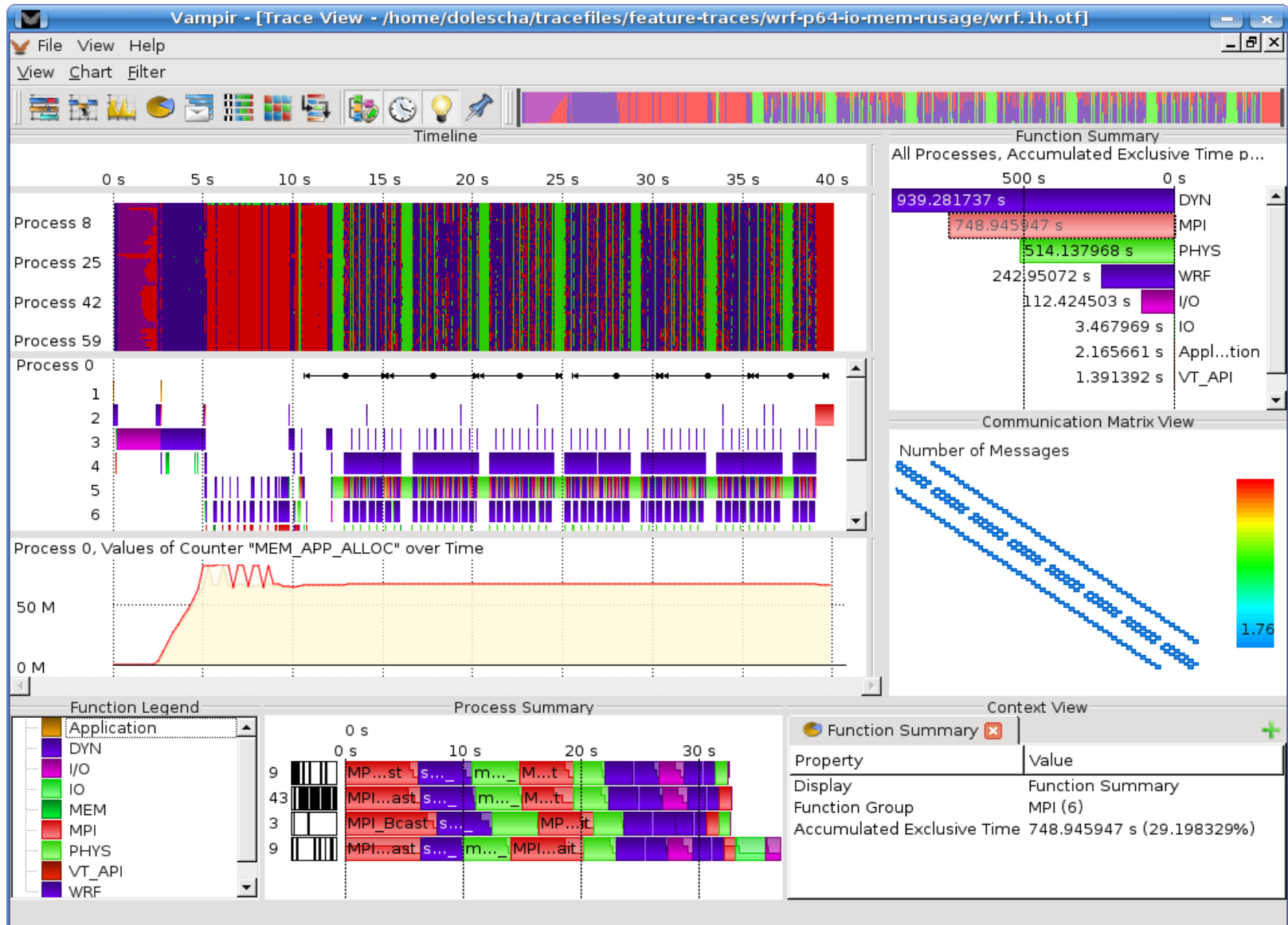
- **ATTENTION:**
  - Traces can quickly become extremely large!
  - Remember to use proper filtering, selective instrumentation, and Score-P memory specification
  - **Before flooding the file system, ask us for assistance!**

# Scalasca Trace Analysis Example





- Offline trace visualization for Score-P's OTF2 trace files
- Visualization of MPI, OpenMP and application events:
  - All diagrams highly customizable (through context menus)
  - Large variety of displays for ANY part of the trace
- <http://www.vampir.eu>
- Advantage:
  - Detailed view of dynamic application behavior
- Disadvantage:
  - Requires event traces (huge amount of data)
  - Completely manual analysis

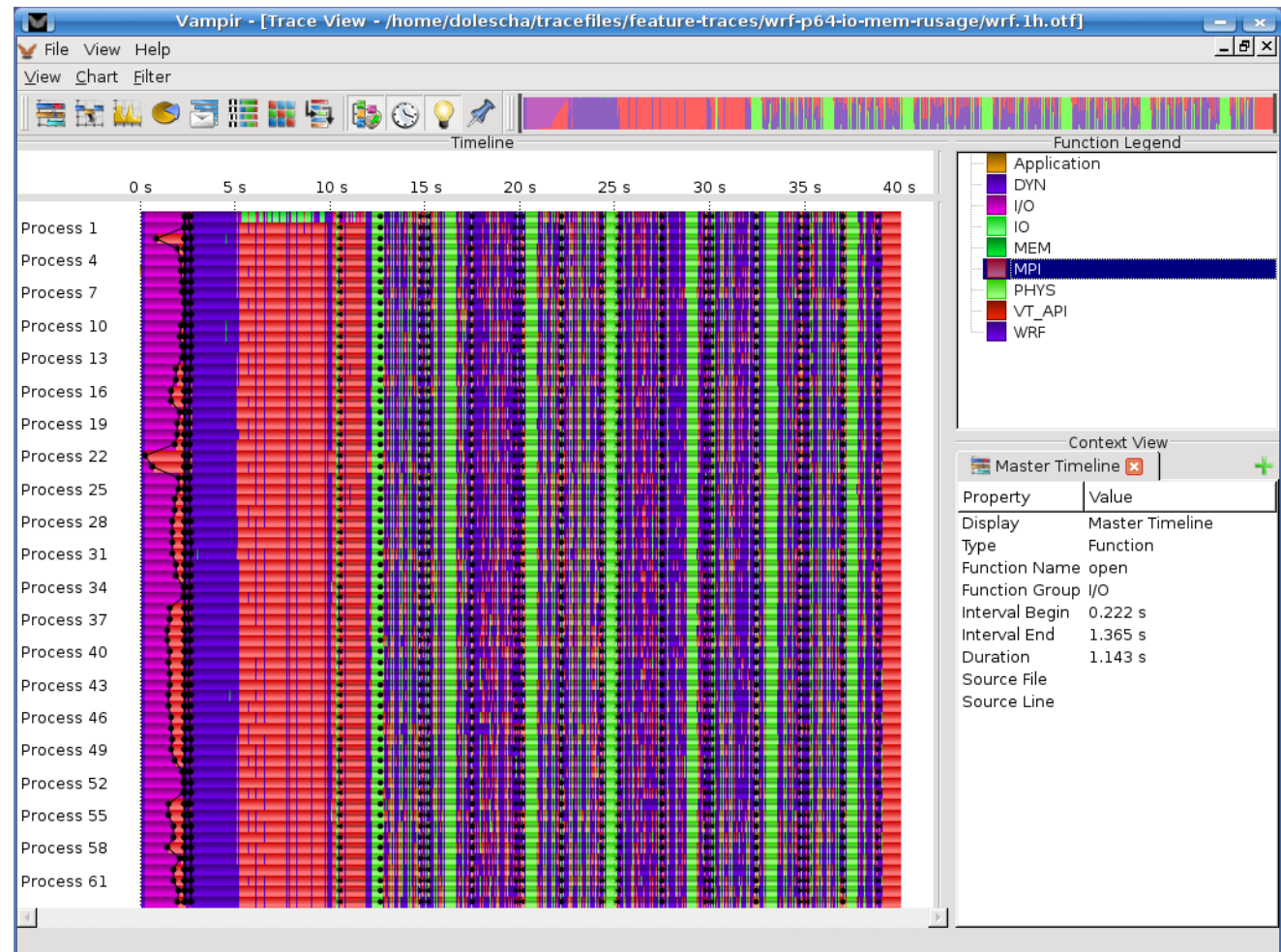


# Vampir: Timeline Diagram

- Functions organized into groups

- Coloring by group

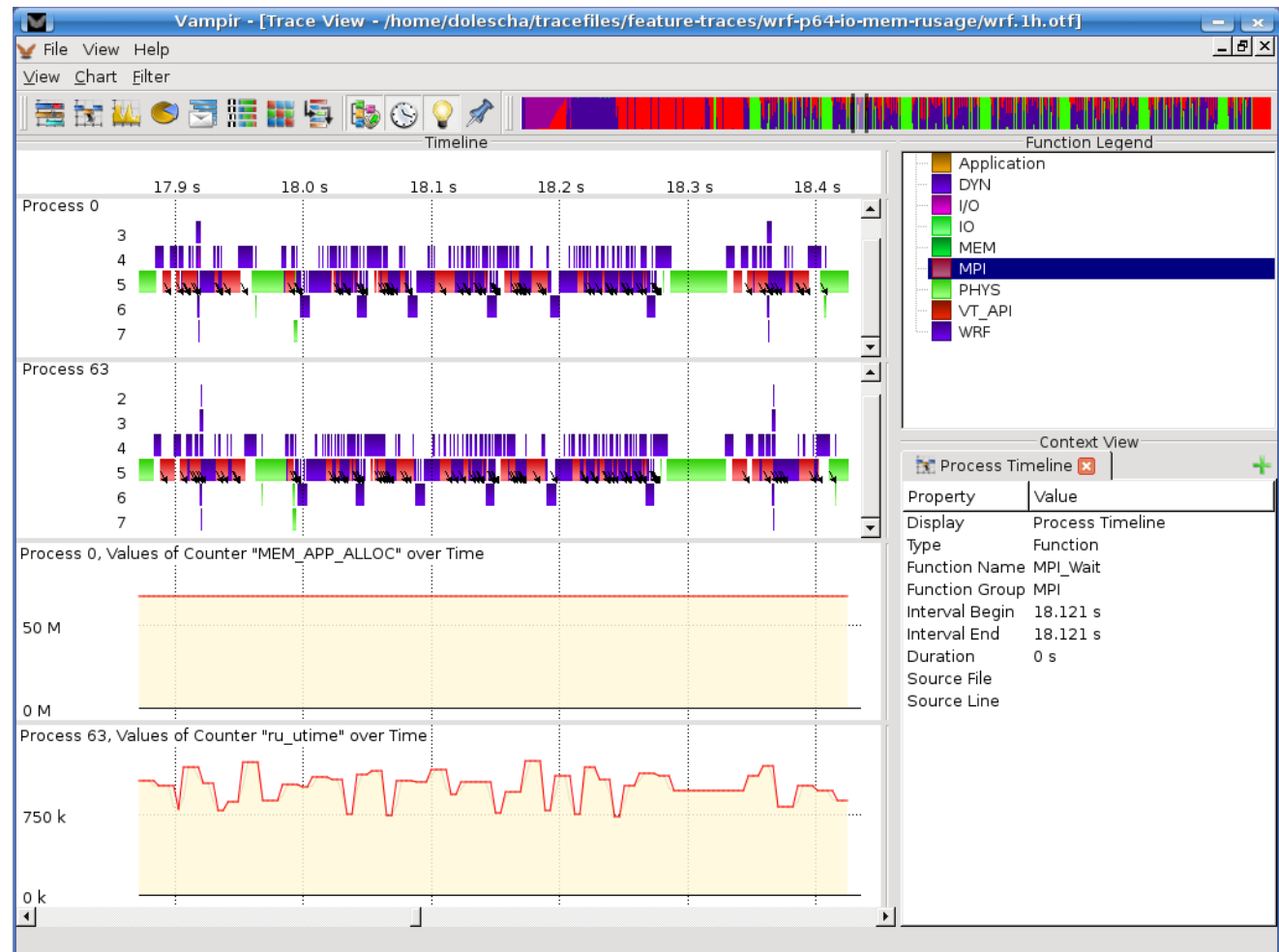
- Message lines can be colored by tag or size



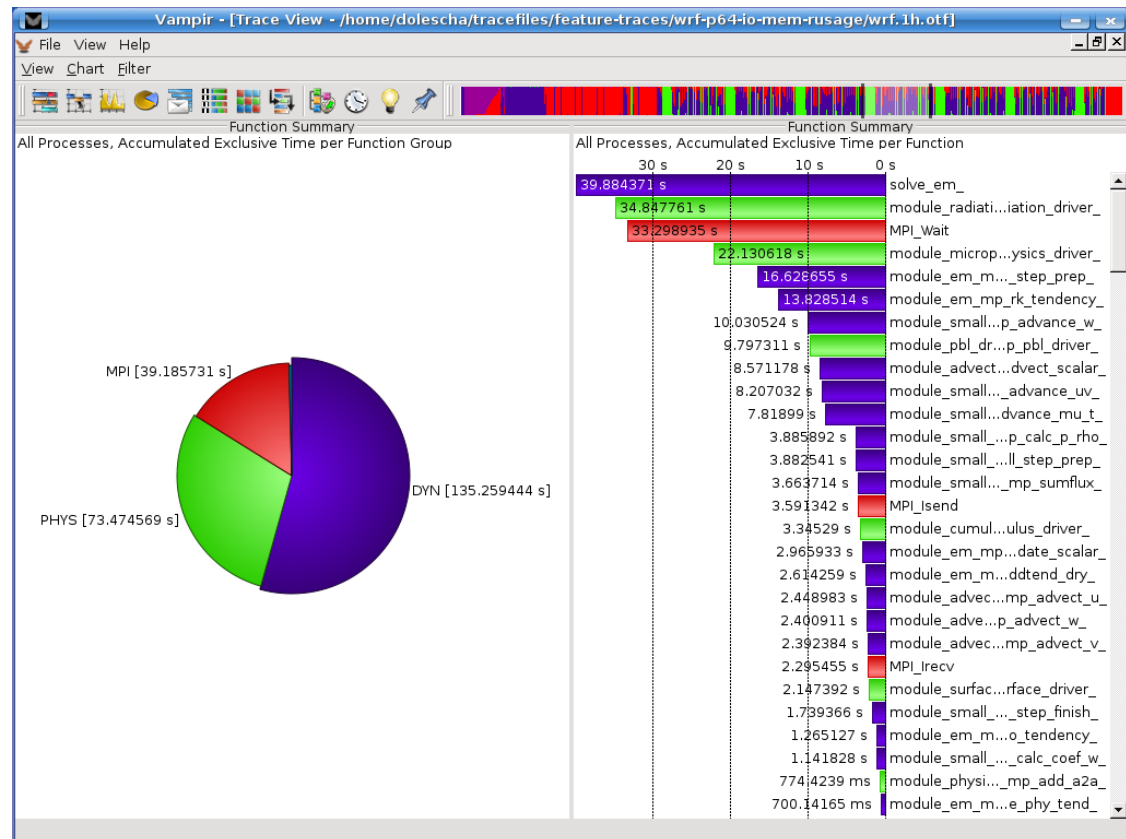
- Information about states, messages, collective and I/O operations available through clicking on the representation

# Vampir: Process and Counter Timelines

- Process timeline show call stack nesting
- Counter timelines for hardware and software counters



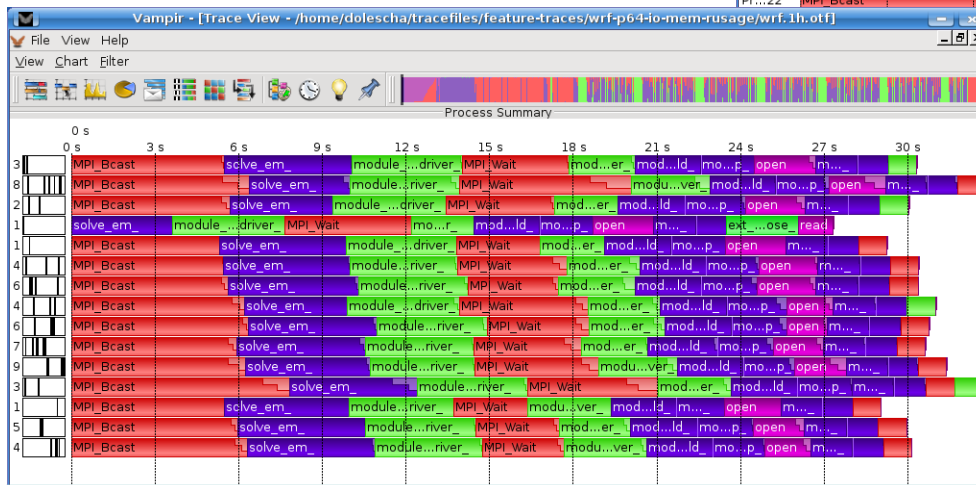
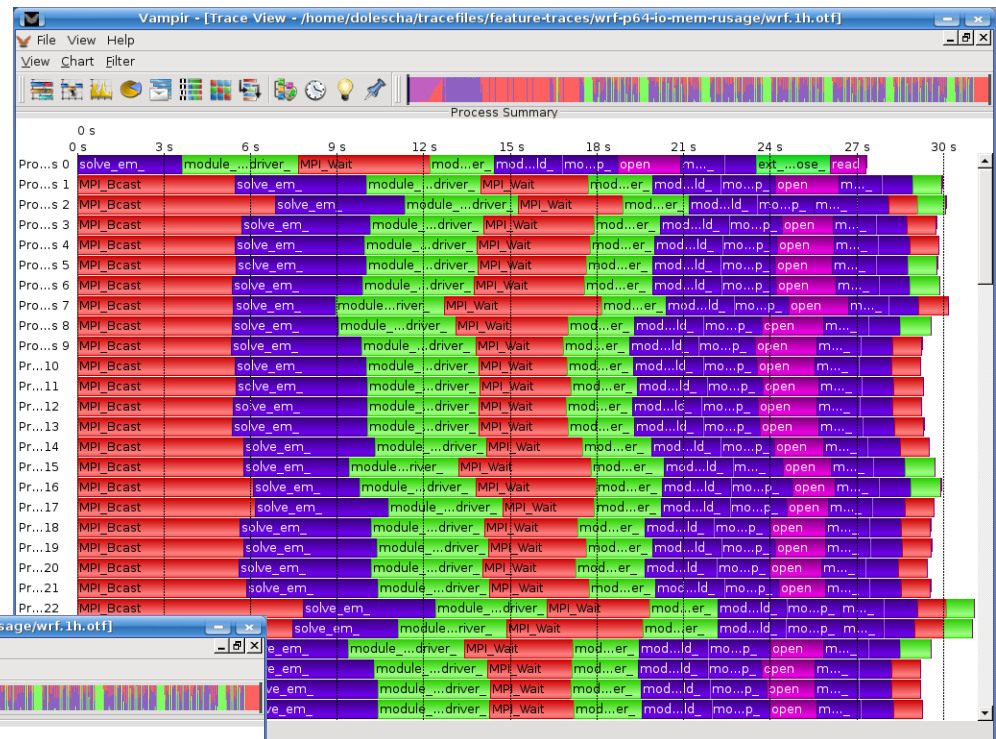
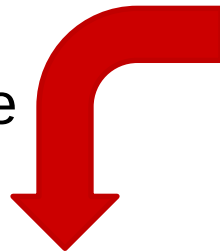
- Aggregated profiling information: execution time, number of calls, inclusive/exclusive
- Available for all / any group (activity) or all routines (symbols)



- Available for any part of the trace  
⇒ selectable through time line diagram

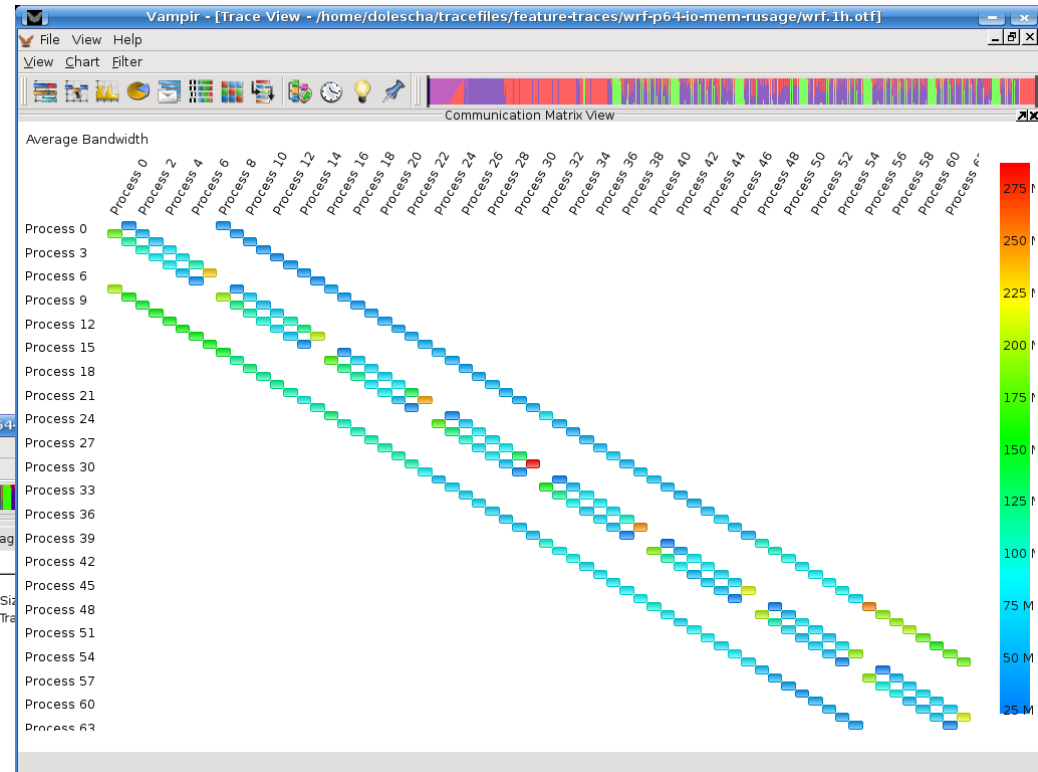
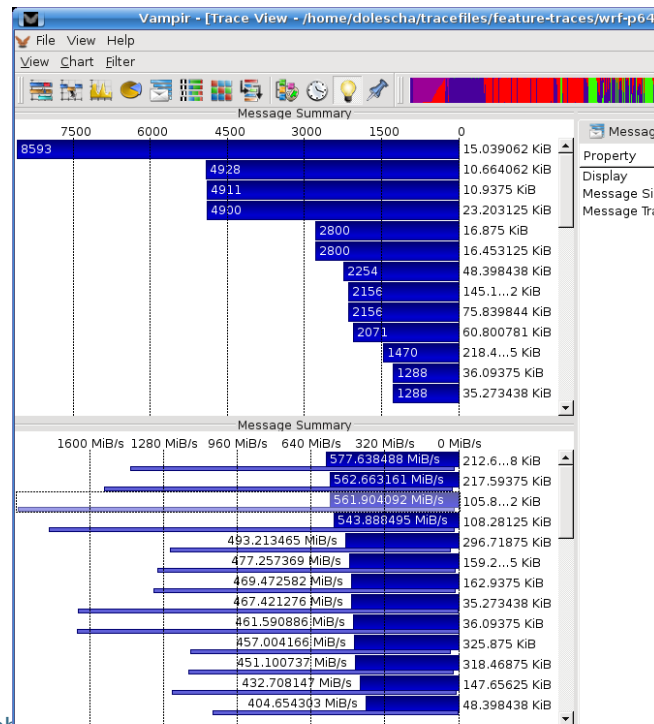
# Vampir: Process Summary

- Execution statistics over all processes for comparison
- Clustering mode available for large process counts



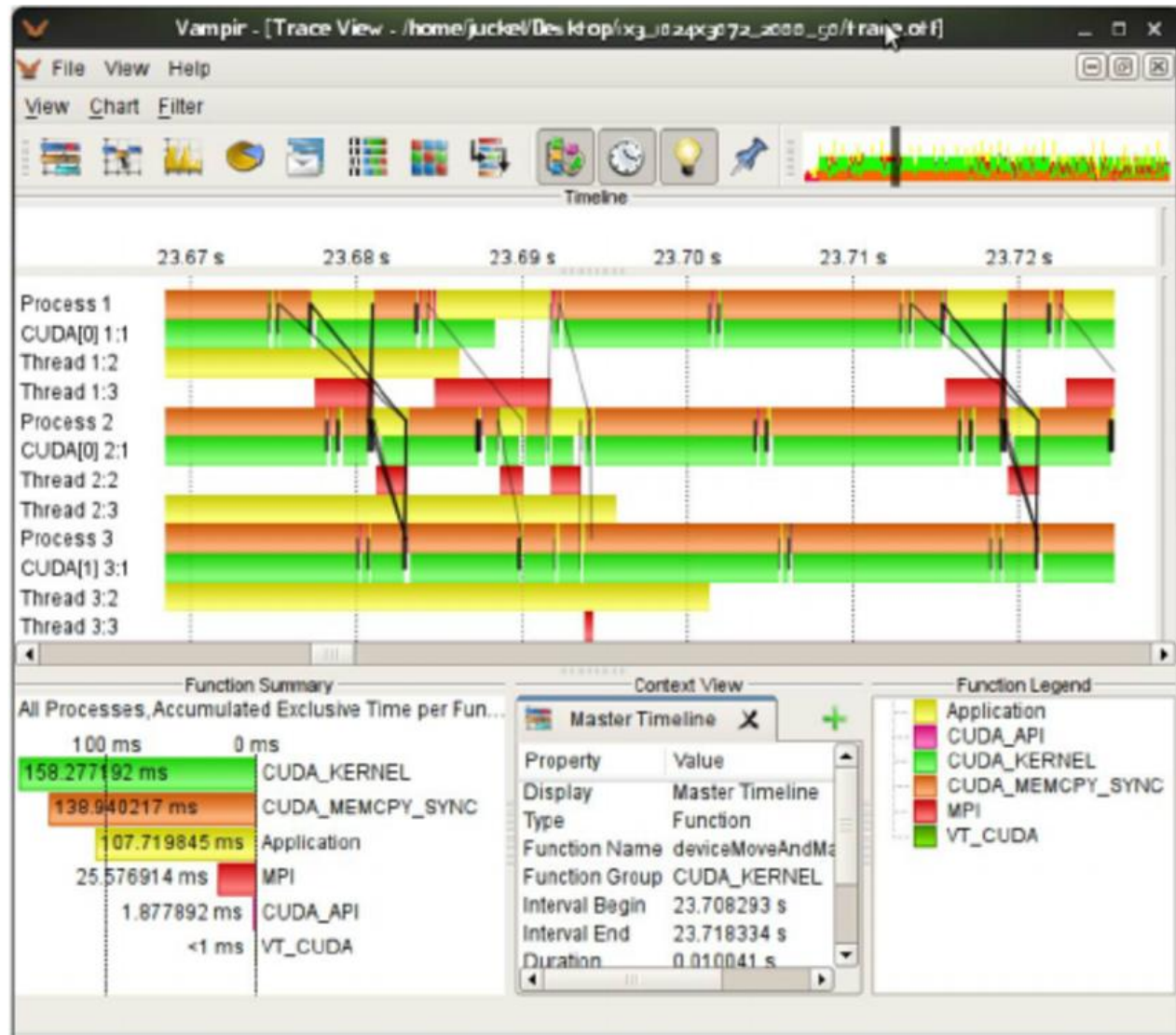
# Vampir: Communication Statistics

- Byte and message count, min/max/avg message length and min/max/avg bandwidth for each process pair
- Message length statistics

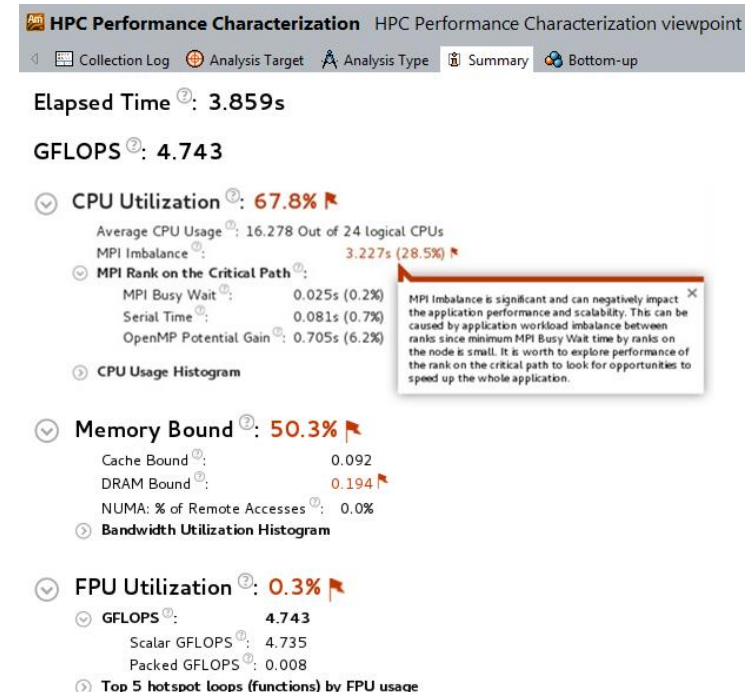


- Available for any part of the trace

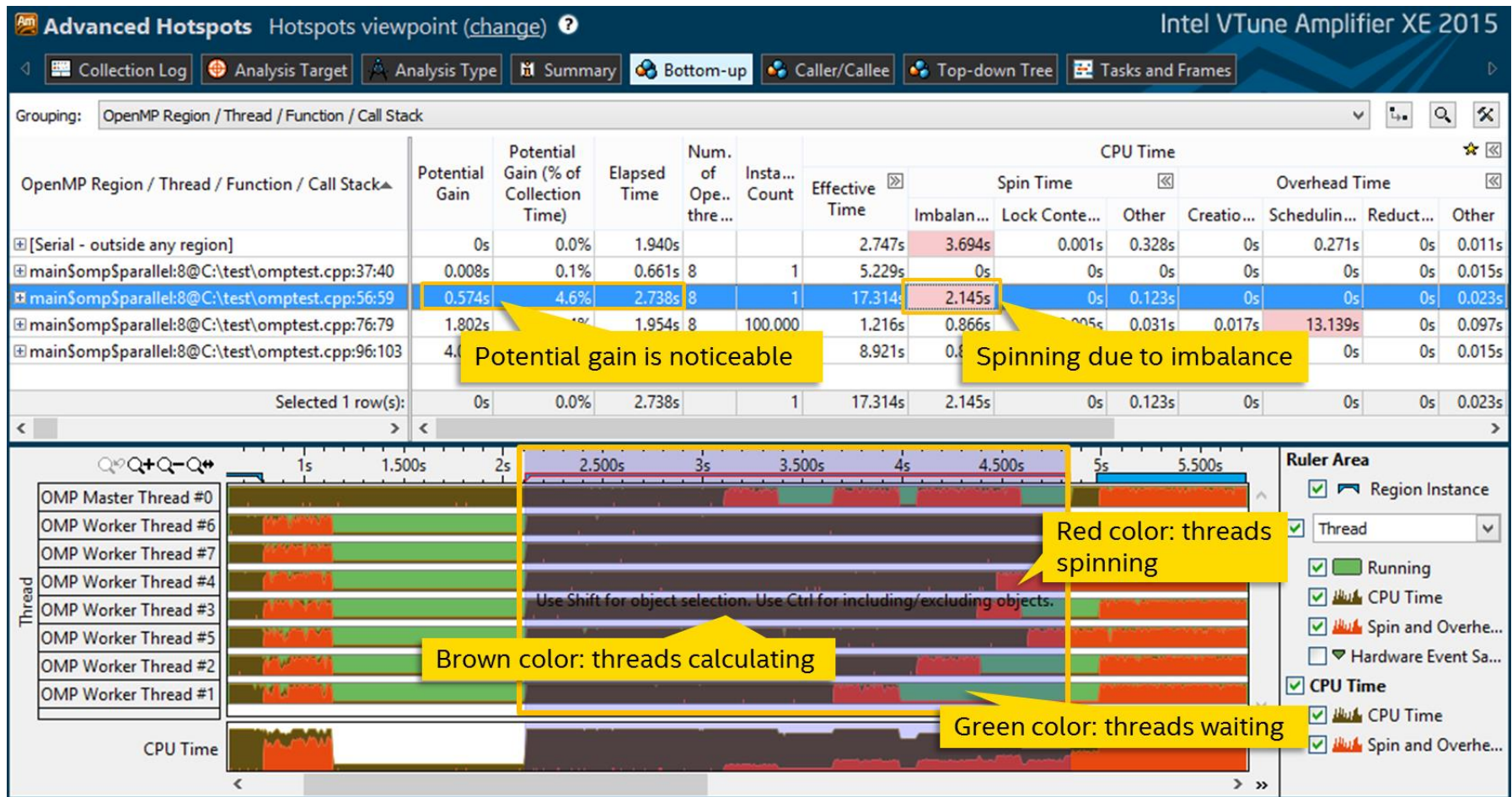
- Detailed information on kernel execution and memory transfers
- All statistics and displays also available for CUDA events



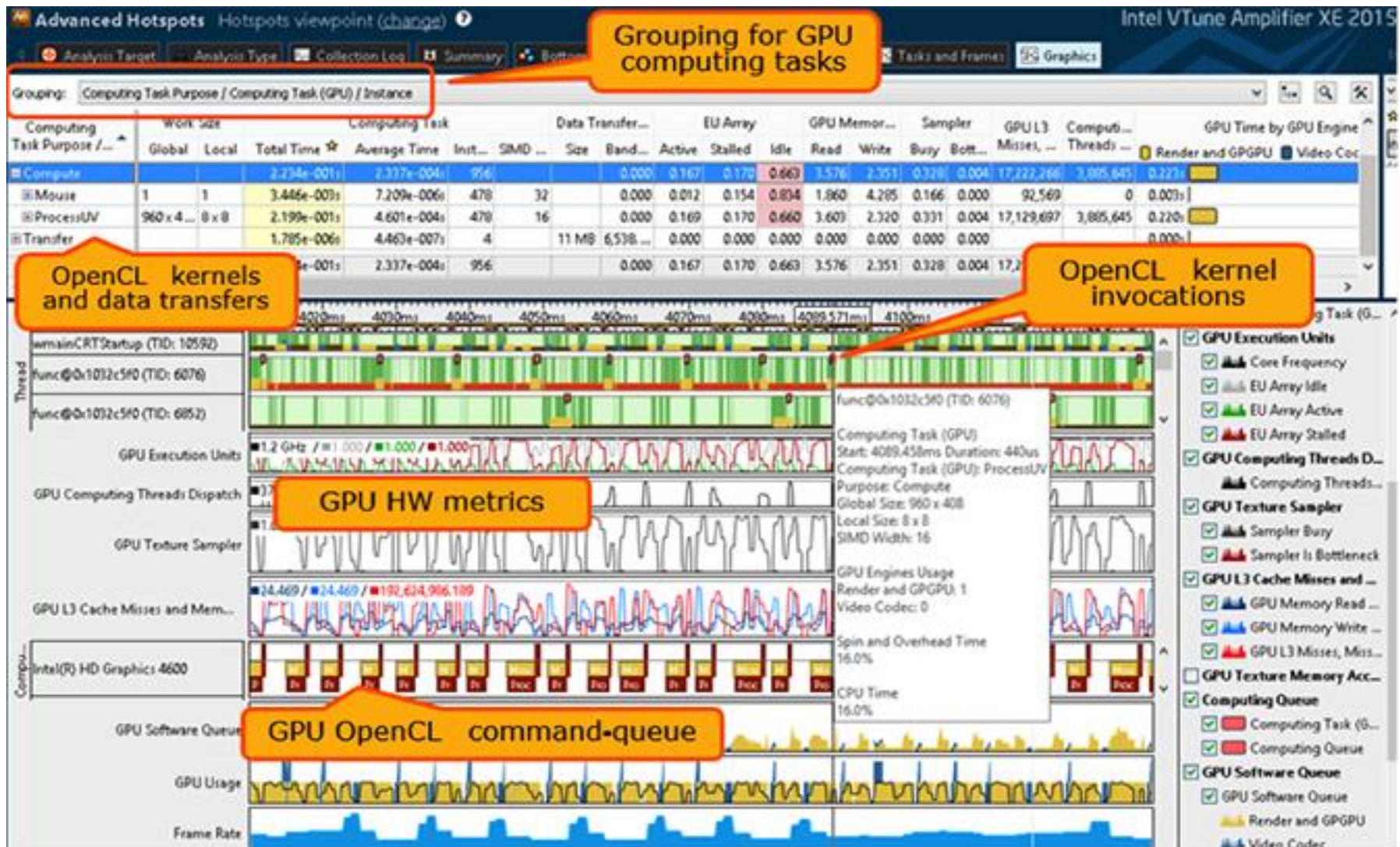
- Feature-rich profiler for Intel platforms
- Supports Python, C/C++ and Fortran
- MPI support continuously improving
- Lock and Wait analysis for OpenMP and TBB
- HPC analysis for quick overview
- Bandwidth and memory analysis
- I/O analysis
- OpenCL and GPU profiling (no CUDA, Intel iGPU only)



# Intel VTune Amplifier GUI



# Intel Vtune – GPU analysis



- Vectorization Advisor
  - Loops-based analysis to identify vectorization candidates
  - Finds save spots to enforce compiler vectorization
  - Roofline analysis to explore performance headroom and co-optimize memory and computation
  
- Threading Advisor
  - Identify issues before parallelization
  - Prototype performance impact of different threading designs
  - Find and eliminate data-sharing issues
  
- Flow-Graph Analysis
  - Speed up algorithm design and express parallelism efficiently
  - Plan, validate, and model application design
  
- C/C++ and Fortran with OpenMP and Intel TBB

**Where should I add vectorization and/or threading parallelism?** Intel Advisor XE 2016

Summary Survey Report Refinement Reports Annotation Report Suitability Report

Program time: 26.54s Vectorized Not Vectorized FILTER: All Modules All Sources **Filters**

| Function Call Sites and Loops        | Self Time | Total Time |   | Loop Type         | Why No Vectorization?               | Vector...<br>Loops | Instruction<br>Set Analysis | Optimization |
|--------------------------------------|-----------|------------|---|-------------------|-------------------------------------|--------------------|-----------------------------|--------------|
| [V] loop at loopstl.cpp:3962 in s... | 0.125s    | 0.125s     |   | Expand            | Expand                              | AVX                | Inserts; Maske...           | Unrolled     |
| [V] loop at loopstl.cpp:6186 in ...  | 0.125s    | 0.125s     | 1 | Collapse          | Collapse                            | AVX                |                             | Unrolled     |
| i> [loop at loopstl.cpp:6186 in s... | 0.062s    | 0.062s     |   | Remainder         |                                     |                    |                             |              |
| i> [V] [loop at loopstl.cpp:...      |           |            |   | Vectorized (Body) |                                     | AVX                |                             | Unrolled     |
| i, [loop at loopstl.cpp:5625 in ...  |           |            |   | Scalar            | loop with early exits cannot be ... |                    |                             |              |

Scalar Loop. Not vectorized. Loop with early exits cannot be vectorized unless it meets search loop id criteria  
No loop transformations were applied

**Loop may have several parts or versions**

**Loop summary**

**Vectorization and compiler optimization details**

Top Down Source Loop Assembly Assistance Recommendations Compiler Diagnostic Details

**Issue: Ineffective peeled/remainder loop(s) present**

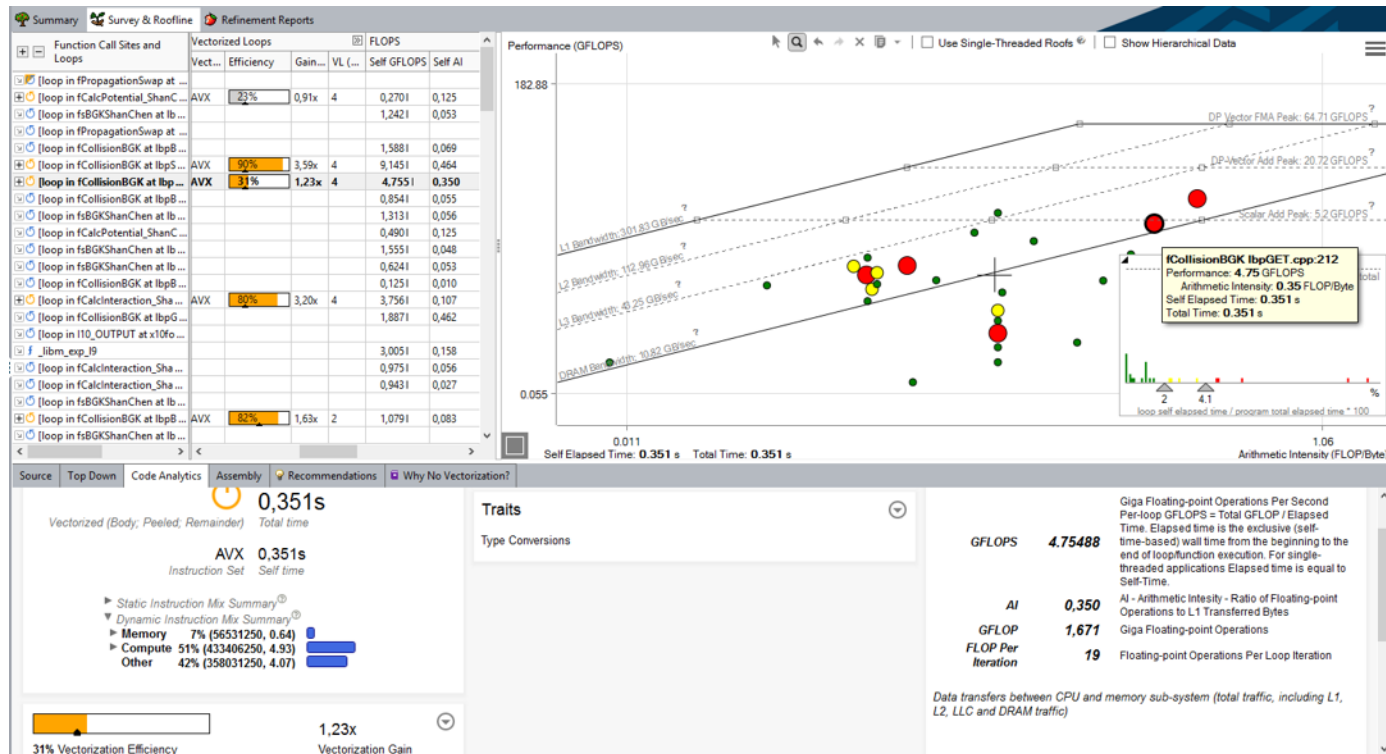
All or some [source loop](#) iterations are not executing in the [loop body](#). Improve performance by moving source loop iterations from [peeled/remainder](#) loops to the loop body.

**Recommendations for optimization**

➤ Add data padding  
Potential performance gain: Information not available  
Confidence this recommendation applies to your code: Information not available until Beta Update release  
The [trip count](#) is not a multiple of [vector length](#). To fix: Do one of the following:

- Increase size of objects and add iterations so the trip count is a multiple of vector length.
- Increase the size of static and automatic objects, and use a compiler option to add data padding.

# Intel Advisor – Roofline



- Multi-platform sampling-based call-path profiler
- Works on unmodified, optimized executables
- <http://hpctoolkit.org>
- Advantages:
  - Overhead can be easily controlled via sampling interval
  - Advantageous for complex C++ codes with many small functions
  - Loop-level analysis (sometimes even individual source lines)
  - Supports POSIX threads
- Disadvantages:
  - Statistical approach that might miss details
  - MPI/OpenMP time displayed as low-level system calls

- Specified via environment variable `HPCRUN_EVENT_LIST`
- General format:  
    `"name@interval [;name@interval ...]"`
- Possible sample sources:
  - WALLCLOCK
  - PAPI counters
  - IO (use w/o interval spec)
  - MEMLEAK (use w/o interval spec)
- Interval: given in microseconds
  - E.g., 10000 → 100 samples per second

# Example: hpcviewer

hpcviewer: sor <@jj28103>

File Debug Help

sor.c

```
670  fkjm1 = Field[k][j-1];
671  rkj   = Rhs[k][j];
672  akj   = Ans[k][j];
673  for (i=1+mod; i<=nxl; i+=2)
674  {
675      delta = omega*( fkj[i+1] + fkj[i-1] +fkjpl[i] + fkjm1[i]
676                  -4.0*fkj[i] - rkj[i] );
677
678      tmpres += fabs(delta);
679
680      fkj[i] = fkj[i] + delta;
681
682      tmperr += fabs(fkj[i] - akj[i]);
683  }
```

associated source code

Calling Context View Callers View Flat View

↑ ↓ 🔥 f(x) 📄 A\* A-

| Scope                        | WALLCLOCK (us).[0.0] (I) | WALLCLOCK (us).[0.0] (E) | WALLCLOCK (us).[1.0] (I) | WALLCLOCK (us).[1.0] (E) |
|------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| Experiment Aggregate Metrics | 4.79e+06 100 %           | 4.79e+06 100 %           | 4.76e+06 100 %           | 4.76e+06 100 %           |
| main                         | 4.79e+06 100 %           |                          | 4.76e+06 100 %           |                          |
| sor_iter                     | 4.68e+06 97.7%           | 4.01e+06 83.7%           | 4.66e+06 97.7%           | 3.95e+06 82.8%           |
| loop at sor.c: 344           | 2.67e+06 55.7%           | 2.00e+06 41.7%           | 2.71e+06 56.8%           | 2.00e+06 41.7%           |
| inlined from sor.c: 658      | 2.00e+06 41.7%           | 2.00e+06 41.7%           | 2.00e+06 42.0%           | 2.00e+06 42.0%           |
| loop at sor.c: 662           | 2.00e+06 41.7%           |                          | 2.00e+06 42.0%           |                          |
| loop at sor.c: 673           | 2.00e+06 41.7%           | 3.55e+04 0.7%            | 2.00e+06 42.0%           |                          |
| loop at sor.c: 673           | 1.96e+06 41.0%           | 1.96e+06 41.0%           | 2.00e+06 42.0%           | 2.00e+06 42.0%           |
| inlined from sor.c: 331      | 8.38e+05 17.5%           | 8.38e+05 17.5%           | 7.06e+05 14.8%           | 7.06e+05 14.8%           |
| sor.c: 675                   | 6.59e+05 13.8%           | 6.59e+05 13.8%           | 6.23e+05 13.1%           | 6.23e+05 13.1%           |
| sor.c: 682                   | 2.40e+05 5.0%            | 2.40e+05 5.0%            | 3.96e+05 8.3%            | 3.96e+05 8.3%            |
| sor.c: 678                   | 1.08e+05 2.2%            | 1.08e+05 2.2%            | 8.39e+04 1.8%            | 8.39e+04 1.8%            |

Callpath to hotspot

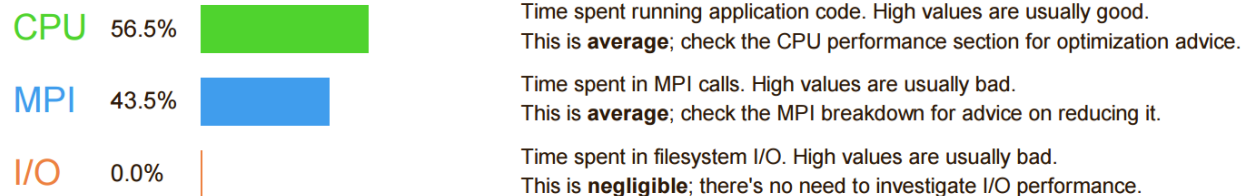
191M of 400M

- **Single page** report provides quick overview of performance issues
- Works on unmodified, optimized executables
- Shows CPU, memory, network and I/O utilization
- Supports MPI, multi-threading and accelerators
- Saves data in HTML, CVS or text form
- <http://www.allinea.com/products/allinea-performance-reports>
- **Note:** License limited to 512 processes (with unlimited number of threads)

# Example Performance Reports

## Summary: cp2k.popt is CPU-bound in this configuration

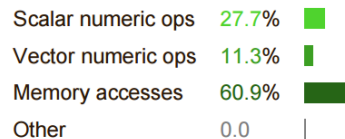
The total wallclock time was spent as follows:



This application run was **CPU-bound**. A breakdown of this time and advice for investigating further is in the **CPU** section below.

### CPU

A breakdown of how the 56.5% total CPU time was spent:

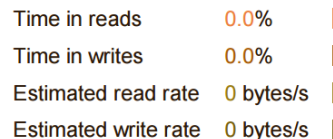


The per-core performance is **memory-bound**. Use a profiler to identify time-consuming loops and check their cache performance.

Little time is spent in **vectorized instructions**. Check the compiler's vectorization advice to see why key loops could not be vectorized.

### I/O

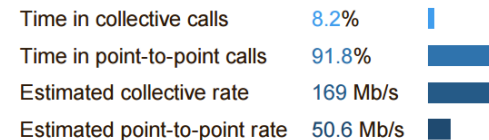
A breakdown of how the 0.0% total I/O time was spent:



No time is spent in **I/O operations**. There's nothing to optimize here!

### MPI

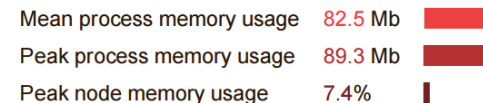
Of the 43.5% total time spent in MPI calls:



The **point-to-point** transfer rate is low. This can be caused by inefficient message sizes, such as many small messages, or by imbalanced workloads causing processes to wait. Use an MPI profiler to identify the problematic calls and ranks.

### Memory

Per-process memory usage may also affect scaling:



The **peak node memory usage** is low. You may be able to reduce the total number of CPU hours used by running with fewer MPI processes and more data on each process.

# Allinea Performance Reports: Example

```
% module load AllineaPerformanceReports

#####
##  In the job script:  ##
#####

perf-report --mpi="slurm" \
  srun --procs-per-node= $P$  --nodes= $n$  [...] ./myprog [args]

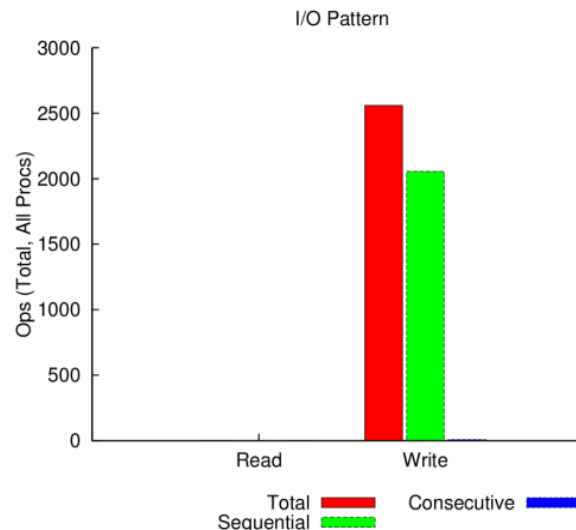
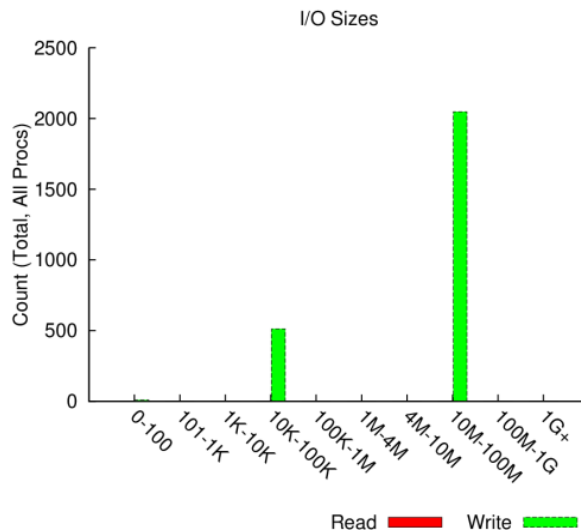
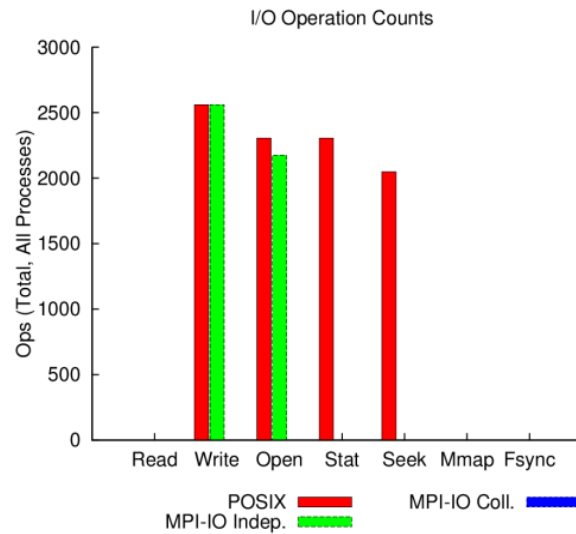
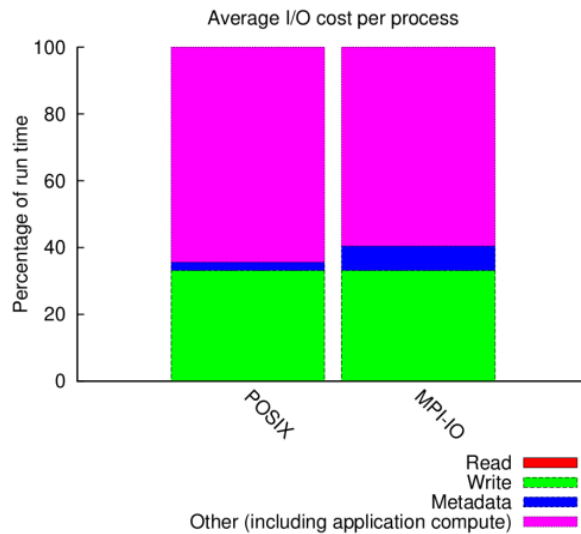
#####
## After job finished: ##
#####

% less myprog_<NP>p_<DATE>.txt
% firefox myprog_<NP>p_<DATE>.html
```

- I/O characterization tool logging parallel application file access
- Summary report provides quick overview of performance issues
- Works on unmodified, optimized executables
- Shows counts of file access operations, times for key operations, histograms of accesses, etc.
- Supports POSIX, MPI-IO, HDF5, PnetCDF, ...
  - Doesn't support mpif90 on BlueGene systems (use mpif77)
- Binary log file written at exit post-processed into PDF report
- <http://www.mcs.anl.gov/research/projects/darshan/>
- Open Source: installed on many HPC systems

# Example Darshan report extract

jobid: | uid: | nprocs: 4096 | runtime: 175 seconds



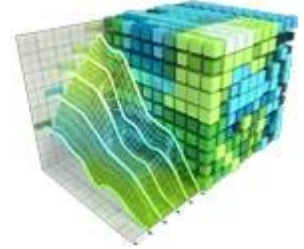
```
% load compiler and MPI module
% module load darshan-runtime darshan-util

#####
## In the job script: ##
#####

export LD_PRELOAD=$EBROOTDARSHANMINRUNTIME/lib/libdarshan.so
export DARSHAN_LOG_PATH=$PWD
export DARSHAN_LOGFILE=darshan.log
srun --tasks-per-node P --ntasks n [...] ./myprog [args]

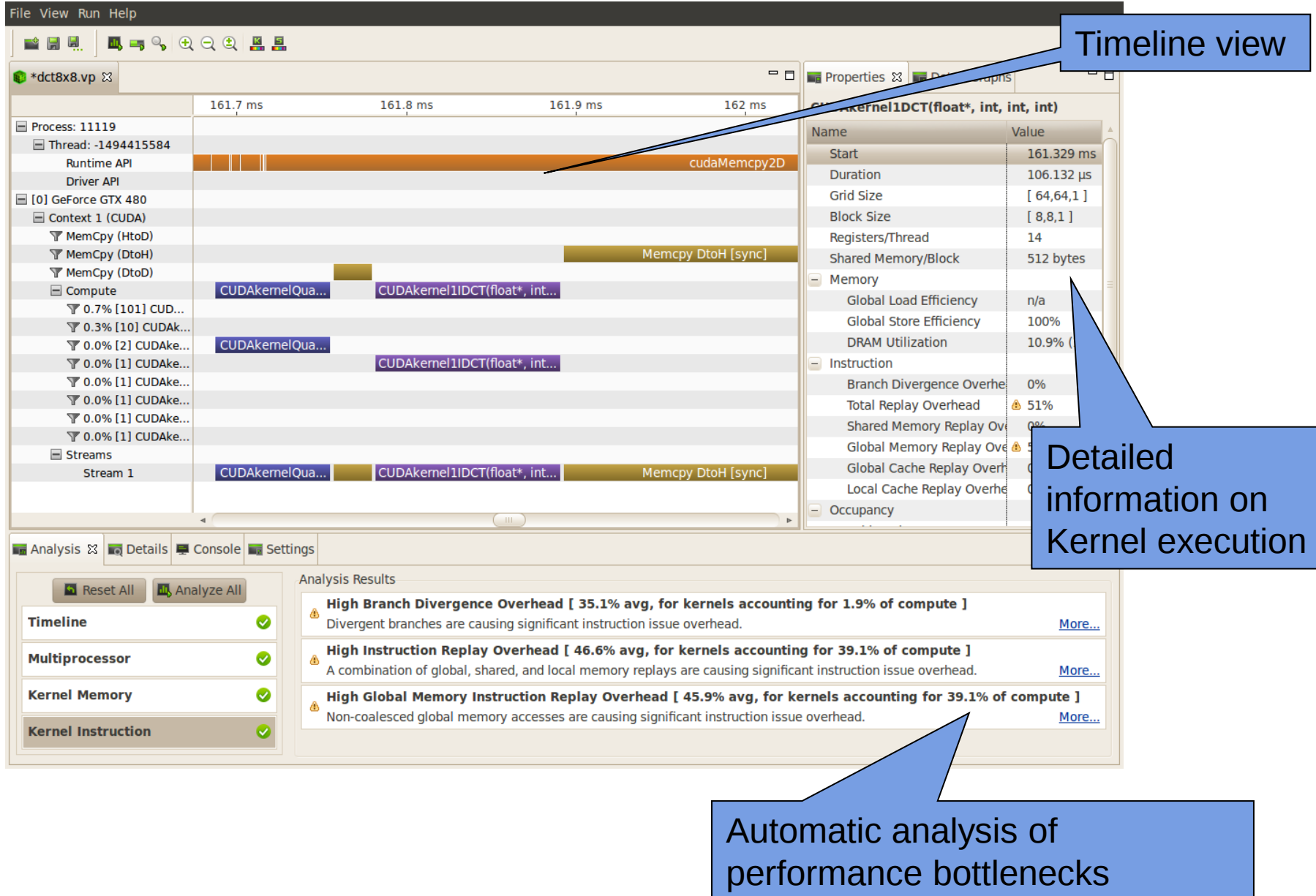
#####
## After job finished: ##
#####

% darshan-job-summary.pl darshan.log
% gv darshan.pdf
```

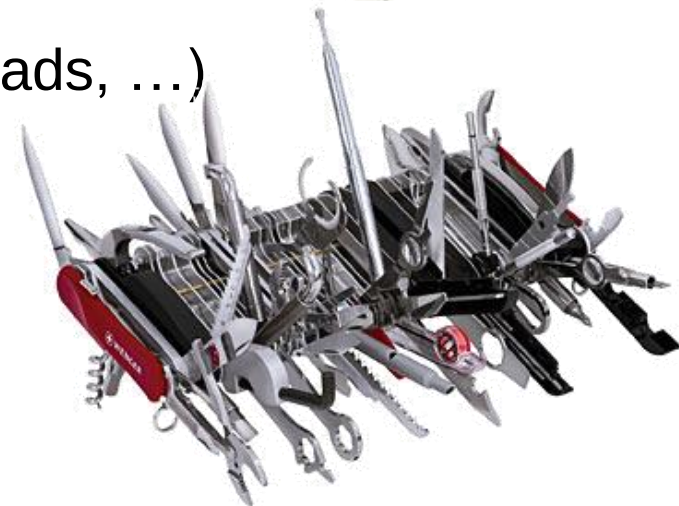
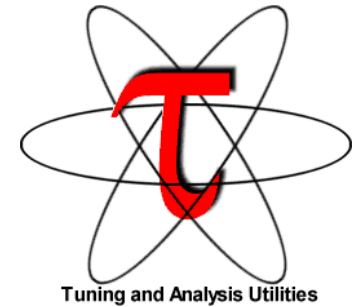


- Part of the CUDA Toolkit
- Supports all CUDA enabled GPUs
- Supports CUDA and OpenACC on Windows, OS X and Linux
- Unified CPU and GPU Timeline
- CUDA API trace
  - Memory transfers, kernel launches, and other API functions
- Automated performance analysis
  - Identify performance bottlenecks and get optimization suggestions
- Guided Application Analysis
- Power, thermal, and clock profiling

# NVIDIA Visual Profiler: Example

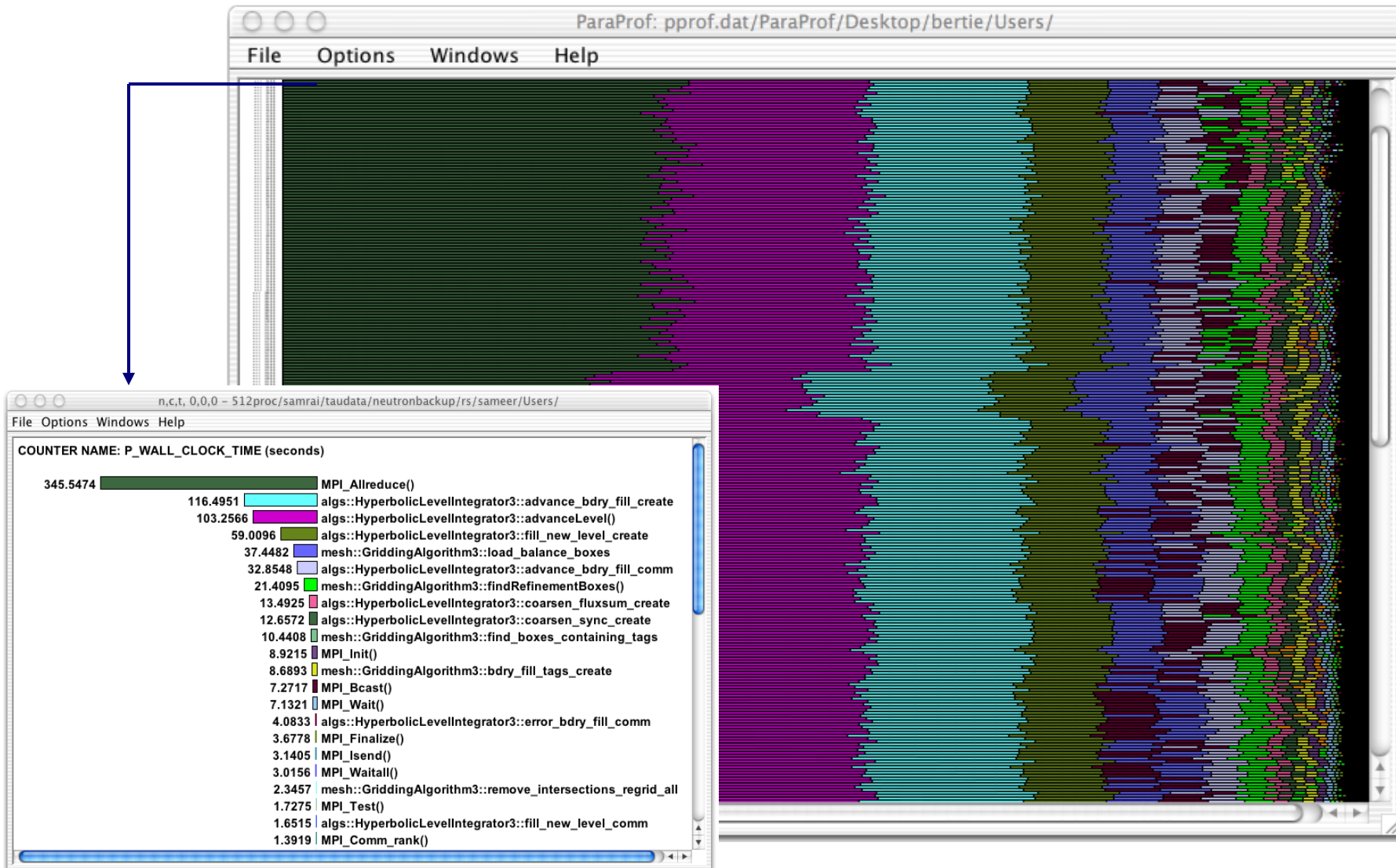


- Very portable tool set for instrumentation, measurement and analysis of parallel multi-threaded applications
- <http://tau.uoregon.edu/>
- Supports
  - Various profiling modes and tracing
  - Various forms of code instrumentation
  - C, C++, Fortran, Java, Python
  - MPI, multi-threading (OpenMP, Pthreads, ...)
  - Accelerators

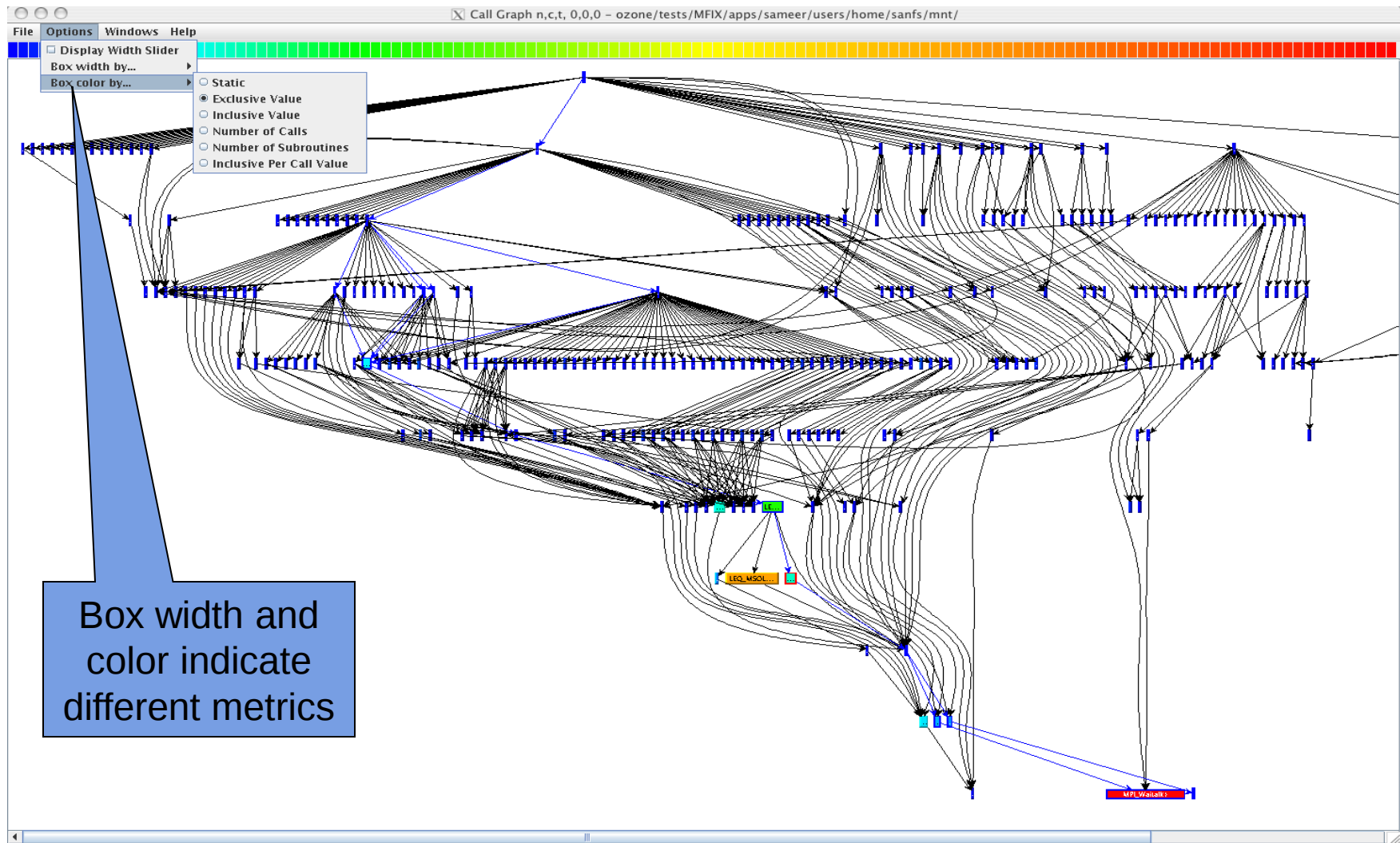


- Flexible instrumentation mechanisms at multiple levels
  - Source code
    - manual
    - automatic
      - C, C++, F77/90/95 (Program Database Toolkit (PDT))
      - OpenMP (directive rewriting with **Opari**)
  - Object code
    - pre-instrumented libraries (e.g., MPI using **PMPI**)
    - statically-linked and dynamically-loaded (e.g., Python)
  - Executable code
    - dynamic instrumentation (pre-execution) (**DynInst**)
    - virtual machine instrumentation (e.g., Java using **JVMPI**)
- Support for **performance mapping**
- Support for **object-oriented** and **generic** programming

# TAU: Basic Profile View

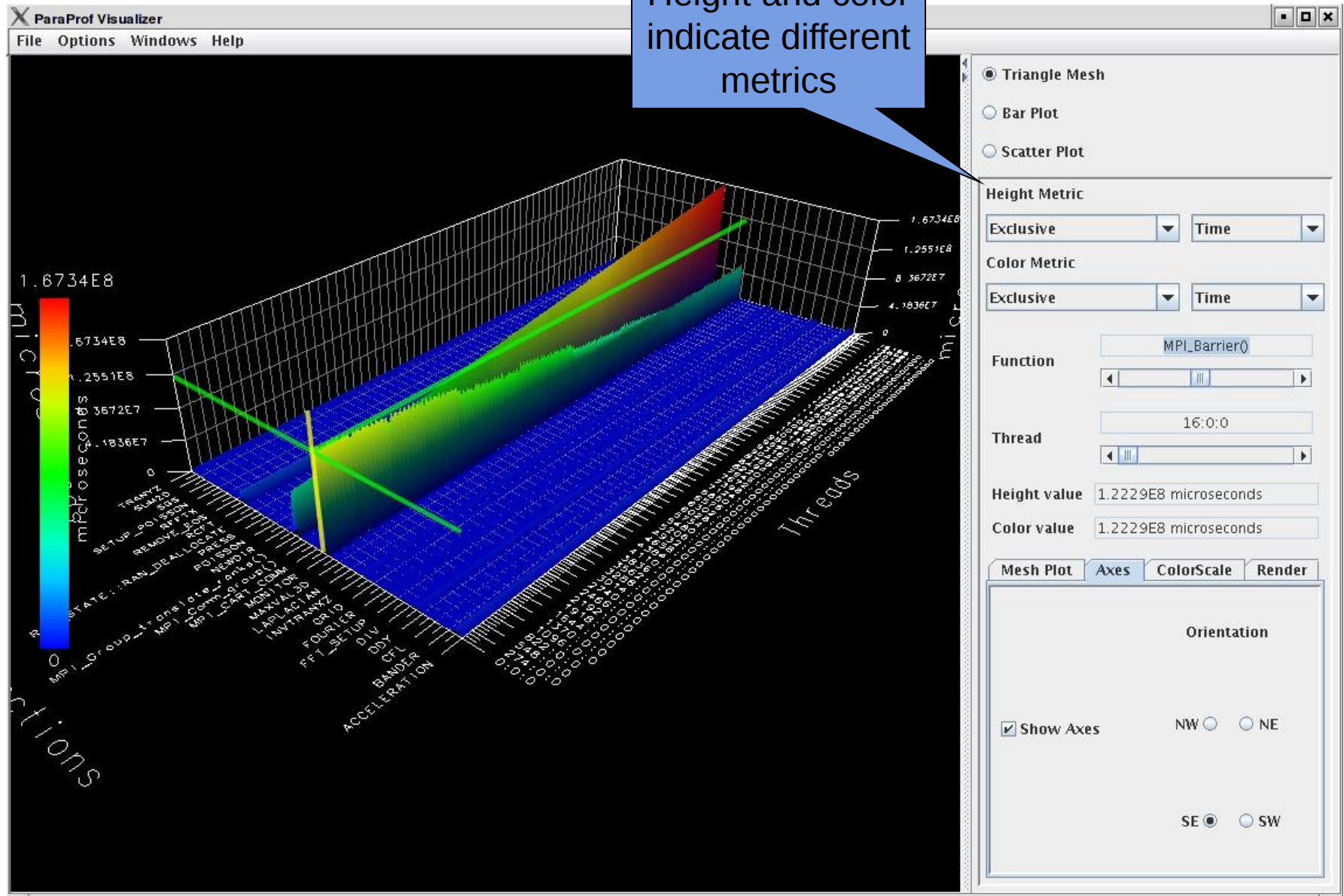


# TAU: Callgraph Profile View

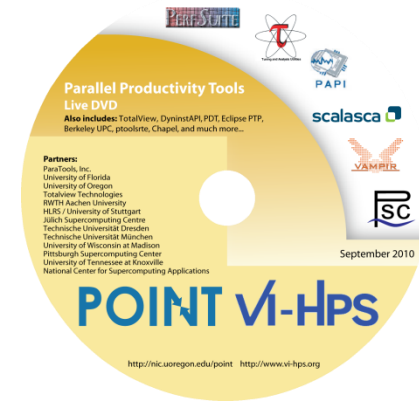


# TAU: 3D Profile View

Height and color  
indicate different  
metrics



- To check latest status and versions
  - “module spider TOOL”
- Websites
  - <http://www.fz-juelich.de/ias/jsc/juwels/>
  - <http://www.fz-juelich.de/ias/jsc/jureca/>
    - User Info
      - Parallel Debugging (  )
      - Parallel Performance Analysis (  )
  - <http://www.vi-hps.org/training/material/>
    - Performance Tools LiveDVD image
    - Links to tool websites and documentation
    - Tutorial slides



- For general support: `sc@fz-juelich.de`
- Tool-specific support via corresponding mailing lists
  - Score-P: `support@score-p.org`
  - Scalasca: `scalasca@fz-juelich.de`
- Workshops and Trainings:
  - Regular VI-HPS Tuning Workshops
    - Several days
    - Multiple tools, e.g. Score-P, Scalasca, Vampir, TAU, ...
    - Bring-your-own-code
    - <http://www.vi-hps.org/training/tws/>
  - JSC Porting and Tuning Workshop Series
  - WS's and trainings at several HPC conferences