Measurement with Score-P

Marc Schlütter, JSC

Performance engineering workflow

- Prepare application with symbols
- Insert extra code (probes/hooks)

- Collection of performance data
- Aggregation of performance data

- Modifications intended to
- eliminate/reduce performance problem

- Calculation of metrics
- Identification of performance problems
- Presentation of results

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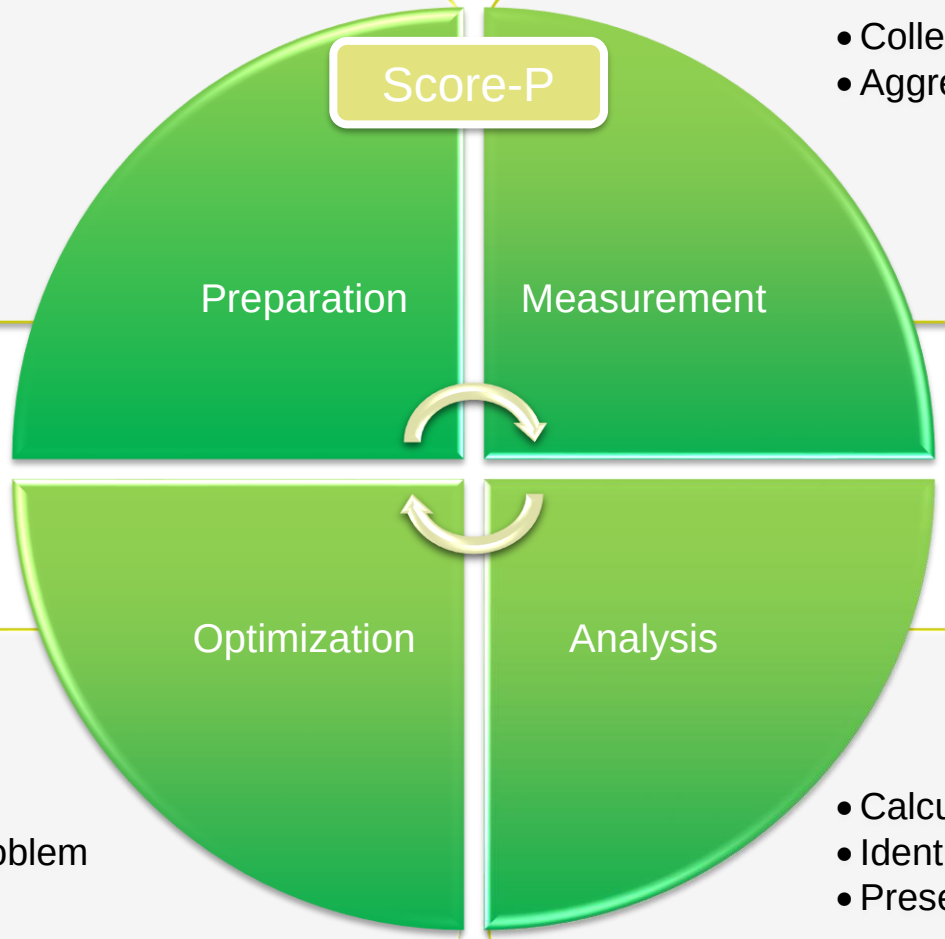

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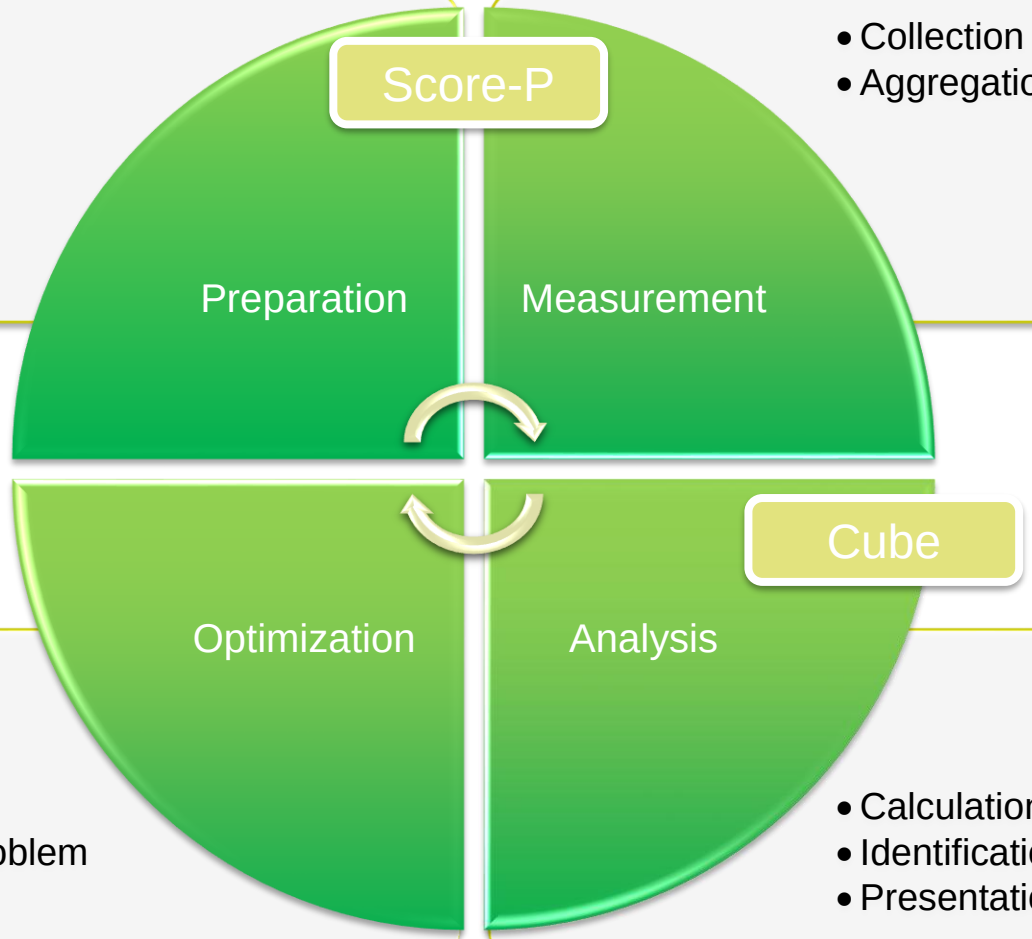

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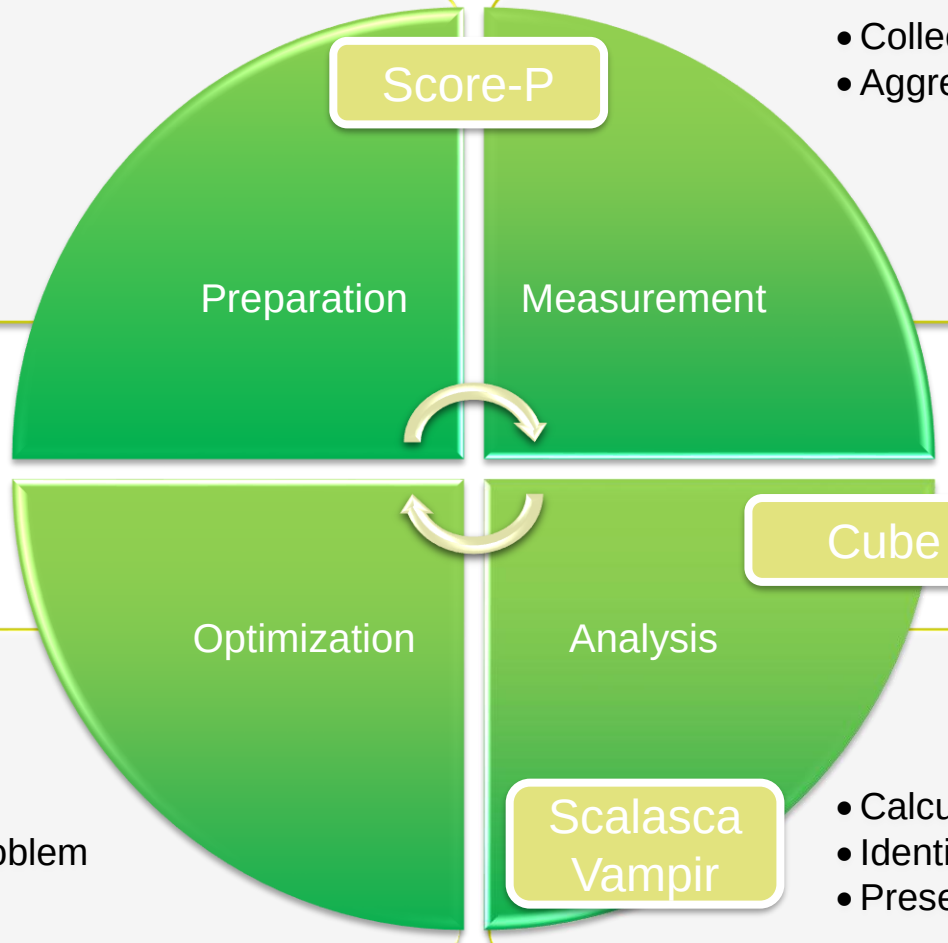

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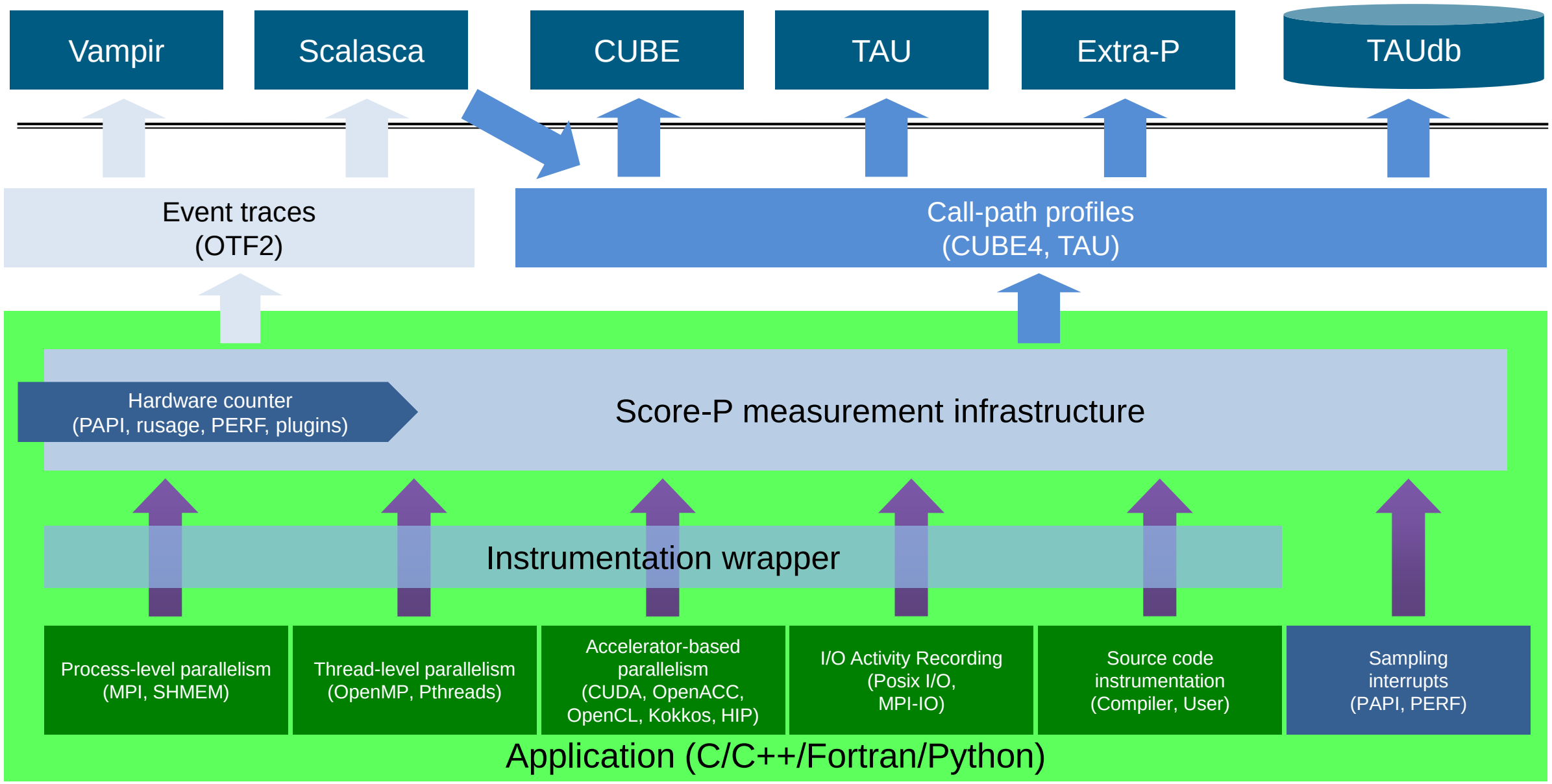
Score-P

- Infrastructure for instrumentation and performance measurements
- Instrumented application can be used to produce several results:
  - Call-path profiling: CUBE4 data format used for data exchange
  - Event-based tracing: OTF2 data format used for data exchange
- Supported parallel paradigms:
  - Multi-process: MPI, SHMEM
  - Thread-parallel: OpenMP, Pthreads
  - Accelerator-based: CUDA, ROCm, OpenCL, OpenACC, Kokkos
- Open Source; portable and scalable to all major HPC systems
- Initial project funded by BMBF
- Close collaboration with PRIMA project funded by DOE

GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung


Vampir
Scalasca
CUBE
TAU
Extra-P
TAUdb
Event traces
(OTF2)
Call-path profiles
(CUBE4, TAU)
Hardware counter
(PAPI, rusage, PERF, plugins)
Score-P measurement infrastructure
Instrumentation wrapper
Process-level parallelism
(MPI, SHMEM)
Thread-level parallelism
(OpenMP, Pthreads)
Accelerator-based
parallelism
(CUDA, OpenACC,
OpenCL, Kokkos, HIP)
I/O Activity Recording
(Posix I/O,
MPI-IO)
Source code
instrumentation
(Compiler, User)
Sampling
interrupts
(PAPI, PERF)
Application (C/C++/Fortran/Python)

Partners

- Forschungszentrum Jülich, Germany
- Gesellschaft für numerische Simulation mbH Braunschweig, Germany
- RWTH Aachen, Germany
- Technische Universität Darmstadt, Germany
- Technische Universität Dresden, Germany
- Technische Universität München, Germany
- University of Oregon, Eugene, USA

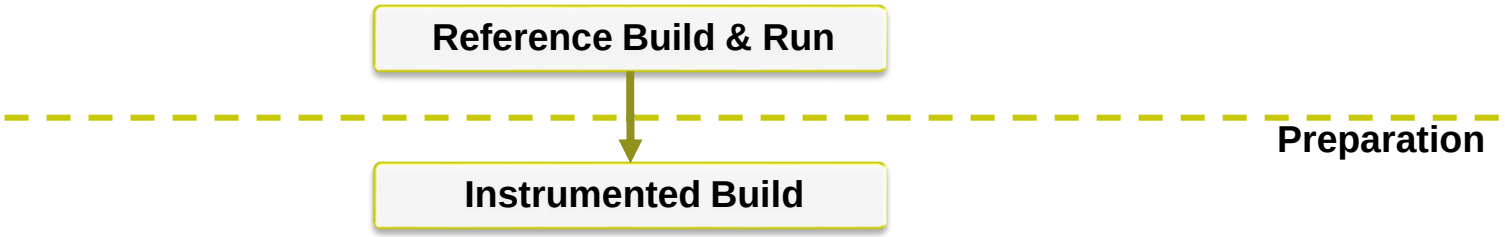
Demo: NPB-MZ-MPI / BT

Performance analysis workflow: Reference Run

Reference Build & Run

- Getting uninstrumented and undisturbed reference execution times
- Verifying a working combination of application and system configuration

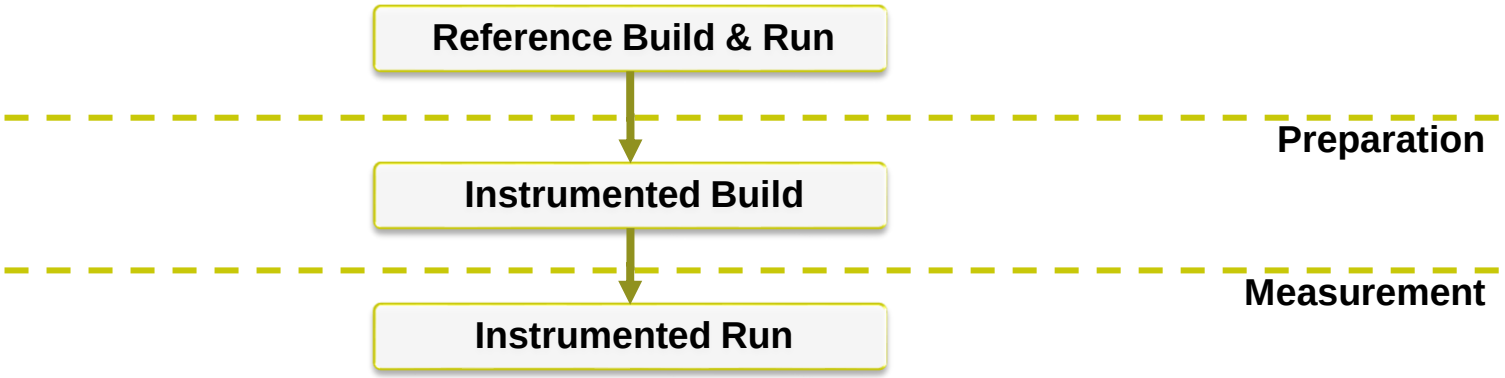
Performance analysis workflow: Application Instrumentation



Instrumented Build

- First instrumentation of the code with Score-P
- Default usage: prefix every compiler call with `scorep`
- Automatic recognition of paradigms in most cases
- Explicit options available in case these fail

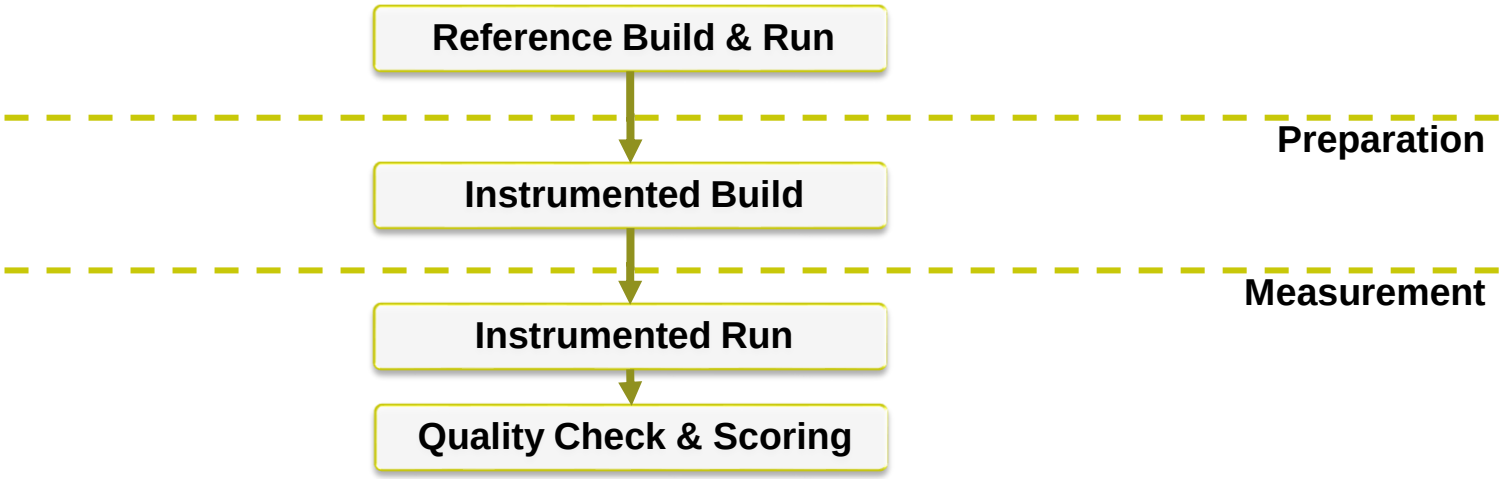
Performance analysis workflow: Instrumented Run



Instrumented Run

- Run possible using the same execution cmds/scripts using Score-P default settings
- Controlled via environment variables
- `scorep-info config-vars` for a list of all variables
- Measurement directory contains the used configuration
- Using the reference run to compare runtime overhead

Performance analysis workflow: Quality Check & Scoring



Quality Check & Scoring

- Using **`scorep-score`** to evaluate sources of overhead in the execution
- Runtime overhead related to time per visit and visits as most of Score-P's overhead is static per visit
- Information about expected trace sizes for later measurements, a direct function of the number of visits for a region

- **`scorep-score -r`** : listing per region(functions mostly)
- **`scorep-score -g`**: generating an initial filter file (heuristics can be modified)
- **`scorep-score -f filter`**: testing the effects of a proposed filter file

Goals of scoring and filtering

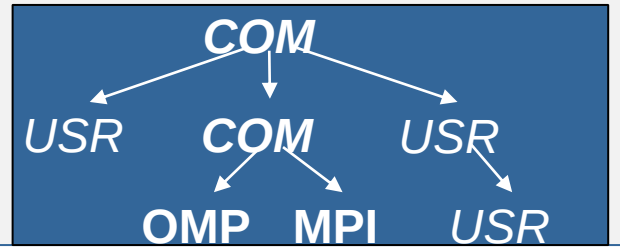
- Evaluate how *expensive* measurement of various regions is
  - Time cost is roughly fixed per event
  - Short functions are relatively more expensive
  - Space cost for tracing is linear in number of events
- Determine which expensive regions are *unnecessary* to measure
  - Frequently called, short execution, and non-scaling behavior
- Repeat the measurement, with those regions *filtered* at runtime to reduce overhead
  - Reduce space cost to zero and time cost to a hash comparison and a couple of branches
- (Optional) Apply the filter at *compile-time* in order to further reduce overhead
  - Eliminates the hash and branches; often not needed

NPB-MZ-MPI / BT summary analysis result scoring

```
% scorep-score scorep-btmz-D-32x7/profile.cubex

Estimated aggregate size of event trace:                   3332GB
Estimated requirements for largest trace buffer (max_buf): 105GB
Estimated memory requirements (SCOREP_TOTAL_MEMORY):       105GB
(warning: The memory requirements cannot be satisfied by Score-P to avoid
 intermediate flushes when tracing. Set SCOREP_TOTAL_MEMORY=4G to get the
 maximum supported memory or reduce requirements using USR regions filters.)

flt     type      max_buf[B]          visits  time[s] time[%] time/visit[us]  region
         ALL 112,035,087,899 137,518,952,689 29382.90   100.0          0.21  ALL
         USR 111,908,772,534 137,419,580,865 11380.33    38.7          0.08  USR
         OMP     121,893,856      95,047,680 17750.19    60.4        186.75  OMP
         COM       2,935,270       3,612,640    14.97     0.1          4.14  COM
         MPI       1,588,606         711,472   237.42     0.8        333.70  MPI
      SCOREP              41              32     0.00     0.0         56.03  SCOREP
```



3332 GB total memory
105 GB per rank!

Region/callpath classification

- **MPI** pure MPI functions
- **OMP** pure OpenMP regions
- **USR** user-level computation
- **COM** "combined" USR+OpenMP/MPI
- **SCOREP** measurement internals
- **ANY/ALL** aggregate of all region types

NPB-MZ-MPI / BT summary analysis report breakdown

```
% scorep-score -r scorep-btmz-D-32x7/profile.cubex
  [...]
  [...]
flt     type      max_buf[B]          visits  time[s] time[%] time/visit[us]  region
         ALL 112,035,087,899 137,518,952,689 29382.90   100.0           0.21  ALL
         USR 111,908,772,534 137,419,580,865 11380.33    38.7           0.08  USR
         OMP     121,893,856      95,047,680 17750.19    60.4         186.75  OMP
         COM       2,935,270       3,612,640    14.97     0.1           4.14  COM
         MPI       1,588,606         711,472   237.42     0.8         333.70  MPI
      SCOREP              41              32     0.00     0.0          56.03  SCOREP

         USR  36,395,971,872  44,677,967,872  5074.31    17.3           0.11  binvcrhs
         USR  36,395,971,872  44,677,967,872  3479.03    11.8           0.08  matmul_sub
         USR  36,395,971,872  44,677,967,872  2510.98     8.5           0.06  matvec_sub
         USR     957,566,506   1,152,495,616   152.76     0.5           0.13  lhsinit
         USR     957,566,506   1,152,495,616   103.12     0.4           0.09  binvrhs
         USR     878,133,152   1,080,078,336    60.03     0.2           0.06  exact_solution
         OMP       9,782,976       3,598,336     0.53     0.0           0.15  !$omp parallel @exch_qbc.f:204
         OMP       9,782,976       3,598,336     0.52     0.0           0.14  !$omp parallel @exch_qbc.f:215
         OMP       9,782,976       3,598,336     0.49     0.0           0.14  !$omp parallel @exch_qbc.f:244
         OMP       9,782,976       3,598,336     0.55     0.0           0.15  !$omp parallel @exch_qbc.f:255
[...]
```

Majority of the 105 GB just for these 6 regions

NPB-MZ-MPI / BT summary analysis report filtering

```
% scorep-score -g scorep-btmz-D-32x7/profile.cubex
An initial filter file template has been generated:
'initial_scorep.filter'
To use this file for filtering at run-time, set the respective
Score-P variable:
    SCOREP_FILTERING_FILE=initial_scorep.filter
For compile-time filtering 'scorep' has to be provided with
the '--instrument-filter' option:
    $ scorep --instrument-filter=initial_scorep.filter
Compile-time filtering depends on support in the used Score-P
installation.
The filter file is annotated with comments, please check if
the selection is suitable for your purposes and add or remove
functions if needed.
```

- Report scoring with prospective filter listing 3 USR regions

NPB-MZ-MPI / BT summary analysis report filtering

```
% scorep-score -r -f initial_scorep.filter \
> scorep-btmz-D-32x7/profile.cubex
flt     type      max_buf[B]          visits  time[s] time[%] time/visit[us]  region
 -       ALL 112,035,087,899 137,518,952,689 29382.90   100.0           0.21  ALL
 -       USR 111,908,772,534 137,419,580,865 11380.33    38.7           0.08  USR
 -       OMP     121,893,856      95,047,680 17750.19    60.4         186.75  OMP
 -       COM       2,935,270       3,612,640    14.97     0.1           4.14  COM
 -       MPI       1,588,606         711,472   237.42     0.8         333.70  MPI
 -    SCOREP              41              32     0.00     0.0          56.03  SCOREP

 *       ALL   2,919,186,417   3,485,049,073 18318.59    62.3           5.26  ALL-FLT
 +       FLT 109,187,915,616 134,033,903,616 11064.32    37.7           0.08  FLT
 *       USR   2,792,819,848   3,385,677,249   316.01     1.1           0.09  USR-FLT
 -       OMP     121,893,856      95,047,680 17750.19    60.4         186.75  OMP-FLT
 *       COM       2,935,270       3,612,640    14.97     0.1           4.14  COM-FLT
 -       MPI       1,588,606         711,472   237.42     0.8         333.70  MPI-FLT
 -    SCOREP              41              32     0.00     0.0          56.03  SCOREP-FLT

+       USR  36,395,971,872  44,677,967,872  5074.31    17.3           0.11  binvcrhs
+       USR  36,395,971,872  44,677,967,872  3479.03    11.8           0.08  matmul_sub
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-       USR     957,566,506   1,152,495,616   103.12     0.4           0.09  binvrhs
-       USR     878,133,152   1,080,078,336    60.03     0.2           0.06  exact_solution
```

Filtered routines marked with '+'

- Score report breakdown by region
- Adapt initial filter file to include the 3 additional routines

NPB-MZ-MPI / BT summary analysis report filtering

```
% scorep-score -r -f initial_scorep.filter \
> scorep-btmz-D-32x7/profile.cubex
Estimated aggregate size of event trace:                   3871MB
Estimated requirements for largest trace buffer (max_buf): 122MB
Estimated memory requirements (SCOREP_TOTAL_MEMORY):       136MB
(hint: When tracing set SCOREP_TOTAL_MEMORY=136MB to avoid intermediate flushes
or reduce requirements using USR regions filters.)
[...]
+       USR  36,395,971,872  44,677,967,872  5063.46    17.2           0.11  binvcrhs
+       USR  36,395,971,872  44,677,967,872  3469.07    11.8           0.08  matmul_sub
+       USR  36,395,971,872  44,677,967,872  2493.53     8.5           0.06  matvec_sub
+       USR     957,566,506   1,152,495,616   152.54     0.5           0.13  lhsinit
+       USR     957,566,506   1,152,495,616   102.90     0.4           0.09  binvrhs
+       USR     878,133,152   1,080,078,336    59.91     0.2           0.06  exact_solution

% cat initial_scorep.filter
SCOREP_REGION_NAMES_BEGIN
 EXCLUDE
   lhsinit
   binvrhs
   exact_solution

   # type=USR max_buf= 36,395,971,872 visits= 44,677,967,872, ...
   # name='binvcrhs'
   # file='BT-MZ/solve_subs.f'
   MANGLED binvcrhs_
```

3.9 GB of memory in total, 136 MB per rank!

Manually added entries, Space separated and bash-like wildcards *, ?, []

- Refined filter reduces the requirements to useful sizes.
- More information on manual and automatic filtering in the user documentation and `scorep-score --help`

Adding PAPI Performance counters

- Estimating the memory requirements due to recorded counters:

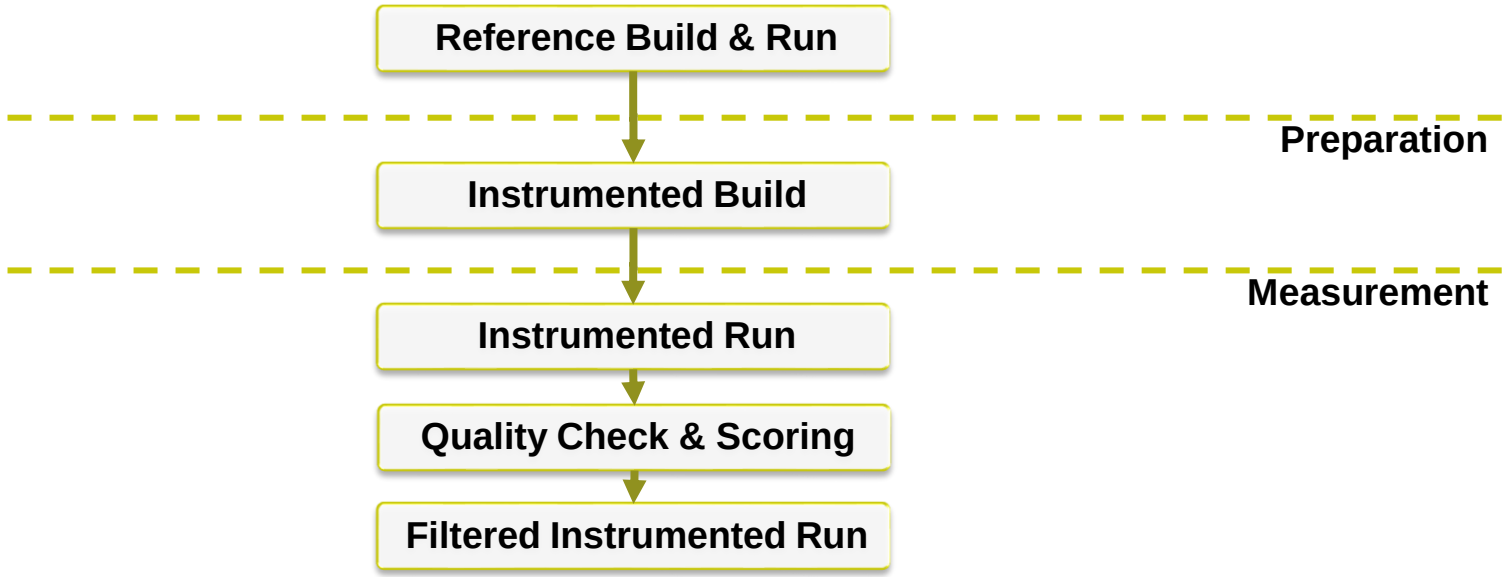
```
% <editor> scorep.slurm
...
#SBATCH -J bt-scorep-filter
% scorep-score -f initial_scorep.filter -c 2 scorep-btmz-D-32x7/profile.cubex

Estimated aggregate size of event trace:                   10GB
Estimated requirements for largest trace buffer (max_buf): 297MB
Estimated memory requirements (SCOREP_TOTAL_MEMORY):       311MB
(hint: When tracing set SCOREP_TOTAL_MEMORY=311MB to avoid intermediate flushes
or reduce requirements using USR regions filters.)
```

Increased memory requirements from the prior 136 MB per rank!

- With a PAPI module loaded: **`papi_avail`** for a list of available counters

```
export SCOREP_METRIC_PAPI=PAPI_TOT_INS,PAPI_TOT_CYC
```

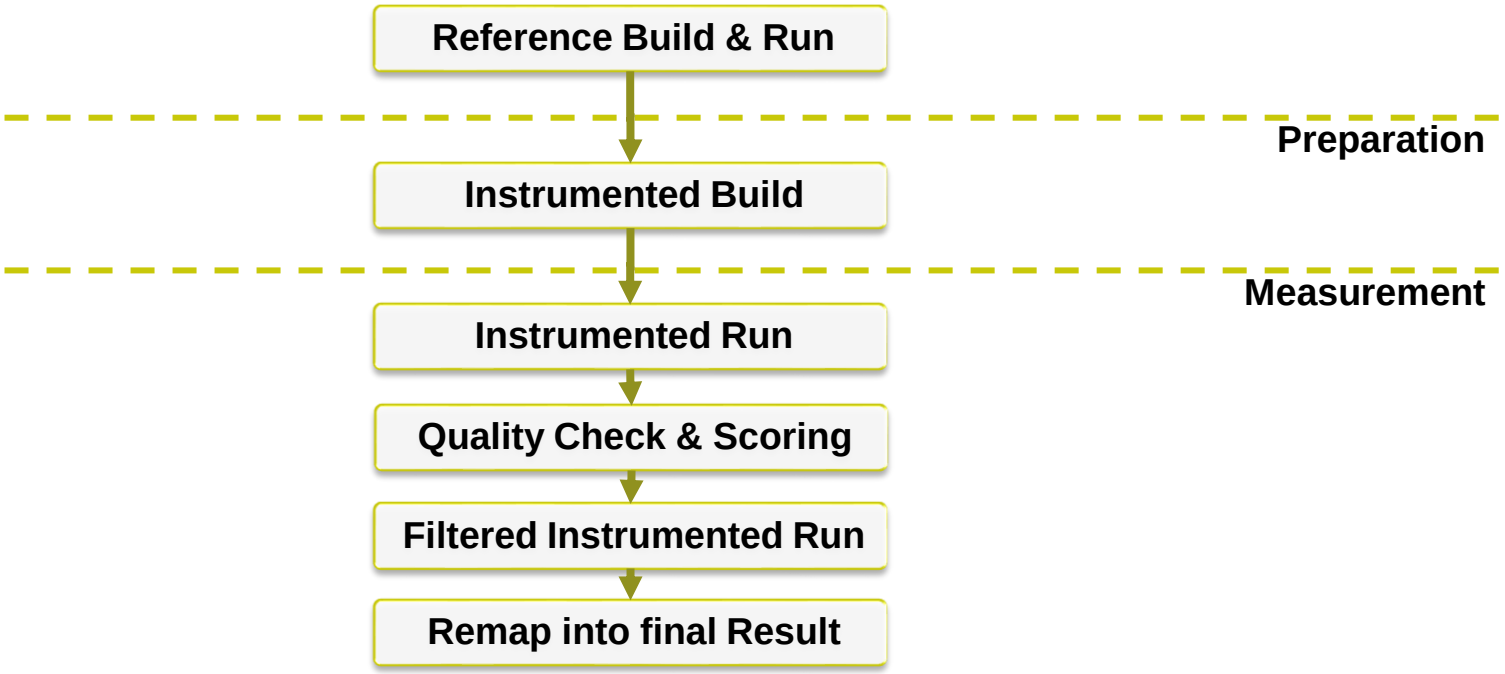
Performance analysis workflow: Filtered Run



Filtered Instrumented Run

- Using the generated and modified filter file via `SCOREP_FILTERING_FILE=name`
- If necessary modify and rerun, but ideally that should work via the scoring preview
- The result should have a `profile.cubex` that is technically usable

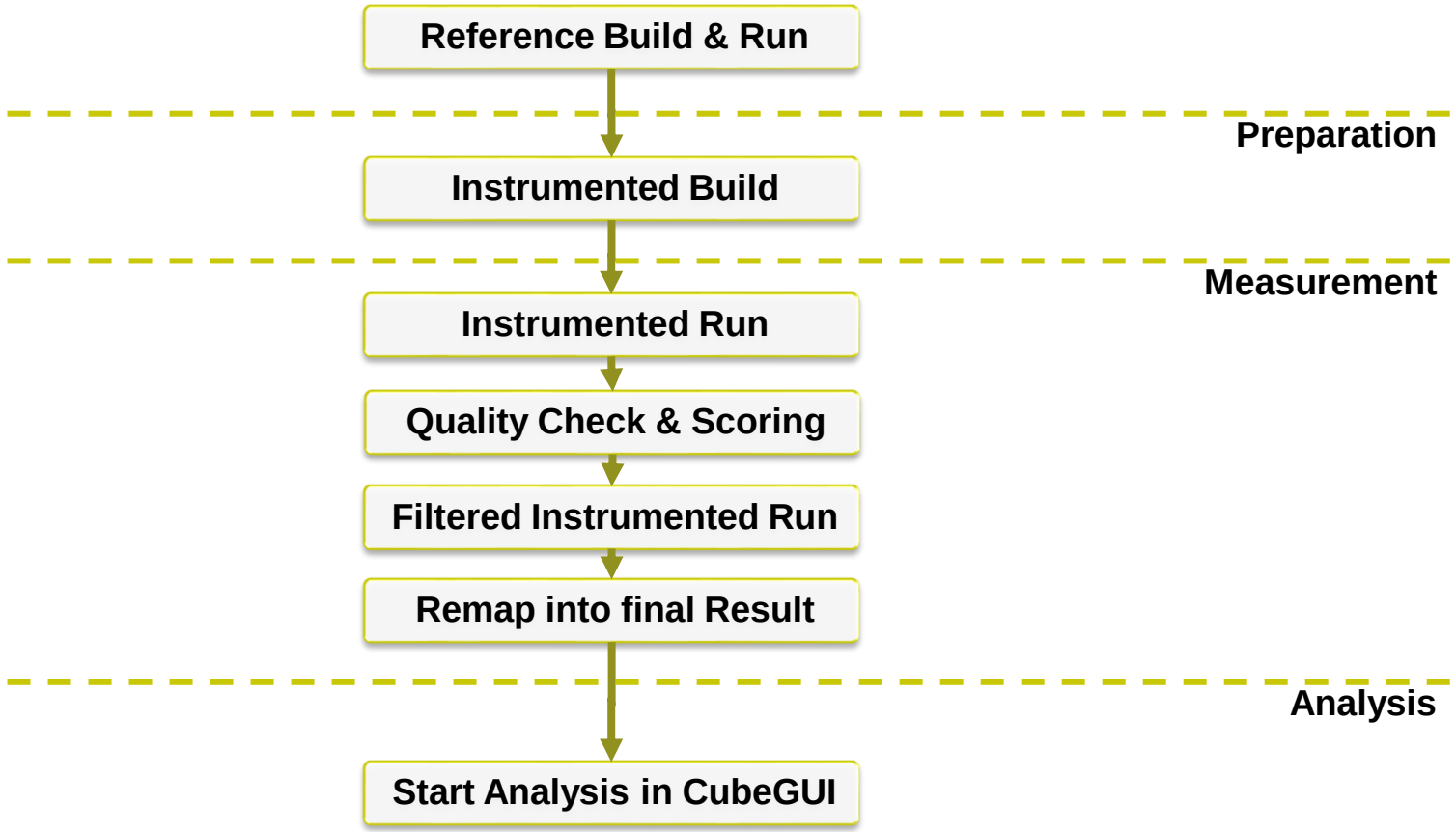
Performance analysis workflow: Postprocessing



Remap into final Result

- Postprocessing step that generates additional metrics and data
- Results in a measurement ready for analysis
- The remap step can be done by `cube_remap2 -s -d profile.cubex`
- `-s`: adds additional metrics
- `-d`: precalculates values (tradeoff size vs. calculation effort while analysing)

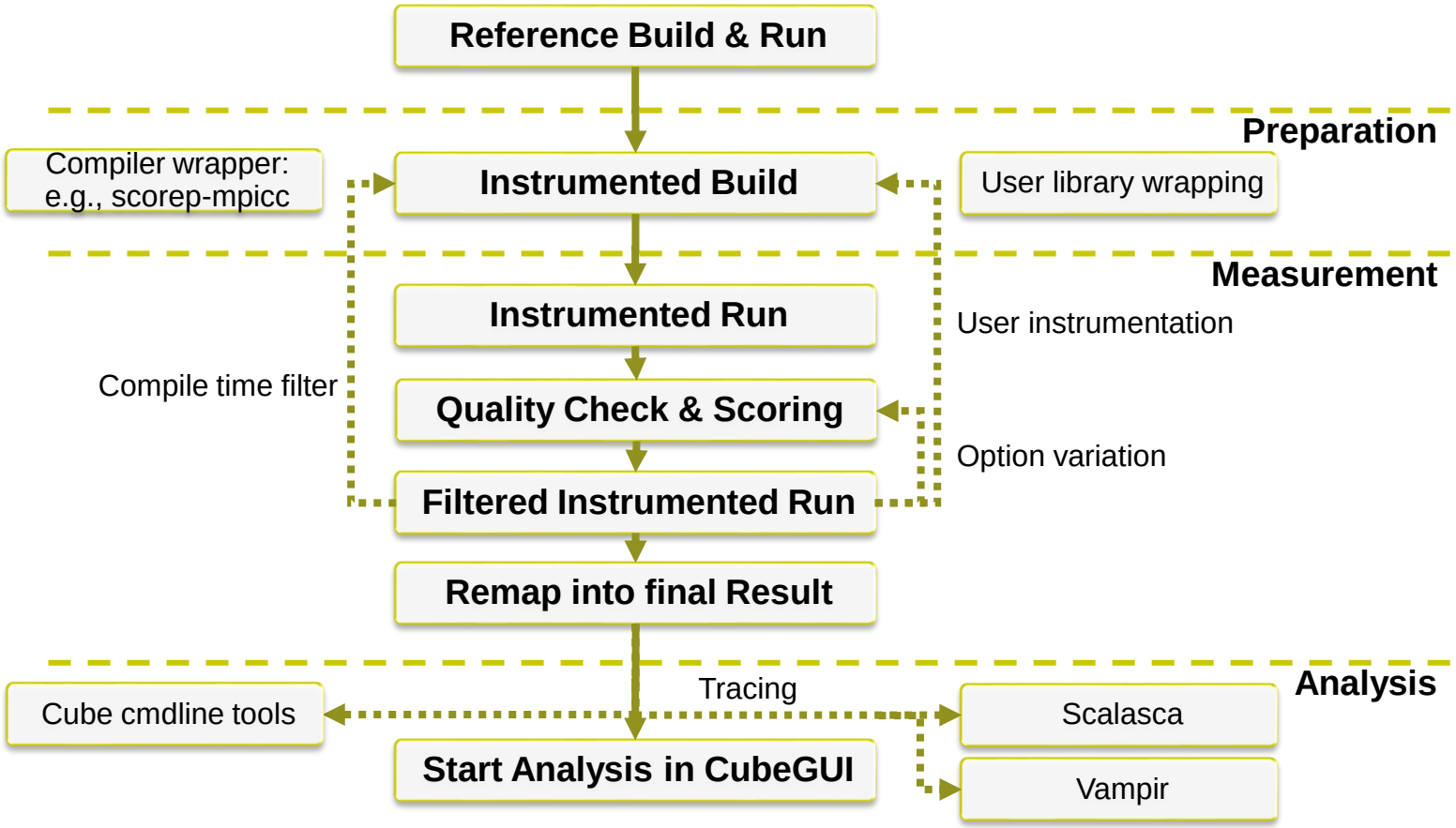
Performance analysis workflow: Start Analysis



Start Analysis in CubeGUI

- Open the result in the CubeGUI
- The GUI is available as:
  - To build from source
  - Various prebuilt executables
- The cubex files are transferable and the only element required to run
- For source code references the application sources need to be accessible

Performance analysis workflow: Outlook

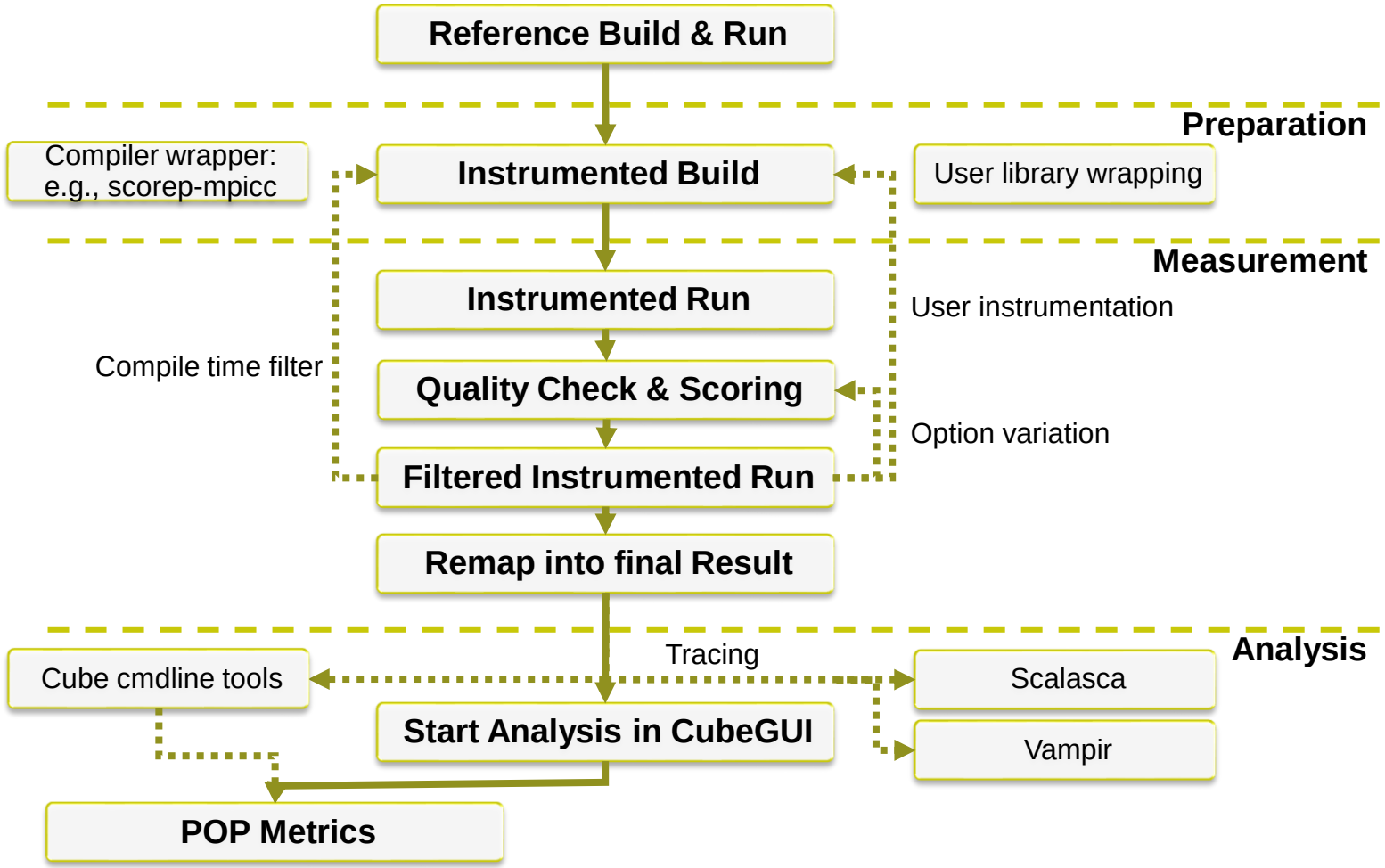


Foreshadowing

- The straightforward linear graph can become more complicated, depending on software environment, application requirements, measured paradigms and various other settings
- Going into tracing as next step will be covered tomorrow

- See reference slides at the end

Performance analysis workflow: POP Metrics



POP Metrics

- Additional Requirements:
  - Hardware Counters
  - (Optional Metrics from Tracing)
    - => Scalasca
- Calculation via GUI or cmd line
  `cube_pop_metrics`
- More complex selections easier in GUI

Calculating POP metrics on the cmd line: `cube_pop_metrics`

```
% cube_pop_metrics -h
Usage: cube_pop_metrics [-i] [-a <pop analysis>] [-c <FOI(s)>] [-h] [-? <pop analysis>] <cube1> <cube2> ..
  -a     Name of the POP analysis. Options: mpi,hybrid-add, hybrid-mult, bsc. Default: mpi
  -c     Name(s) or ID(s) of FOI(s). Default: calltree root(s). Comma separated
  -i     Performs the calculation individually for every listed FOI.
         Default: if omitted, the calculation is performed in an accumulated manner
  -h     Help; Output a brief help message.
  -?     Help; Output a long detailed help message.
```

```
POP Metric                                  Profile 0
-----------------------------------
Hybrid Parallel Efficiency                  0.770967
 * Hybrid Load Balance Efficie              0.851013
 * Hybrid Communication Effici              0.905941
MPI Parallel Efficiency                     0.896192
 * MPI Load Balance                         0.949225
 * MPI Communication Efficienc              0.944130
 * * * MPI Serialisation Effic              nan
 * * * MPI Transfer Efficiency              nan
OpenMP Parallel Efficiency                  0.860270
 * OpenMP Load Balance Efficie              0.896534
 * OpenMP Communication Effici              0.959551
…
```

Some values not available in pure profile measurements => Provided by Scalasca through tracing

Score-P: Further information

- Scalable Performance Measurement Infrastructure for Parallel Codes
  - Instrumenter, libraries, and tools to generate profile and trace measurements
  - Bundled with OTF2 (tracing), OPARI2 (OpenMP instrumentation), CubeWriter, and CubeLib (profiling)
- Available under 3-clause BSD open-source license
- Documentation & sources:
  - https://score-p.org
- User guide also part of installation:
  - <prefix>/share/doc/scorep/pdf/scorep.pdf
- Contact:
  - mailto: support@score-p.org

Reference Material:
Specialized Measurements and Analysis Options

Mastering build systems

- Hooking up the Score-P instrumenter `scorep` into complex build environments like *Autotools* or *CMake* was always challenging
- Score-P provides convenience wrapper scripts to simplify this
- *Autotools* and *CMake* need the used compiler already in the *configure step,* but instrumentation should not happen in this step, only in the *build step*

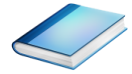
```
% SCOREP_WRAPPER=off \
>   cmake .. \
>   -DCMAKE_C_COMPILER=scorep-icc \
>   -DCMAKE_CXX_COMPILER=scorep-icpc
```

Disable instrumentation in the *configure step*

Specify the wrapper scripts as the compiler to use

- Allows to pass addition options to the Score-P instrumenter and the compiler via environment variables without modifying the *Makefiles*
- Run `scorep-wrapper --help` for a detailed description and the available wrapper scripts of the Score-P installation

User instrumentation



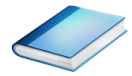
- No replacement for automatic compiler instrumentation

- Can be used to further subdivide functions
  - E.g., multiple loops inside a function
- Can be used to partition application into coarse grain phases
  - E.g., initialization, solver, & finalization

- Enabled with `--user` flag to Score-P instrumenter

- Available for Fortran / C / C++

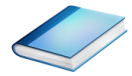
User instrumentation: Fortran



```
#include <scorep/SCOREP_User.inc>

subroutine foo(…)
  ! Declarations
  SCOREP_USER_REGION_DEFINE( solve )

  ! Some code…
  SCOREP_USER_REGION_BEGIN( solve, "<solver>", \
                            SCOREP_USER_REGION_TYPE_LOOP )
  do i=1,100
    [...]
  end do
  SCOREP_USER_REGION_END( solve )
  ! Some more code…
end subroutine
```

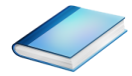
- Requires processing by the C preprocessor
  - For most compilers, this can be automatically achieved by having an uppercase file extension, e.g., `main.F` or `main.F90`

User instrumentation: C/C++



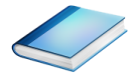
```
#include <scorep/SCOREP_User.h>

void foo()
{
  /* Declarations */
  SCOREP_USER_REGION_DEFINE( solve )

  /* Some code… */
  SCOREP_USER_REGION_BEGIN( solve, "<solver>",
                            SCOREP_USER_REGION_TYPE_LOOP )
  for (i = 0; i < 100; i++)
  {
    [...]
  }
  SCOREP_USER_REGION_END( solve )
  /* Some more code… */
}
```

User instrumentation: C++



```
#include <scorep/SCOREP_User.h>

void foo()
{
  // Declarations

  // Some code…
  {
    SCOREP_USER_REGION( "<solver>",
                        SCOREP_USER_REGION_TYPE_LOOP )
    for (i = 0; i < 100; i++)
    {
      [...]
    }
  }
  // Some more code…
}
```

Score-P measurement control API



- Can be used to temporarily disable measurement for certain intervals
  - Annotation macros ignored by default
  - Enabled with `--user` flag

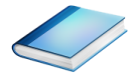
```
#include <scorep/SCOREP_User.inc>

subroutine foo(…)
  ! Some code…
  SCOREP_RECORDING_OFF()
  ! Loop will not be measured
  do i=1,100
    [...]
  end do
  SCOREP_RECORDING_ON()
  ! Some more code…
end subroutine
```

Fortran (requires C preprocessor)

```
#include <scorep/SCOREP_User.h>

void foo(…) {
  /* Some code… */
  SCOREP_RECORDING_OFF()
  /* Loop will not be measured */
  for (i = 0; i < 100; i++) {
    [...]
  }
  SCOREP_RECORDING_ON()
  /* Some more code… */
}
```

C / C++

Enriching measurements with performance counters



- Record metrics from PAPI:

```
% export SCOREP_METRIC_PAPI=PAPI_TOT_CYC
% export SCOREP_METRIC_PAPI_PER_PROCESS=PAPI_L3_TCM
```

  - Use PAPI tools to get available metrics and valid combinations:

```
% papi_avail
% papi_native_avail
```

- Record metrics from Linux perf:

```
% export SCOREP_METRIC_PERF=cpu-cycles
% export SCOREP_METRIC_PERF_PER_PROCESS=LLC-load-misses
```

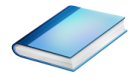
  - Use the `perf` tool to get available metrics and valid combinations:

```
% perf list
```

- Write your own metric plugin
  - Repository of available plugins: https://github.com/score-p

Only the master thread records the metric (assuming all threads of the process access the same L3 cache)

Mastering application memory usage

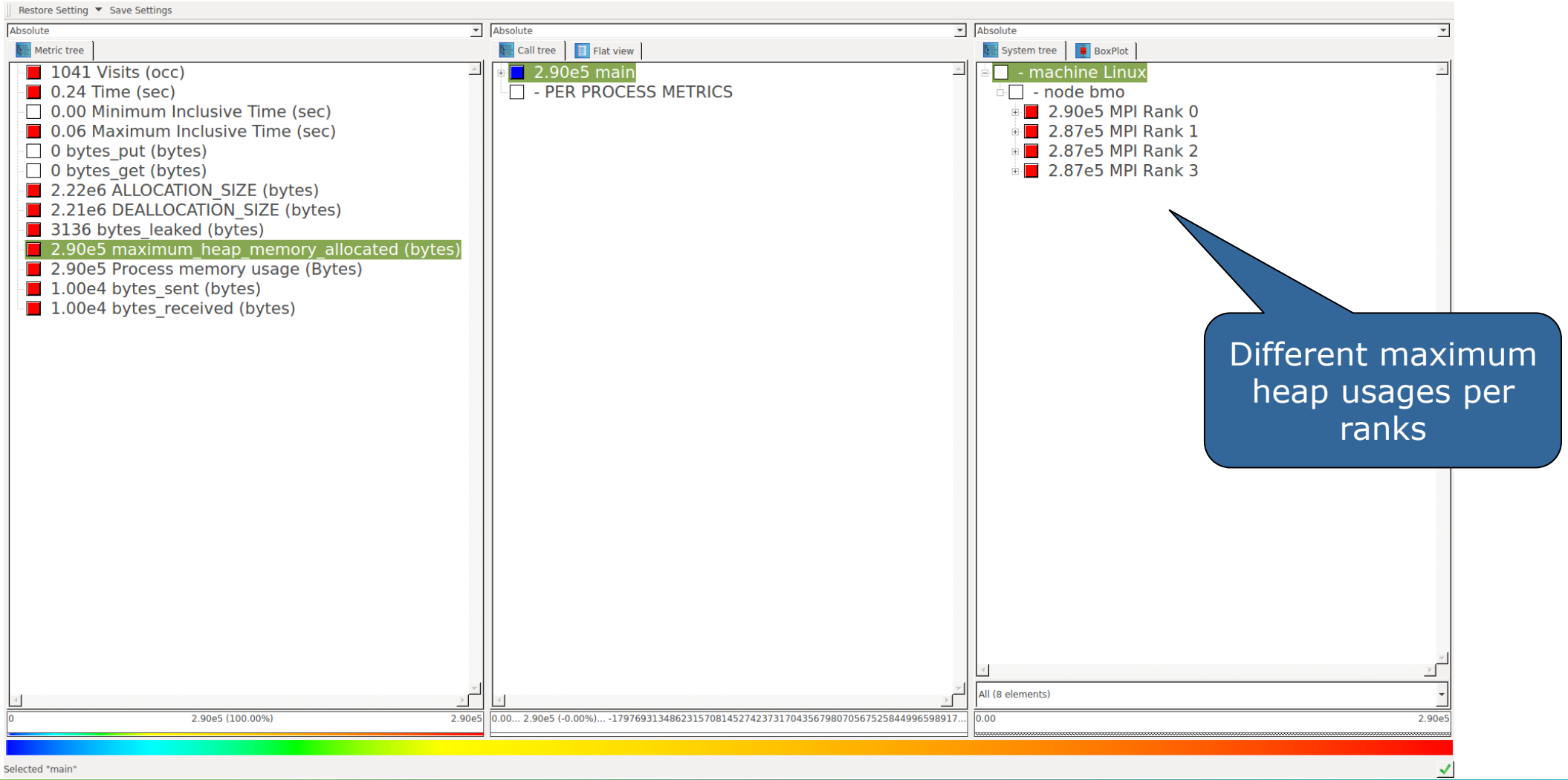


- Determine the maximum heap usage per process
- Find high frequent small allocation patterns
- Find memory leaks
- Support for:
  - C, C++, MPI, and SHMEM
  - Profile and trace generation (profile recommended)
    - Memory leaks are recorded only in the profile
    - Resulting traces are not supported by Scalasca yet

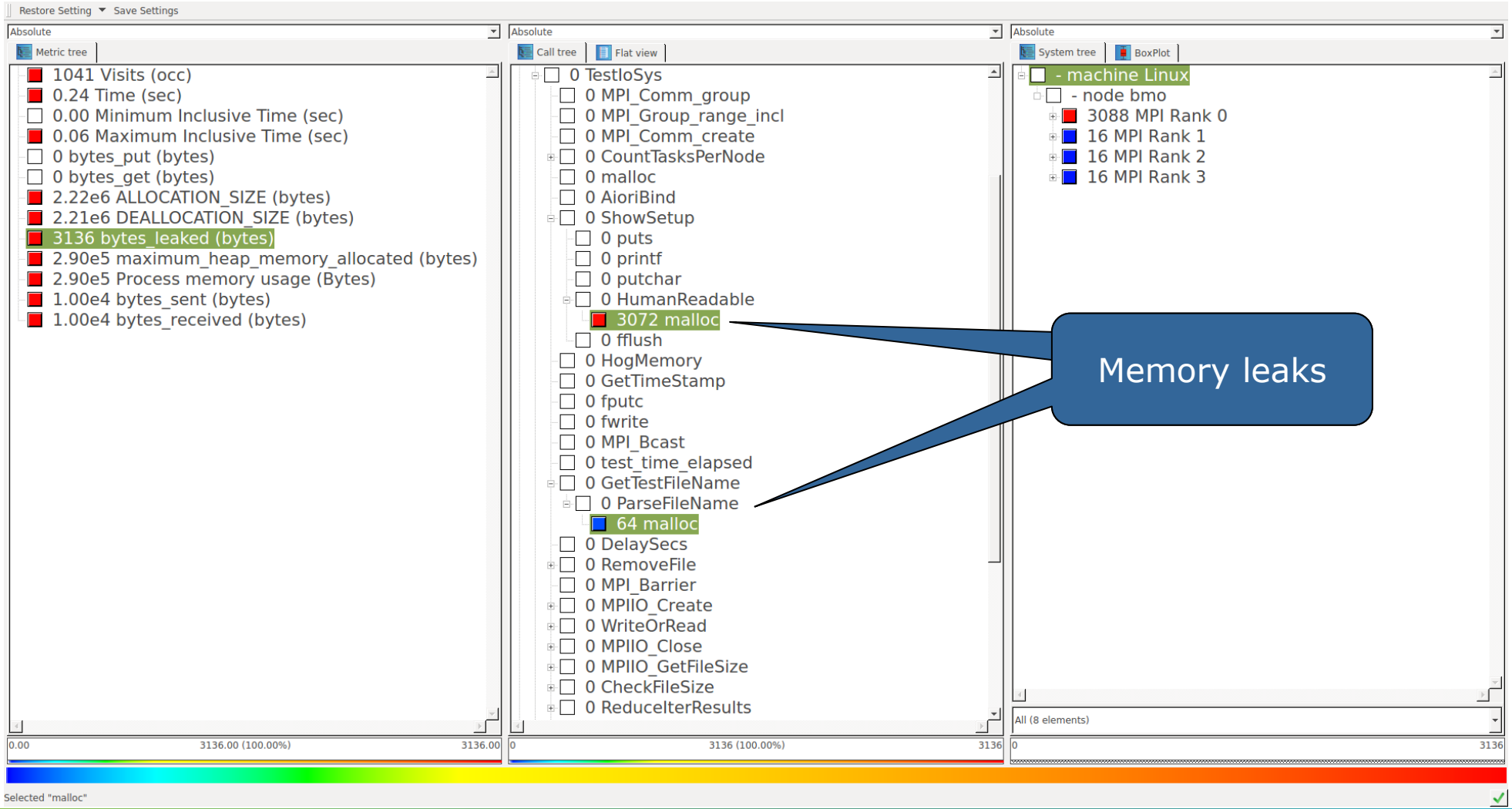
```
% export SCOREP_MEMORY_RECORDING=true
% export SCOREP_MPI_MEMORY_RECORDING=true
```

- Set new configuration variable to enable memory recording

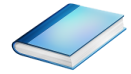
Mastering application memory usage



Mastering application memory usage



Mastering accelerators



- Record CUDA applications and device activities

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

- Record HIP applications and device activities

```
% export SCOREP_HIP_ENABLE=all
```

- Record OpenCL applications and device activities

```
% export SCOREP_OPENCL_ENABLE=api,kernel
```

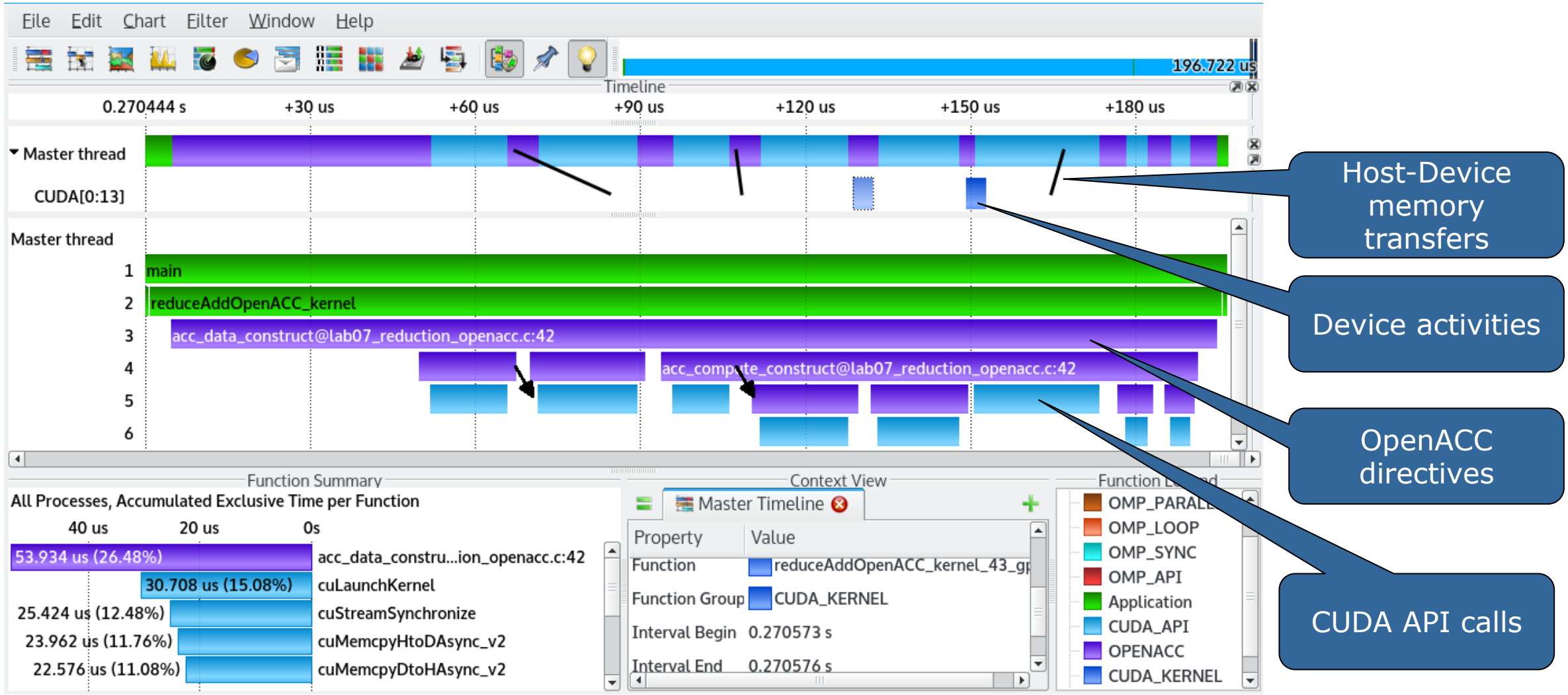
- Record OpenACC applications

```
% export SCOREP_OPENACC_ENABLE=yes
```

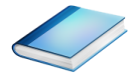
  - Can be combined with CUDA if it is a NVIDIA device

```
% export SCOREP_CUDA_ENABLE=kernel
```

Mastering accelerators



Hybrid measurement with sampling

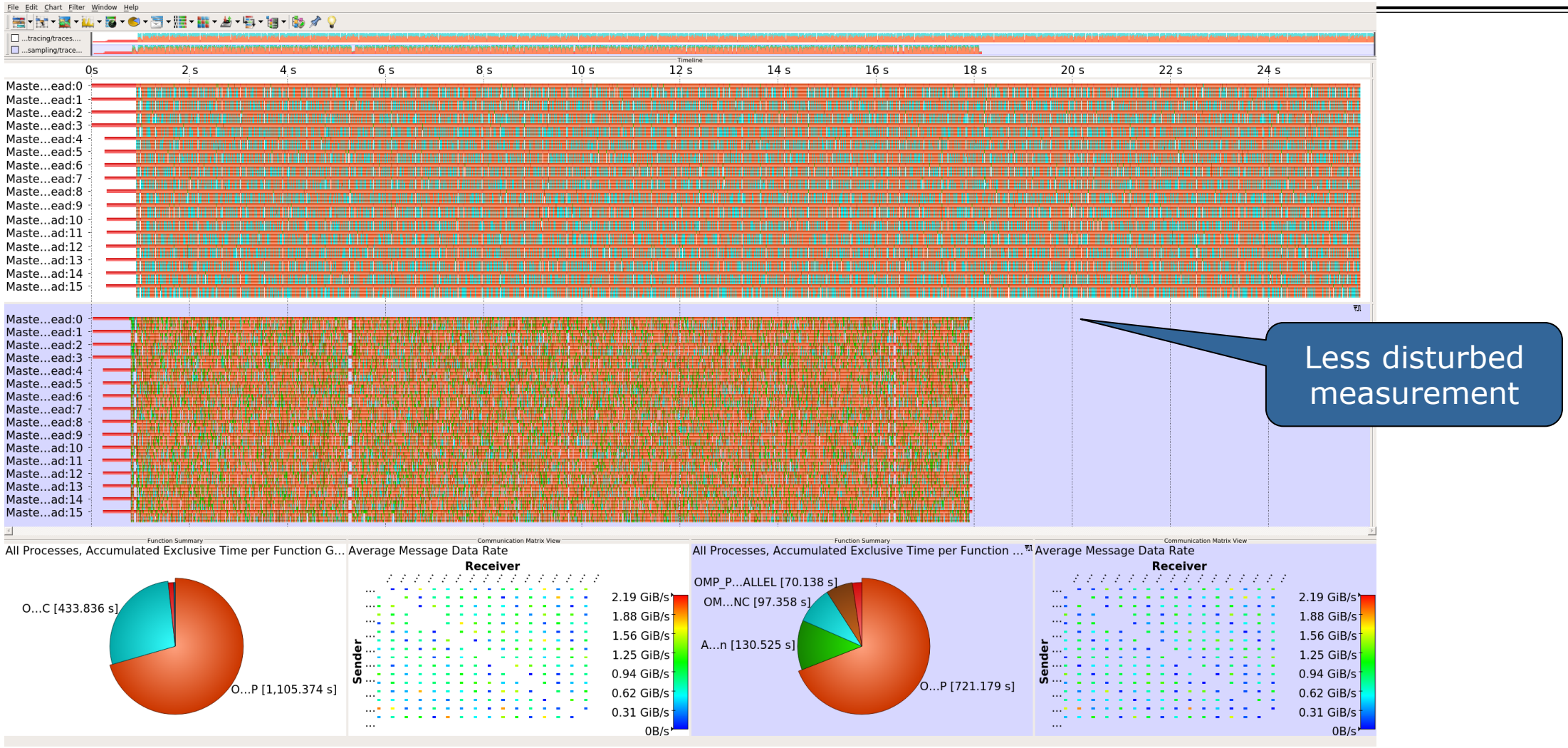


- Automatic compiler instrumentation greatly disturbs C++ applications because of frequent/short function calls ⇒ Use sampling instead
- Novel combination of sampling events and instrumentation of MPI, OpenMP, …
  - Sampling replaces only compiler instrumentation (use `--nocompiler`)
  - Instrumentation is still used for parallel activities (MPI, OpenMP, CUDA, I/O)
- Supports profile and trace generation

```
% export SCOREP_ENABLE_UNWINDING=true
% # use the default sampling frequency
% #export SCOREP_SAMPLING_EVENTS=perf_cycles@2000000
```

- Set new configuration variable to enable sampling

Mastering C++ applications



Instrumenting calls to 3rd party libraries

- Score-P does not record function calls to non-instrumented external libraries
- Increase insight into the behavior of the application
  - How does the application use the external library?
  - How does this compares to the usage of other libraries?
- Manual user instrumentation of the application using the library should be avoided
- Vendor provided libraries cannot be instrumented, but API is provided in headers

Instrumenting calls to 3rd party libraries: Library wrapper generator

- Workflow to generate library wrappers for most C/C++ libraries
- Tailored towards users of the external library, not users of Score-P
- Results can be shared with multiple users
- Workflow driver `scorep-libwrap-init --help` provides instructions

Only once

Library wrapper creator

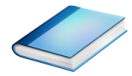
1. Initialize the working directory
2. Add library headers
3. Create a simple example application
4. Further configure the build parameters
5. Build the wrapper
6. Verify the wrapper
7. Install the wrapper
8. Verify the installed wrapper

Library wrapper user

9. Use the wrapper

Often

Instrumenting calls to 3rd party libraries: Workflow



- Start workflow by telling `scorep-libwrap-init` how you would compile and link an application, e.g., using FFTW

```
% scorep-libwrap-init          \
>   --name=fftw                 \
>   --prefix=$PREFIX            \
>   -x c                        \
>   --cppflags="-O3 -DNDEBUG -openmp -I$FFTW_INC" \
>   --ldflags="-L$FFTW_LIB"     \
>   --libs="-lfftw3f -lfftw3" \
>   working_directory
```

Omit to install into Score-P

Flags used to compile/link

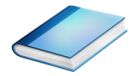
Working directory can be archived for later rebuild

- Generate and build wrapper

```
% cd working_directory
% ls                    # (Check README.md for instructions)
% make                  # Generate and build wrapper
% make check            # See if header analysis matches symbols
% make install          #
% make installcheck     # More checks: Linking etc.
```

Tells you how to use the wrapper with Score-P

Instrumenting calls to 3rd party libraries: Usage and result



- List of available wrappers:

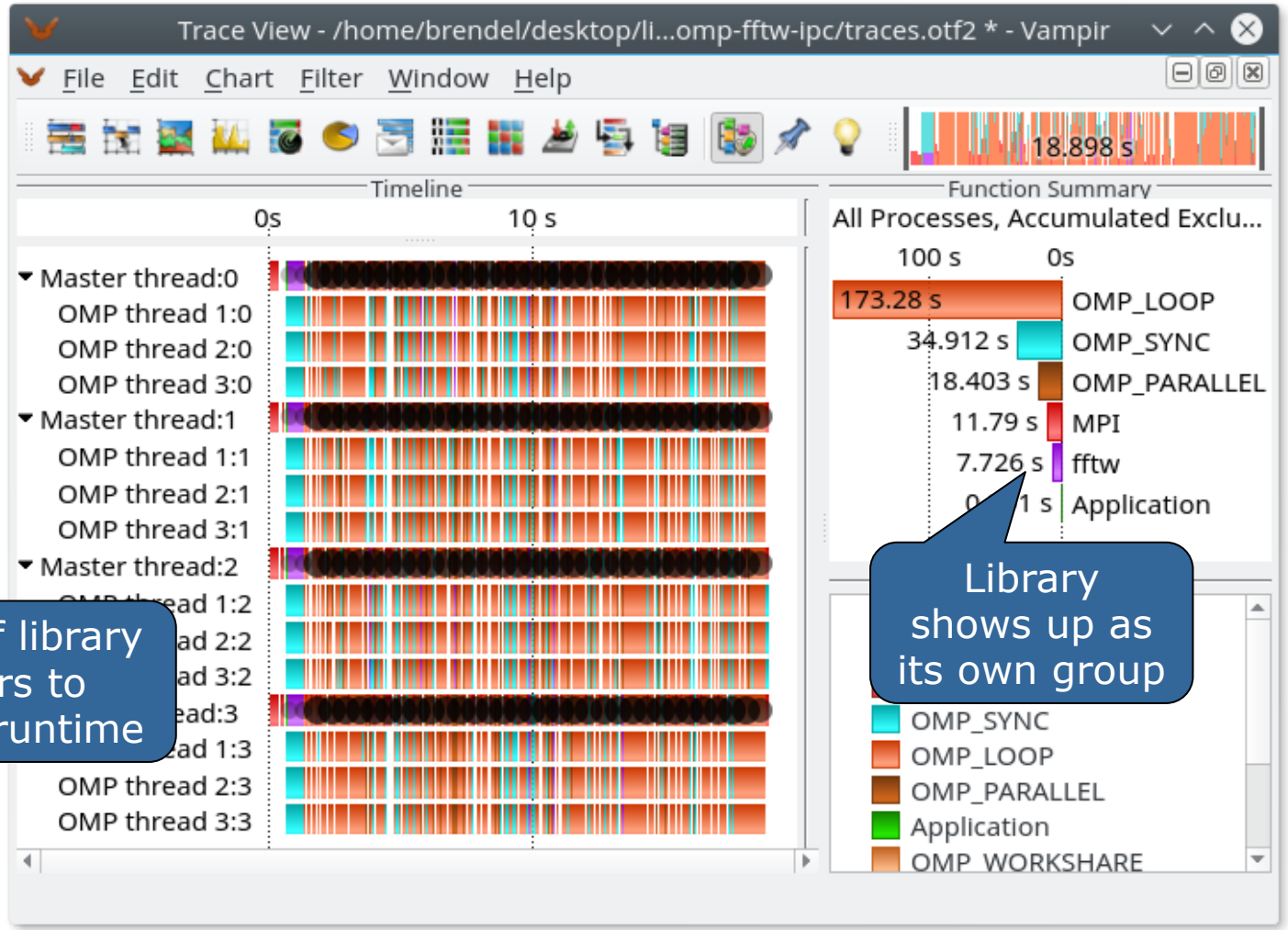
```
% scorep-info libwrap-summary
```

- Instrumentation:

```
# instrument application as usual
% cd <application>
% make clean
% make
% export \
SCOREP_LIBWRAP_ENABLE=fftw
# run application as usual
```

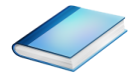
- MPI + OpenMP
- Calls to FFTW library

Pass list of library wrappers to enable at runtime



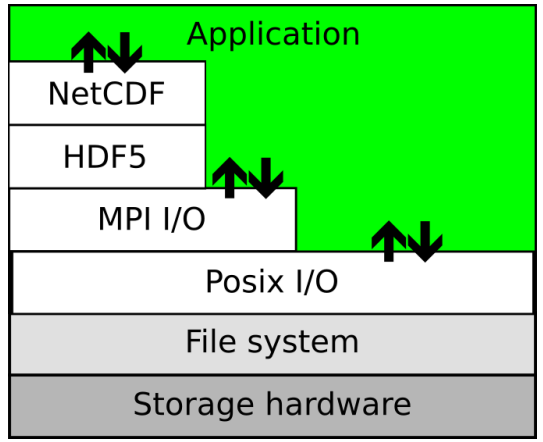
Library shows up as its own group

Mastering File I/O



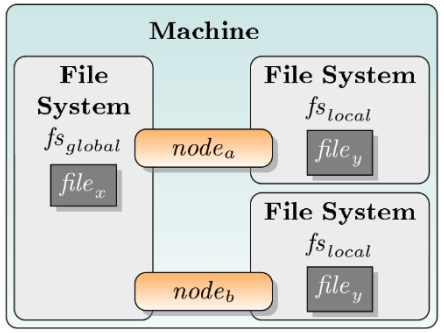
- Omnipresent in todays HPC applications

- Record interaction between multiple layers
  - MPI I/O (`MPI_File_open`)
  - ISO C I/O (`fopen`)
  - POSIX I/O (`open`, interface to OS)

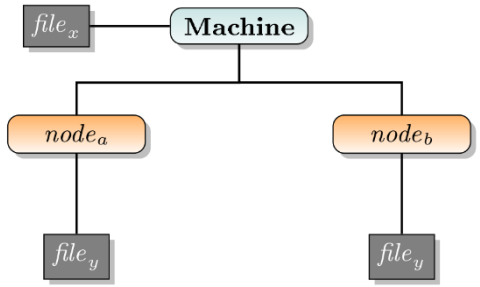


- System tree information determine whether file resides in a shared file system

- High level of detail
  => Trace data might increase dramatically



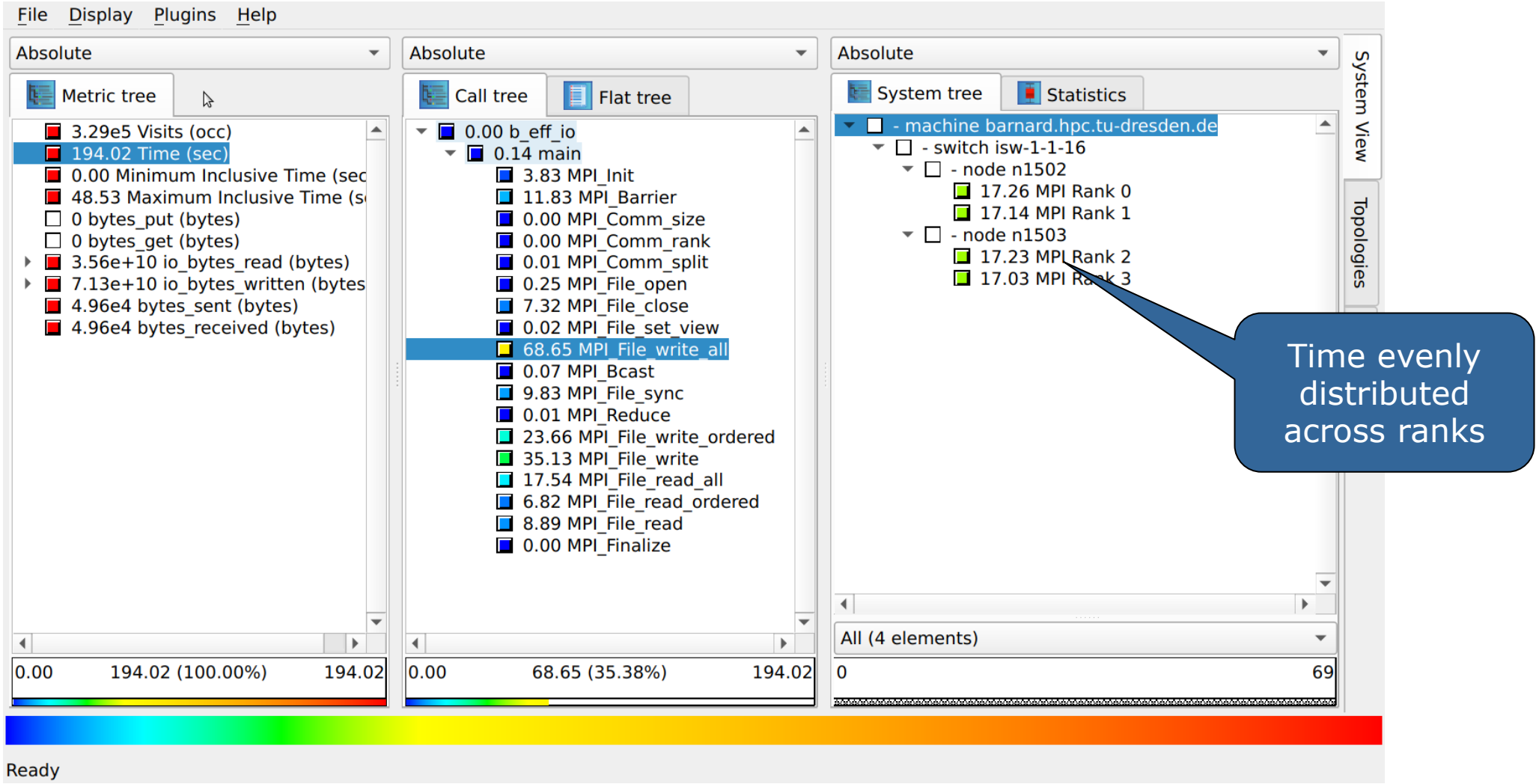
(a) Hardware topology



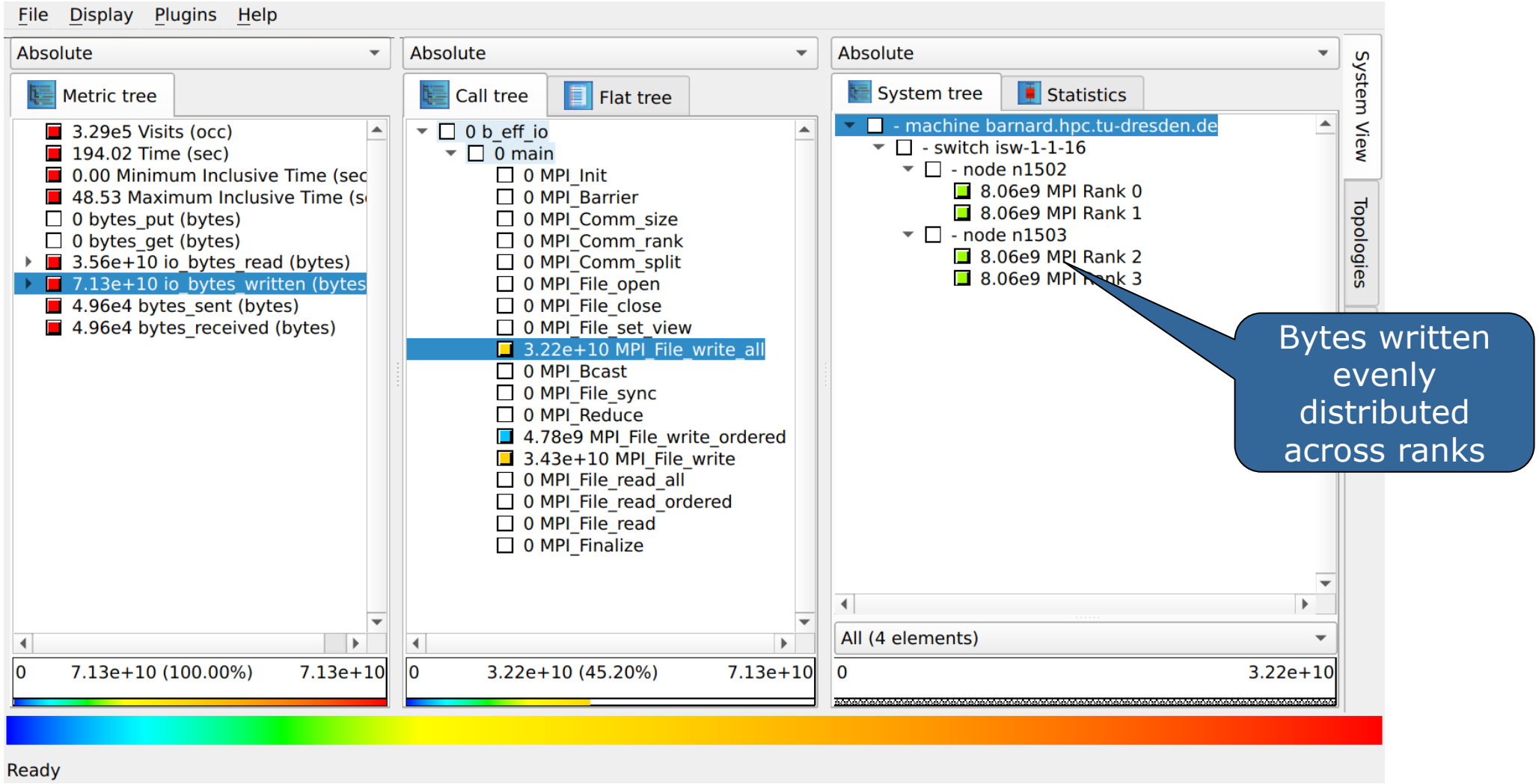
(b) System tree representation

NetCDF & HDF5 will be supported later

Mastering File I/O: Result visualization



Mastering File I/O: Result visualization



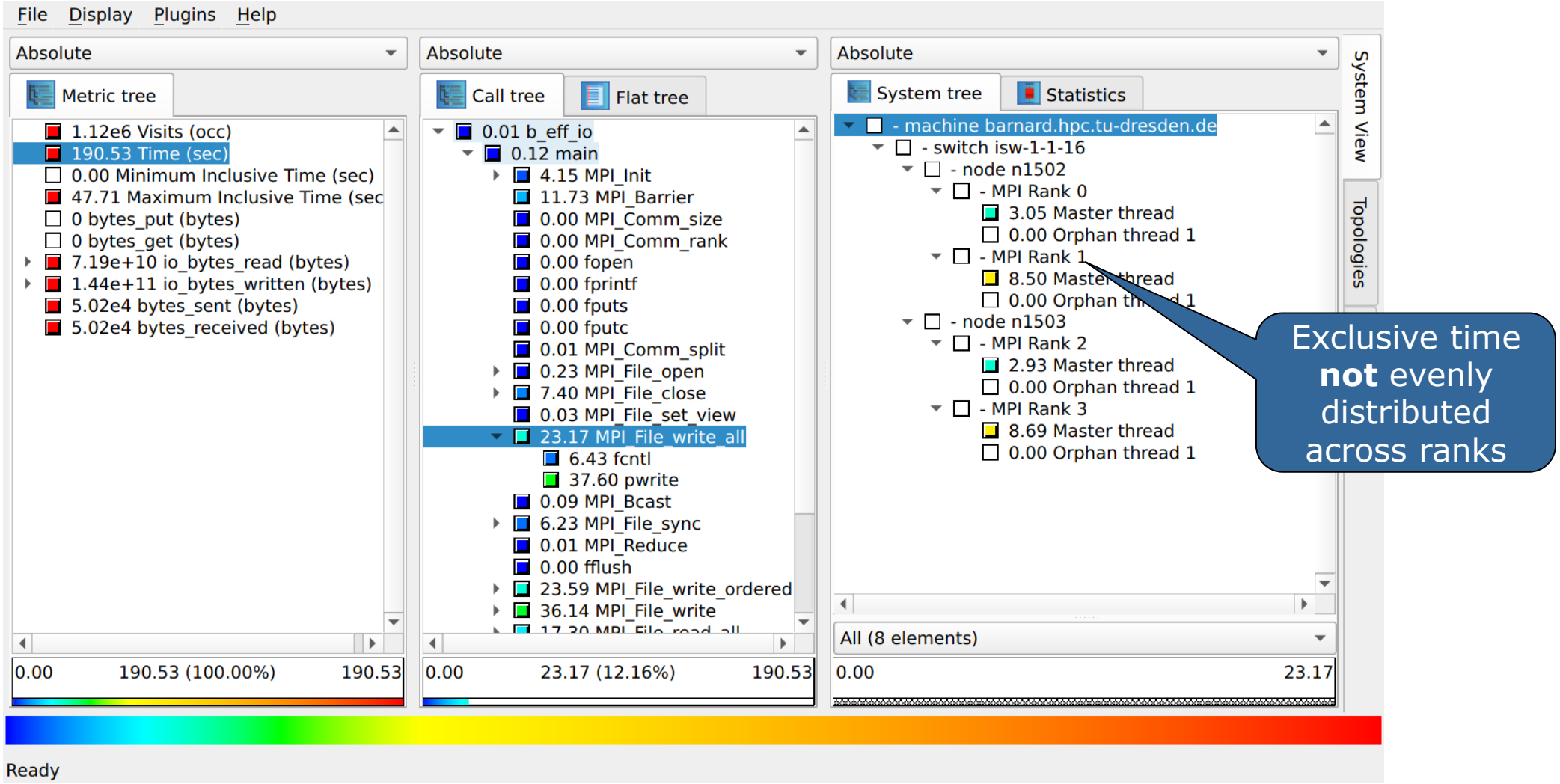
Mastering File I/O: B_EFF I/O hands-on

- Enabling ISO C and POSIX I/O instrumentation

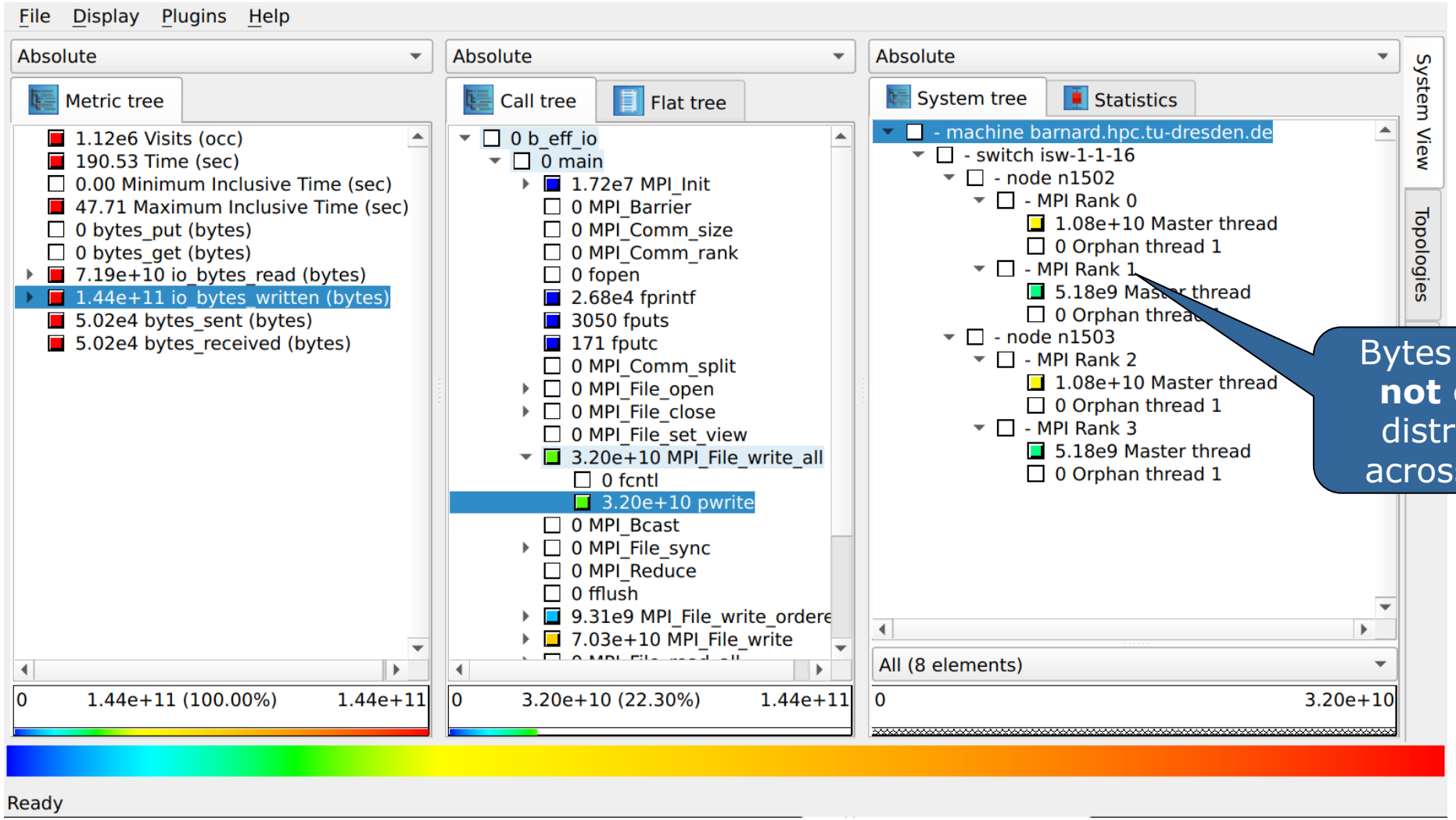
- Instrumentation does require threading support

```
% scorep-mpiicc -g -O3 -o b_eff_io b_eff_io.c
% export SCOREP_EXPERIMENT_DIRECTORY=scorep-b_eff_io-4-profile+posix
% export SCOREP_IO_POSIX=yes
# run with 4 tasks and 6 threads each ./run.sh b_eff_io
% cube scorep-b_eff_io-4-profile+posix/profile.cubex
```

Mastering File I/O: Result visualization



Mastering File I/O: Result visualization



Mastering Python

- Install Score-P Python bindings via

```
pip install --user scorep
```

- Execute Score-P as a module via

```
python -m scorep …
```

- Score-P environment variables are still valid and needed

```
#!/bin/env bash

export SCOREP_EXPERIMENT_DIRECTORY=…

export SCOREP_FILTERING_FILE=…

python –m scorep <path/to/my_script.py>
```

Fig.: Vampir – module import

Mastering Python: Score-P options

- Accepts additional switches `-m scorep <options>`
- These include
  - `--thread=pthread`
  - `--mpp=mpi`
  - `--cuda` / `--hip`

```
#!/bin/env bash

python –m scorep <path/to/my_script.py>
```

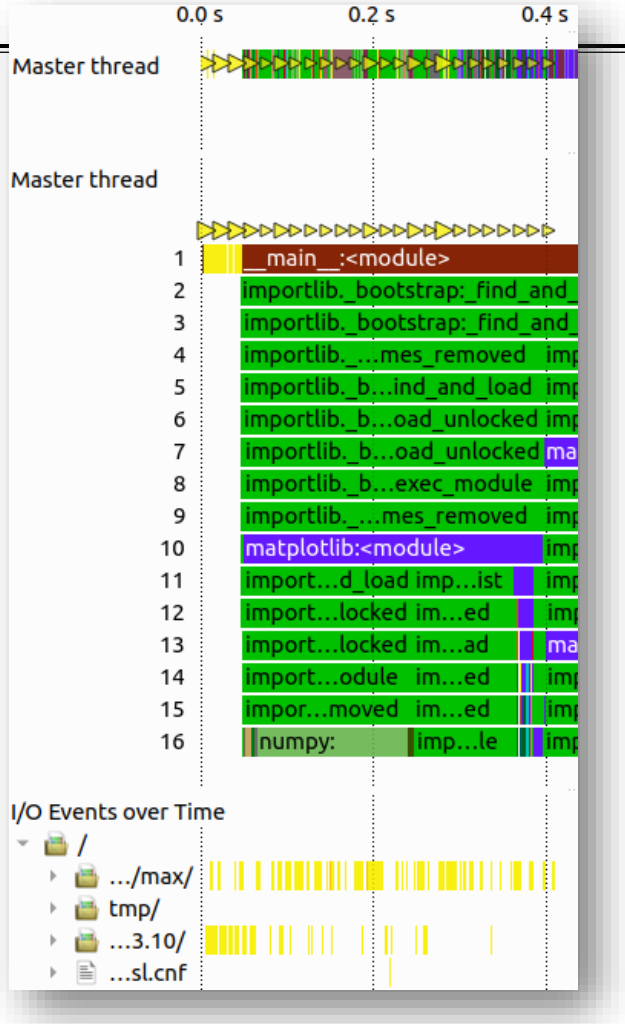


Fig.: Trace with POSIX-I/O

Mastering Python: Selective instrumentation

- Enable/Disable instrumentation for certain functions
- Via decorator or context

```
import scorep

@scorep.instrumenter.enable()/disable()

with scorep.instrumenter.enable()/disable():
```

- [No] data is collected for these sections
- Disabling is useful for
  - Import of modules
  - Known uninteresting functions
  - Very ‘hot’ functions to reduce overhead
- Hint: name ‘disabled’ blocks for attribution in output

```
%%file 02_matmul.py
import scorep
with scorep.instrumenter.disable():
    import numpy as np
…

@scorep.instrumenter.disable()
def add(a,b)
    return a + b

def compute_diagonal_sum(A):
    sum_diag = 0
    for i in range(min(A.shape[0], A.shape[1])):
         sum_diag = add(sum_diag,A[i][i])
    return sum_diag

def main():
    A = generate_random_matrix(64, 64)
    diag_sum = compute_diagonal_sum(A)
…
```

Mastering Python: Selective instrumentation

- Selective enabling of functions
- If only certain region is of interest
- Make sure to execute Score-P with

`--noinstrumenter`

```
#!/bin/env bash
…
python –m scorep --noinstrumenter \
     02_matmul.py
```

```
%%file 02_matmul.py
import scorep
import numpy as np
…
def add(a,b)
    return a + b
def compute_diagonal_sum(A):
    sum_diag = 0
    for i in range(min(A.shape[0], A.shape[1])):
         sum_diag = add(sum_diag,A[i][i])
    return sum_diag

def main():
    A = generate_random_matrix(64, 64)
    with scorep.instrumenter.enable():
        diag_sum = compute_diagonal_sum(A)
…
```

Mastering Python: Selective instrumentation hands-on

- Run application with

```
% export SCOREP_EXPERIMENT_DIRECTORY=scorep-python-matmul
% srun … python -m scorep ./02_matmul.py
% cube scorep-python-matmul/profile.cubex
```

- Use selective instrumentation

```
% <editor> 02_matmul.py
# comment-in "scorep" statements and "fix" indentation
% export SCOREP_EXPERIMENT_DIRECTORY=scorep-python-matmul+selective
% srun … python -m scorep ./02_matmul.py
% cube scorep-python-matmul+selective/profile.cubex
```

Mastering Python: MPI

- MPI must be enabled explicitly via `--mpp=mpi`

```
srun –np 4 python –m scorep --mpp=mpi <path/to/my_script.py>
```

- Caveats
  - No support for `MPI_Mprobe/Mrecv`, default for `mpi4py` -> disable usage
  - No support for `MPI_THREAD_MULTIPLE`, default for `mpi4py` -> disable usage

```
#!/bin/env bash

# disables the use of MPI_Mprobe & MPI_Mrecv
export MPI4PY_RC_RECV_MPROBE=False

# Promise the MPI library (and Score-P) that the funneled mode is
# used at most
export MPI4PY_RC_THREAD_LEVEL=funneled

srun –np 4 python –m scorep --mpp=mpi <path/to/my_script.py>
```

Mastering Python: MPI hands-on

- Run application with

```
% export SCOREP_EXPERIMENT_DIRECTORY=scorep-python-mpi
% export MPI4PY_RC_RECV_MPROBE=False
% export MPI4PY_RC_THREAD_LEVEL=funneled
% srun … python -m scorep --mpp=mpi ./03_mpi.py
% cube scorep-python-mpi/profile.cubex
```

Mastering Python: Accelerators

- Score-P can be used to instrument accelerators (GPUs)
- `SCOREP_[CUDA|HIP]_ENABLE=yes` use default set of features

```
...
export SCOREP_CUDA_ENABLE=yes
export SCOREP_CUDA_BUFFER=1M # Increase if necessary

python -m scorep --cuda <path/to/my_script.py>
```

```
...
export SCOREP_HIP_ENABLE=yes
export SCOREP_HIP_ACTIVITY_BUFFER_SIZE=1M # Increase if necessary

python -m scorep --hip <path/to/my_script.py>
```

Analysis report examination with Cube

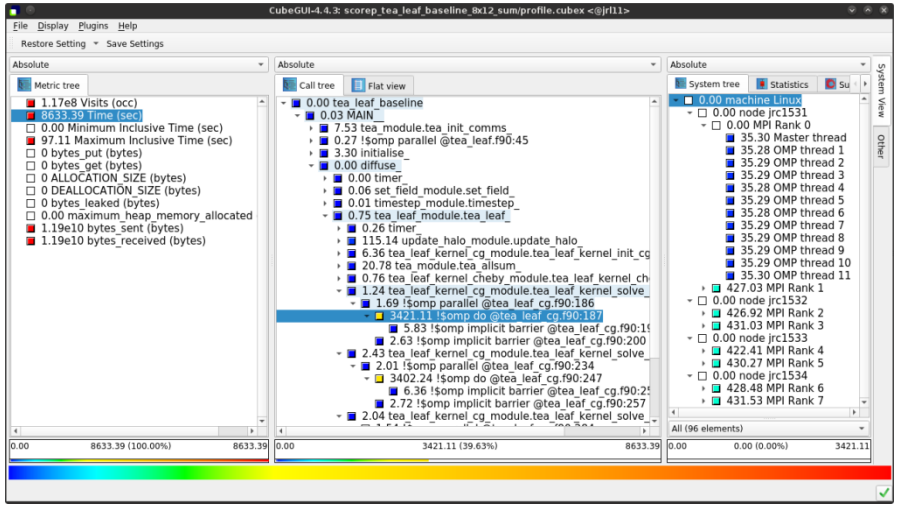
Marc Schlütter
Jülich Supercomputing Centre

cube
scalasca

Cube

CubeLib DOI 10.5281/zenodo.15051777
CubeGUI DOI 10.5281/zenodo.15051823

- Parallel program analysis report exploration tools
  - Libraries for XML+binary report reading & writing
  - Algebra utilities for report processing
  - GUI for interactive analysis exploration
    - Requires Qt ≥ 5



- Originally developed as part of the Scalasca toolset

- Now available as a separate components
  - Can be installed independently of Score-P, e.g., on laptop or desktop
  - Latest release: Cube v4.9.1 (December 2025)

Note: source distribution tarballs for Linux, as well as binary packages provided for Windows & MacOS, from **www.scalasca.org** website in software/Cube-4x

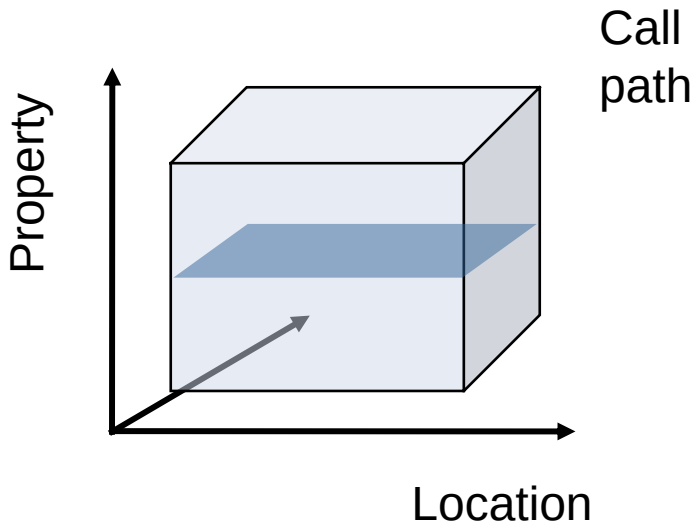
Cube GUI – Client Options & Usage

- Client Options:
  - User installation from tarball
  - **Running binary:**
    - win32 binary, Mac OS .dmg, Linux binary .AppImage
  - Available in Fedora distribution
  - POP3: Making Cube tools available on HPC Systems
  - JupyterLab/Webassembly integration
- Accessing Cube files
  - copy .cubex file (or entire scorep directory) to desktop from remote system via scp
  - **locally mount remote filesystem via sshfs**
  - Running a `cube_server` on the remote system and connect to it

All download options:
https://www.scalasca.org/scalasca/software/cube-4.x/download.html

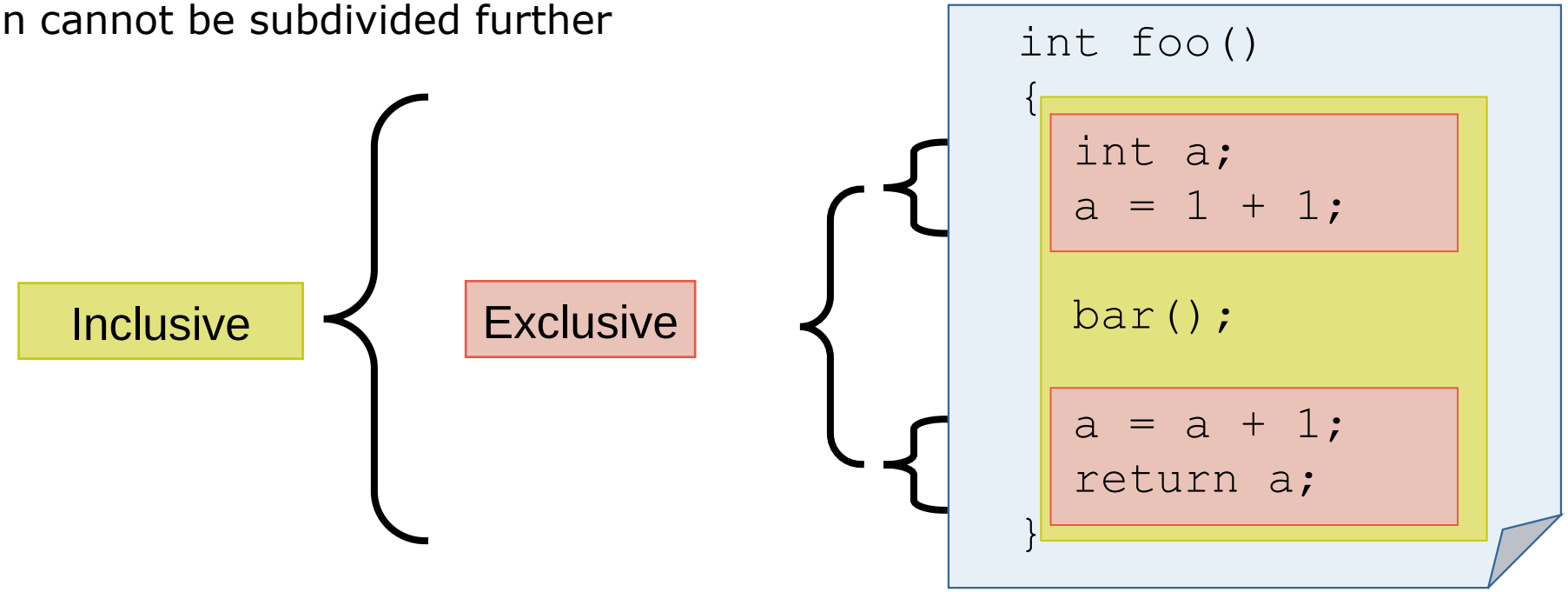
Analysis presentation and exploration

- Representation of values (severity matrix) on three hierarchical axes
  - Performance property (metric)
  - Call path (program location)
  - System location (process/thread)
- Three coupled tree browsers
- Cube displays severities
  - As *value*: for precise comparison
  - As *colour*: for easy identification of hotspots
  - *Inclusive* value when closed & *exclusive* value when expanded
  - Customizable via display *modes*



Inclusive vs. exclusive values

- Inclusive
  - Information of all sub-elements aggregated into single value
- Exclusive
  - Information cannot be subdivided further



Demo:
TeaLeaf case study

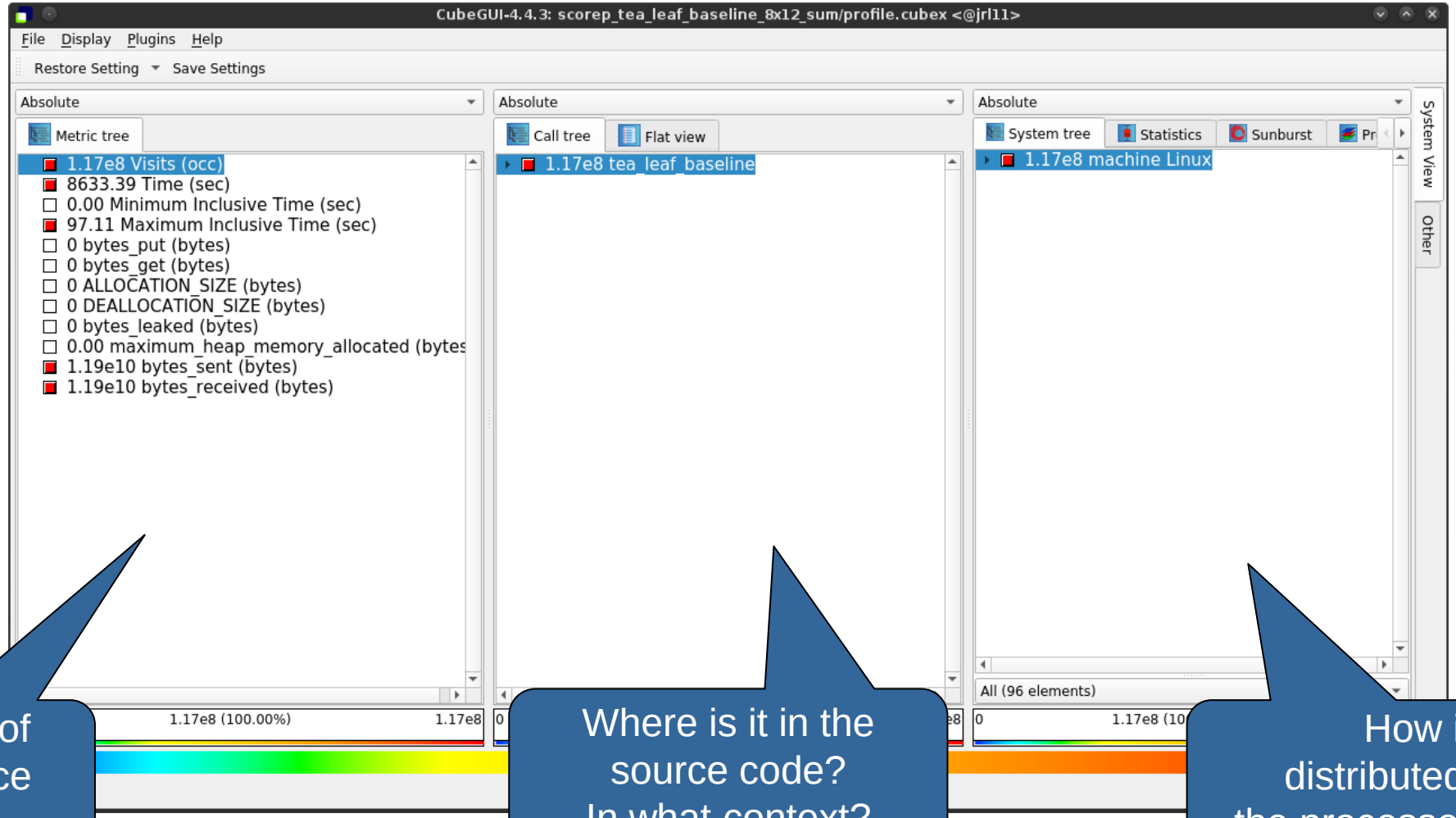
Case study: TeaLeaf

- HPC mini-app developed by the UK Mini-App Consortium
  - Solves the linear 2D heat conduction equation on a spatially decomposed regular grid using a 5 point stencil with implicit solvers
  - Part of the Mantevo 3.0 suite
  - Available on GitHub: http://uk-mac.github.io/TeaLeaf/

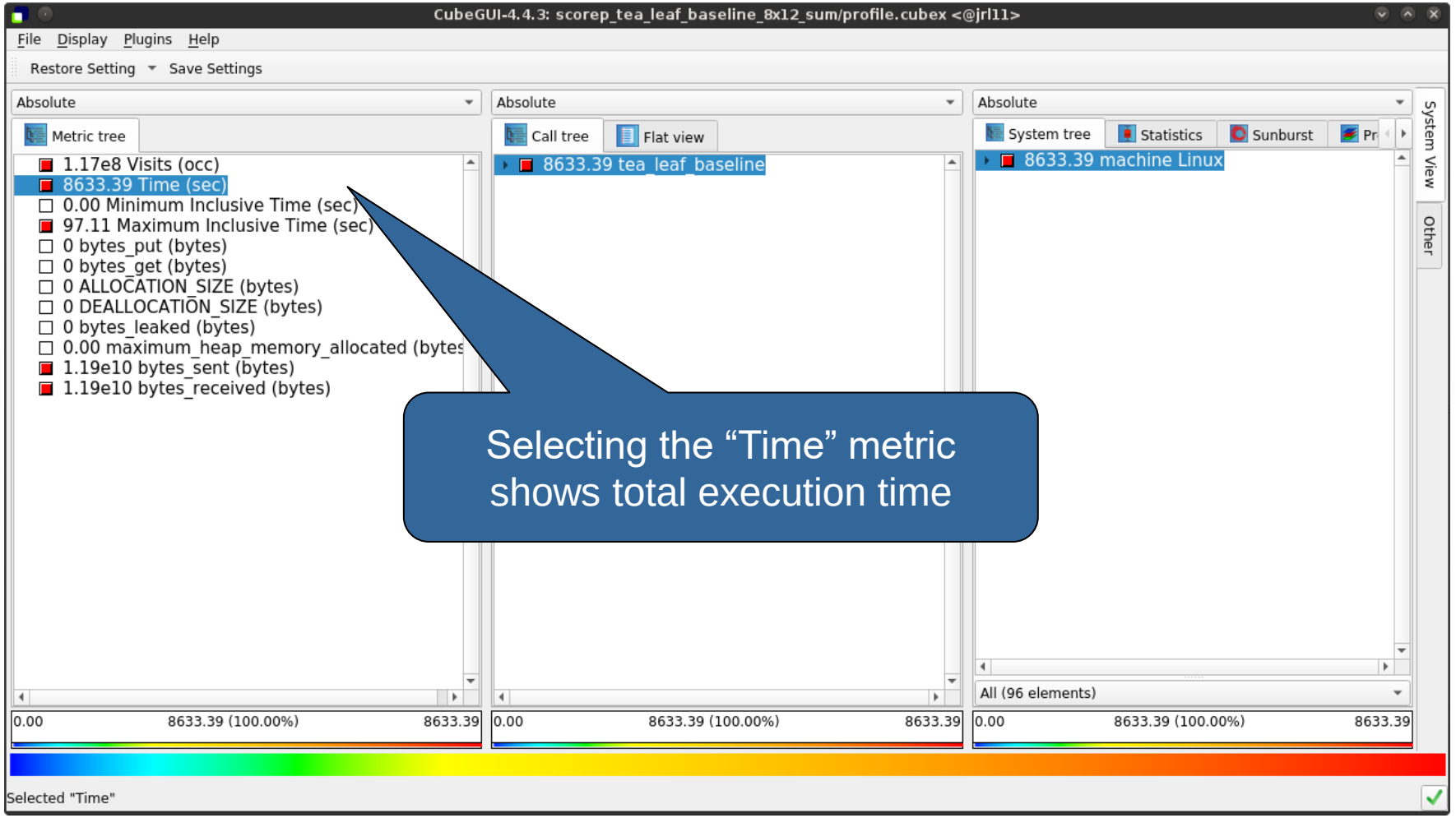
- Measurements of TeaLeaf reference v1.0 taken on Jureca cluster @ JSC
  - Using Intel 19.0.3 compilers, Intel MPI 2019.3, and Score-P 5.0
  - Run configuration
    - 8 MPI ranks with 12 OpenMP threads each

```
% cd ~/workshop-vihps/Experiments
% cube scorep_tea_leaf_baseline_8x12_sum/profile.cubex
                                    [GUI showing summary analysis report]
```

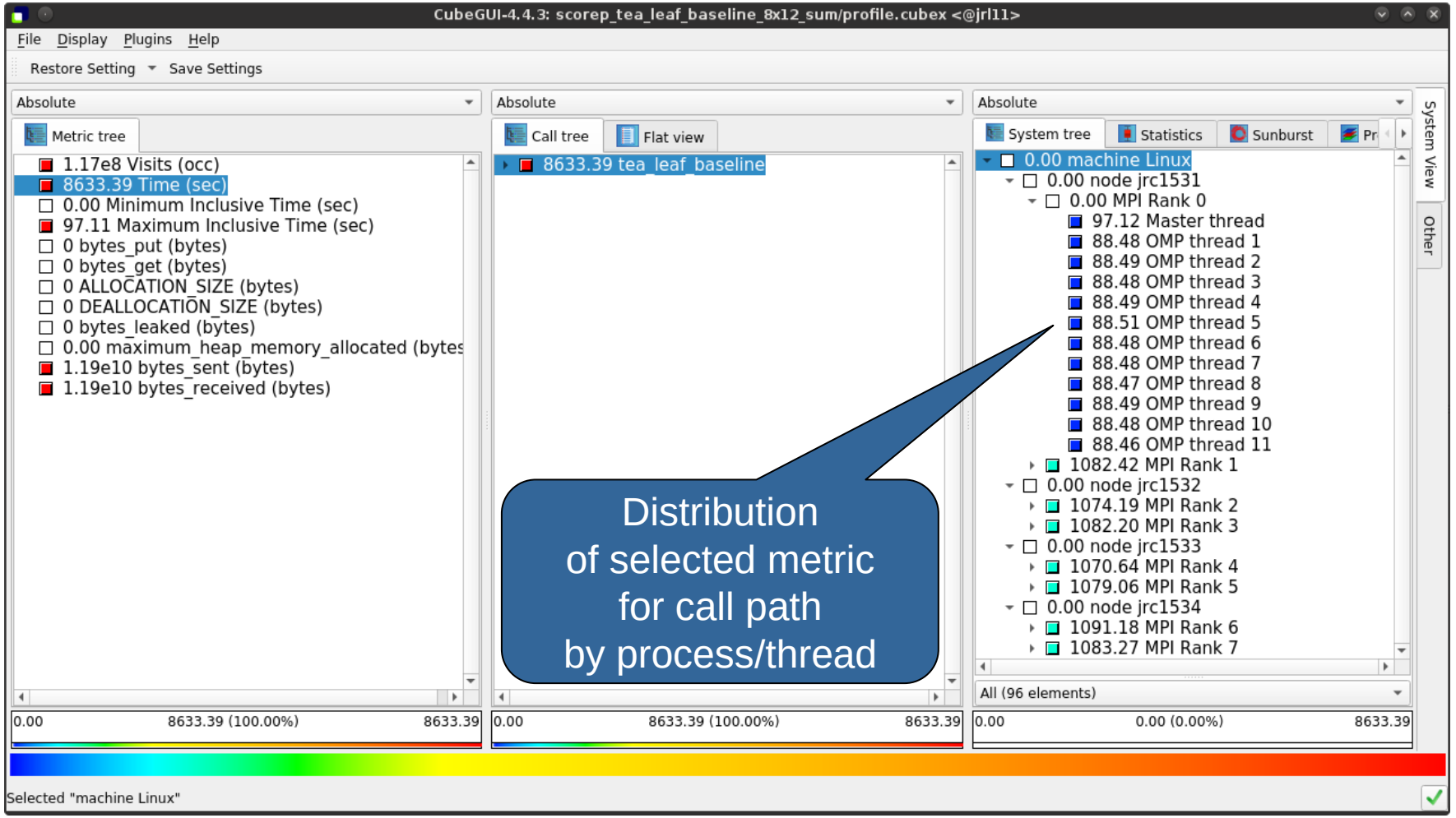
Score-P analysis report exploration (opening view)



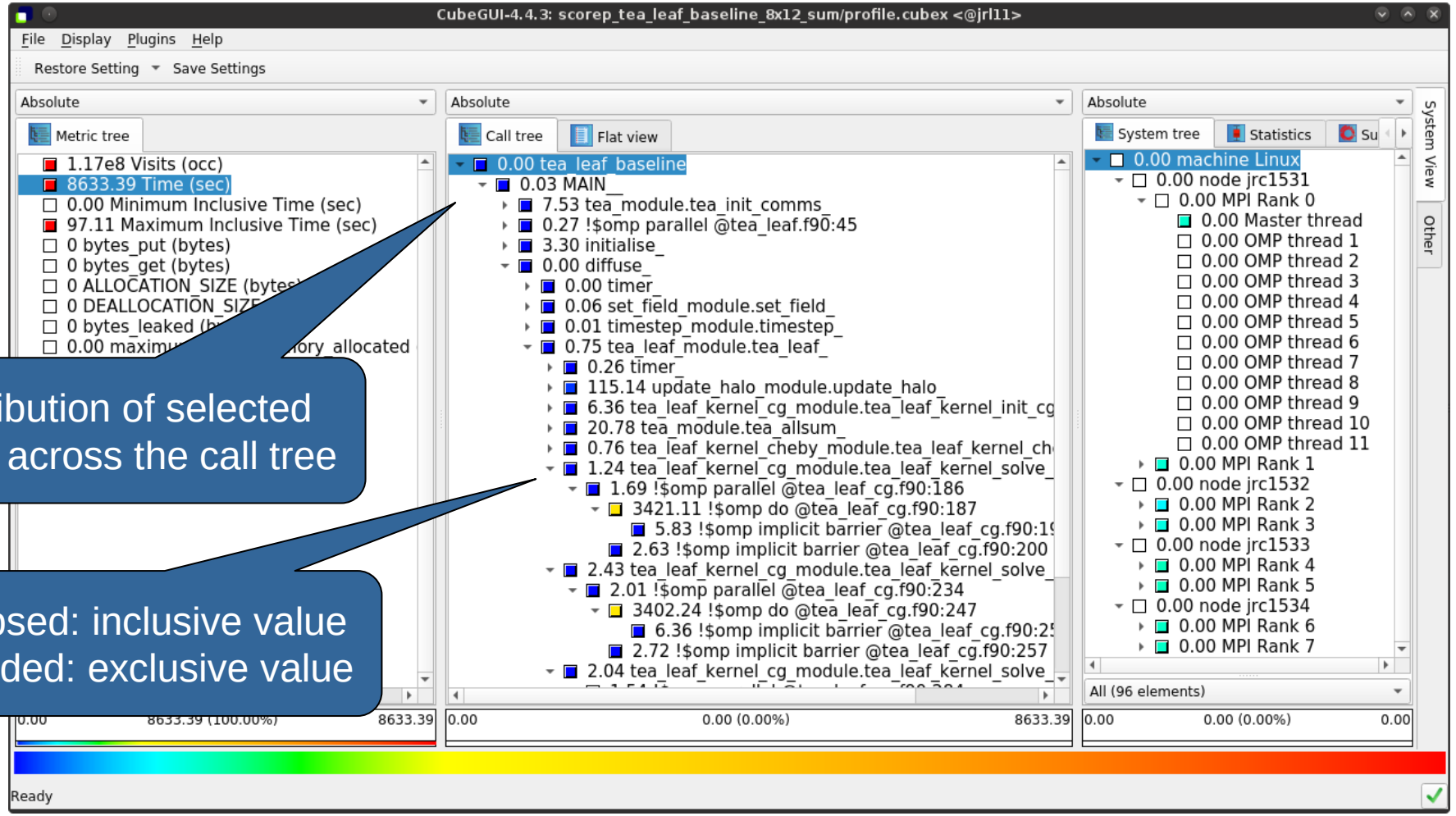
Metric selection



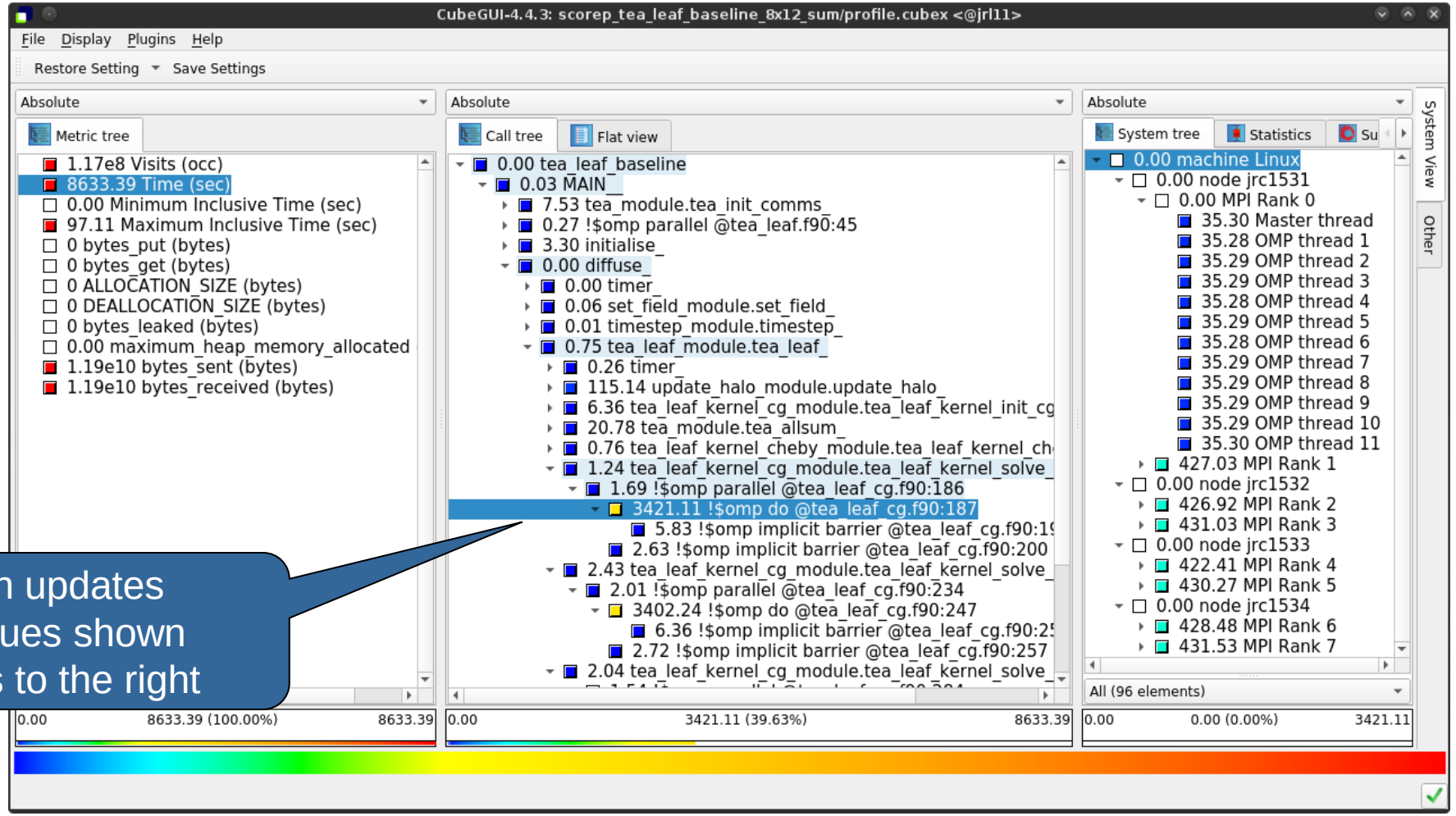
Expanding the system tree



Expanding the call tree

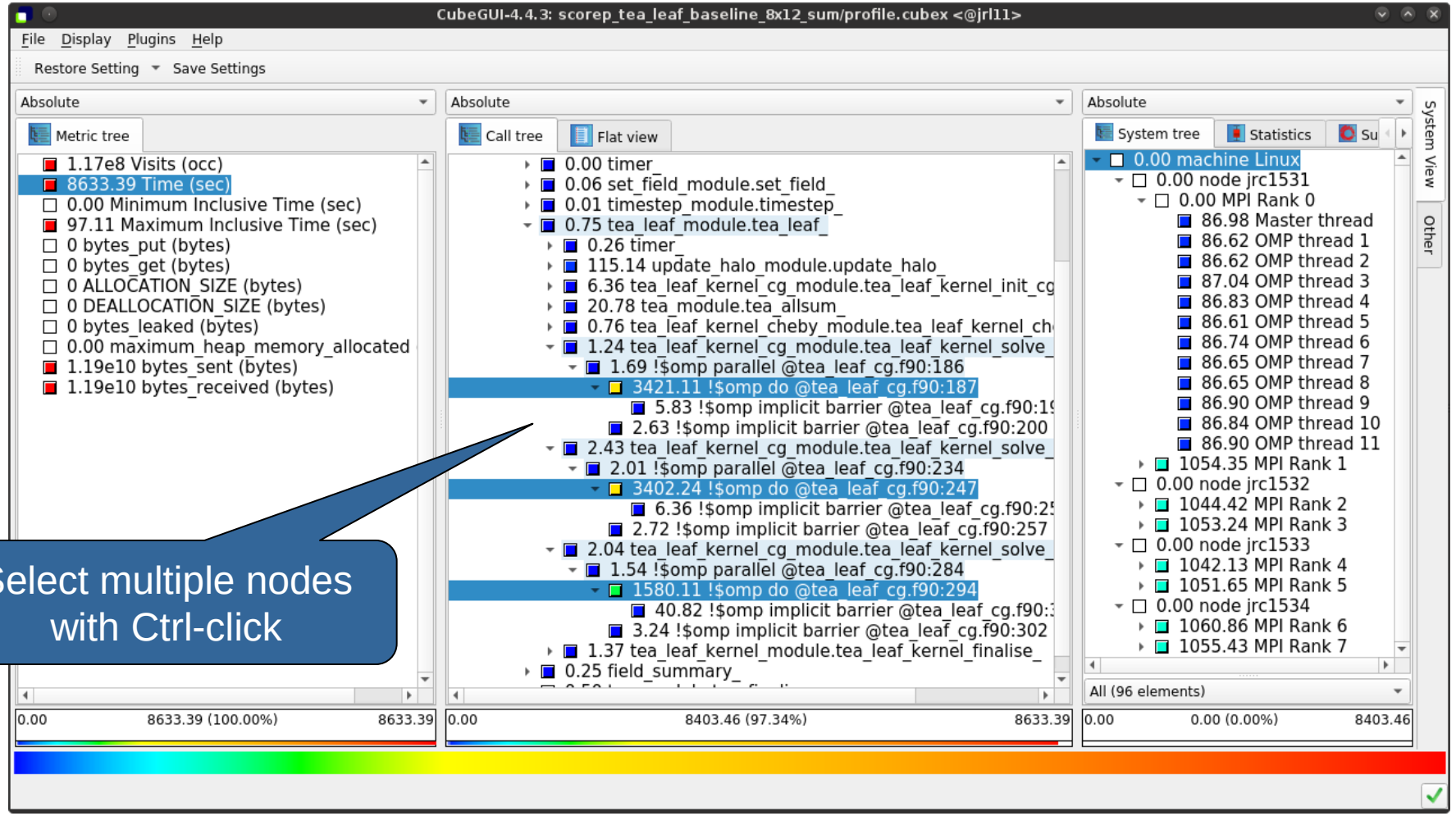


Selecting a call path

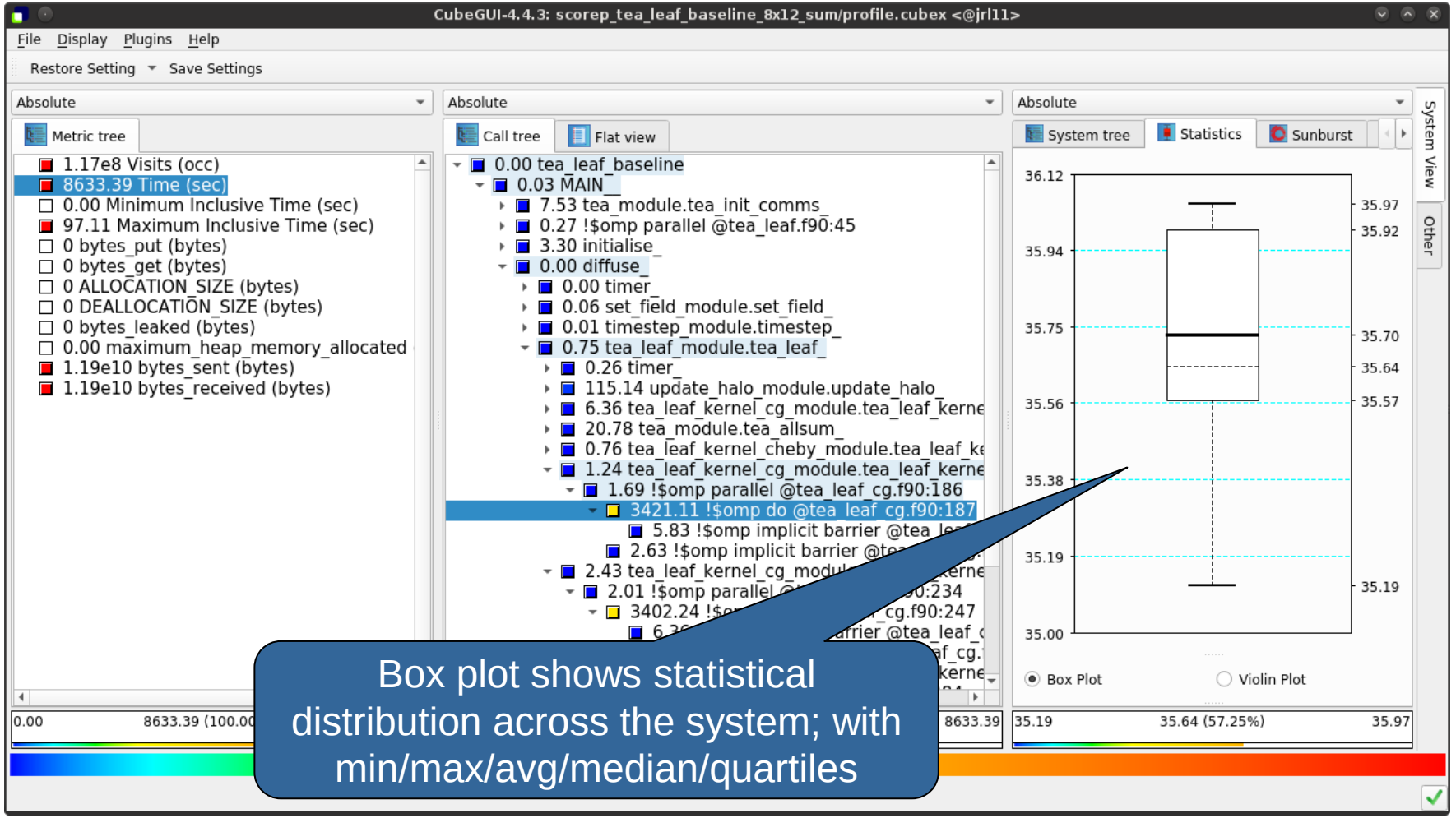


Selection updates metric values shown in columns to the right

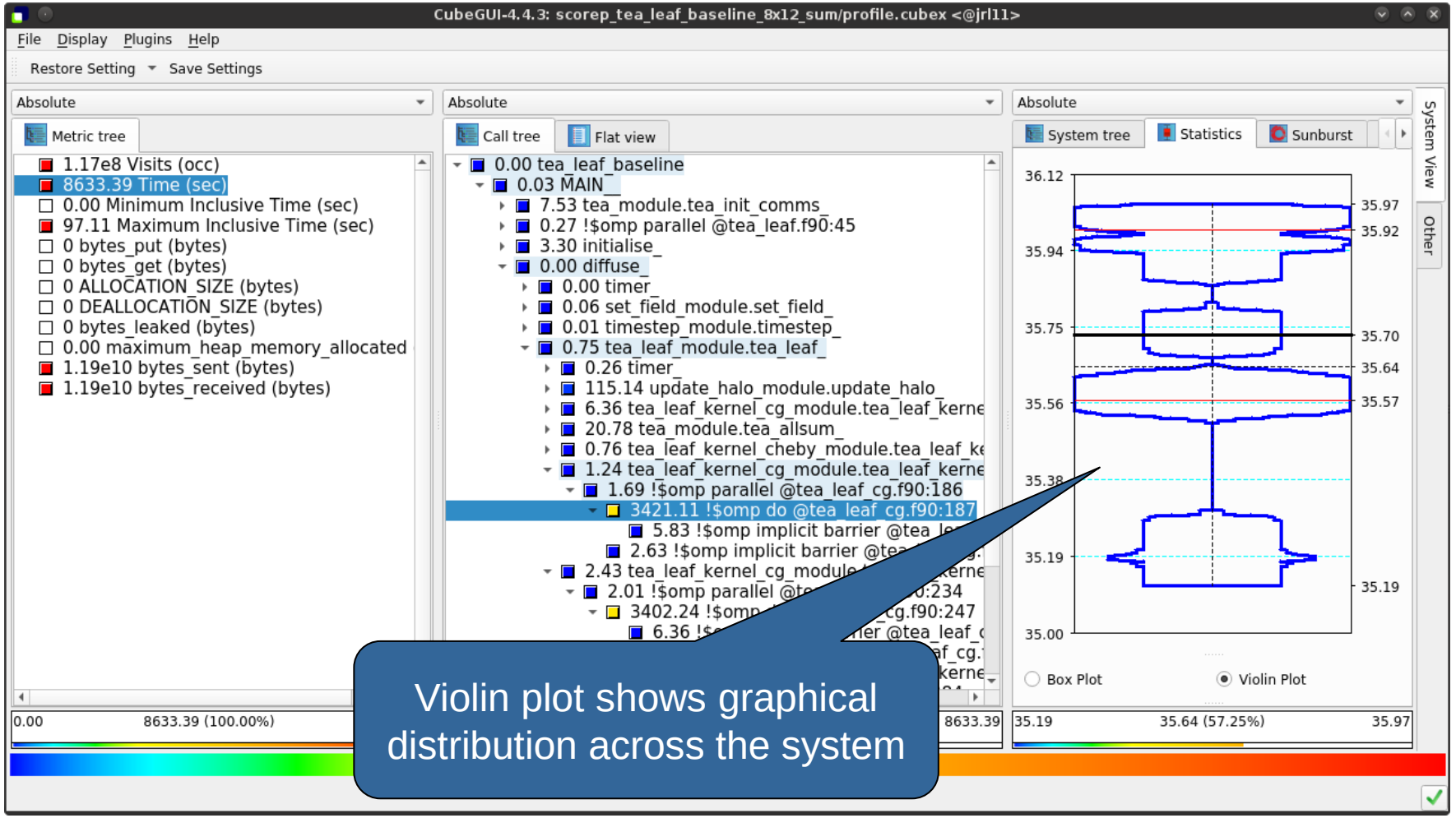
Multiple selection



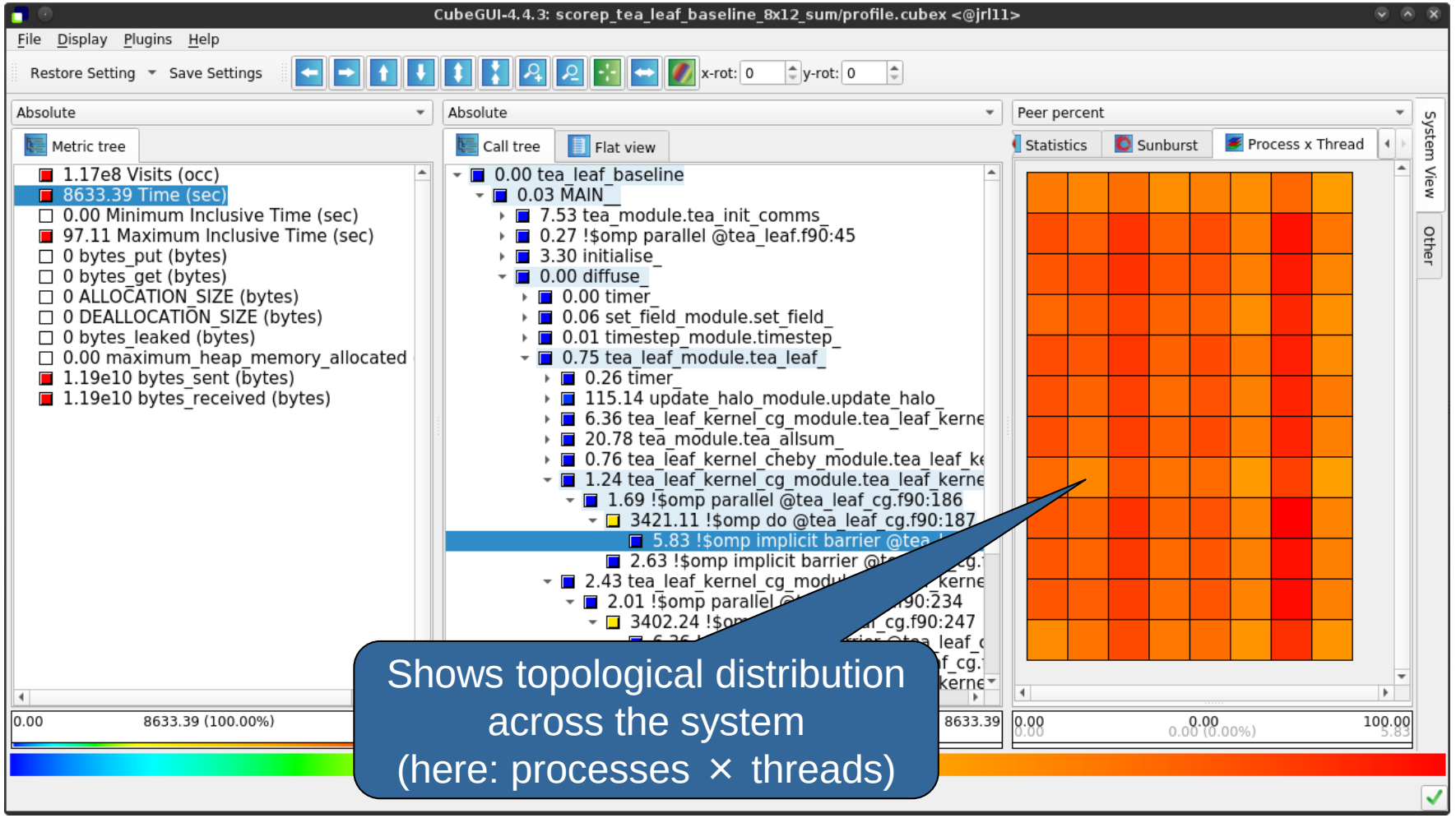
Box plot view



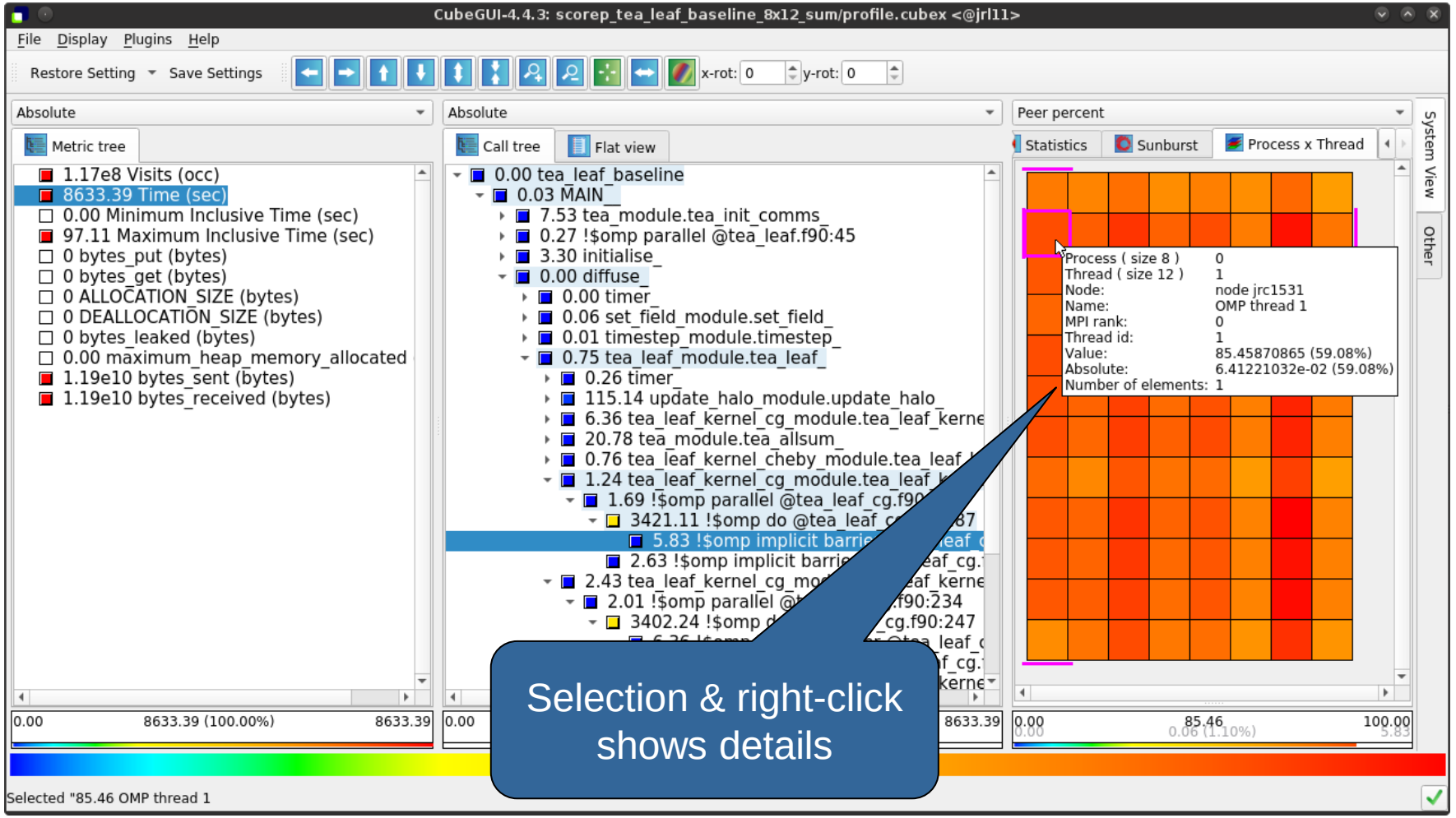
Violin plot view



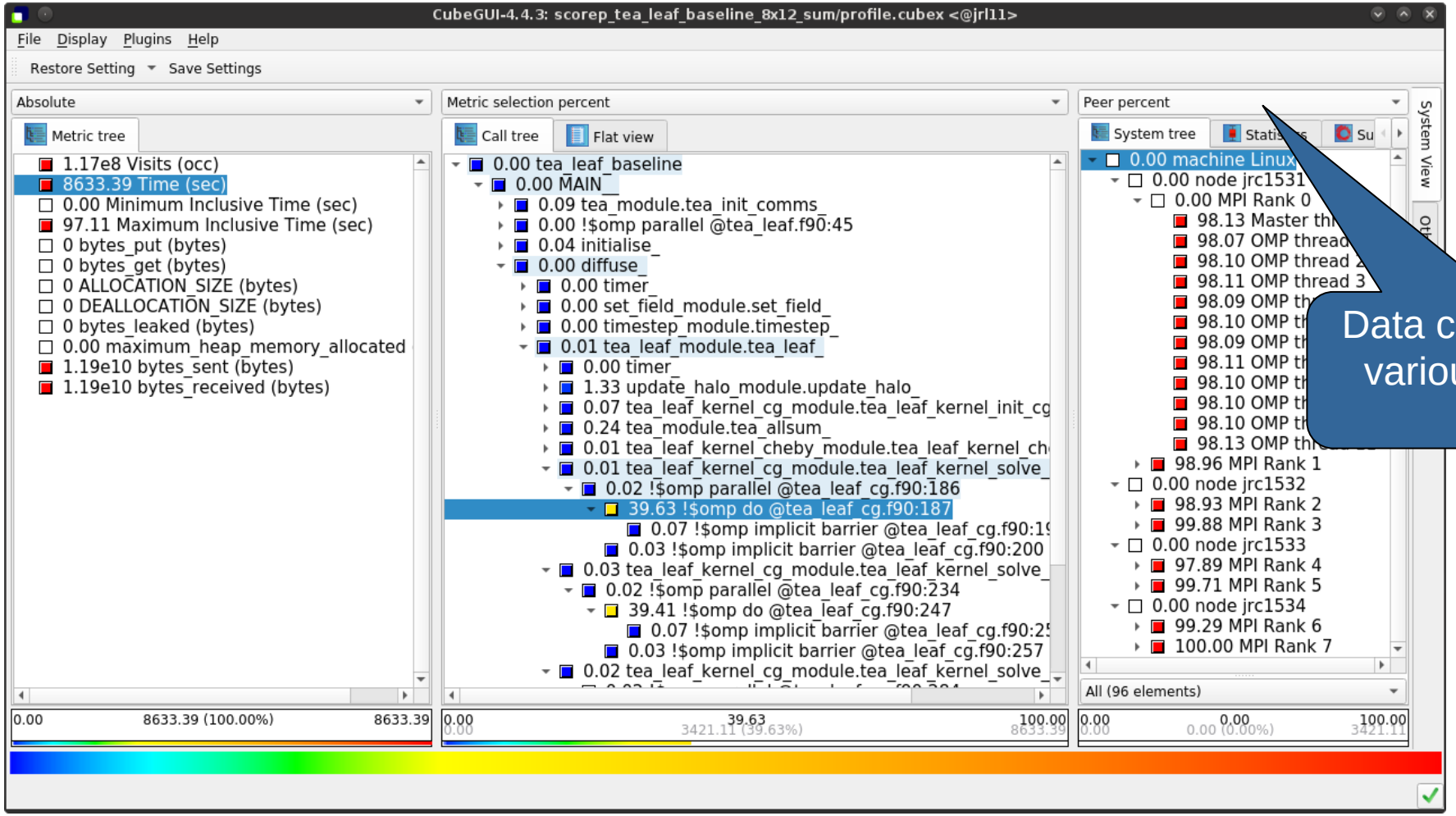
Topology view



Topology view (cont.)



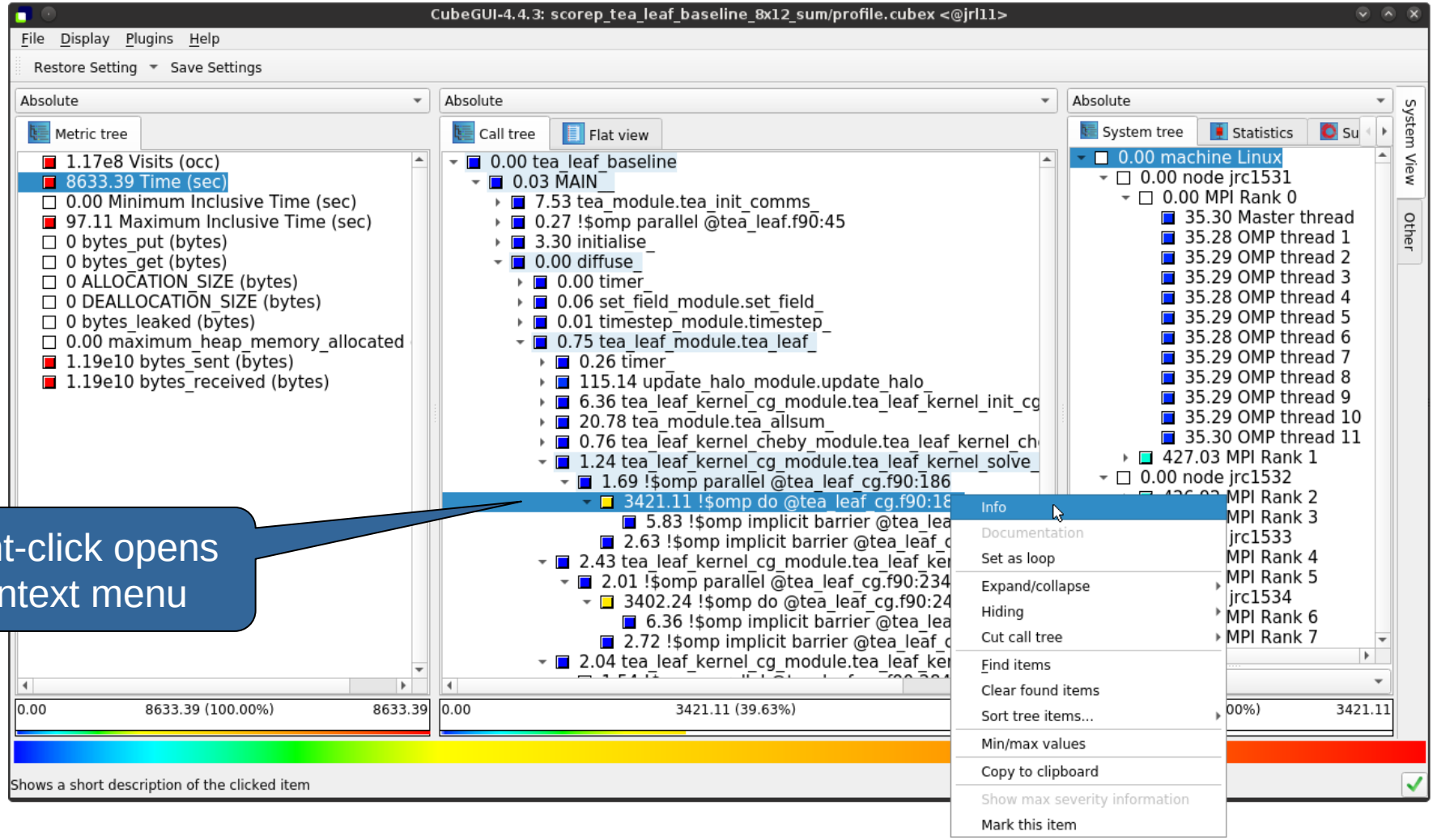
Alternative display modes



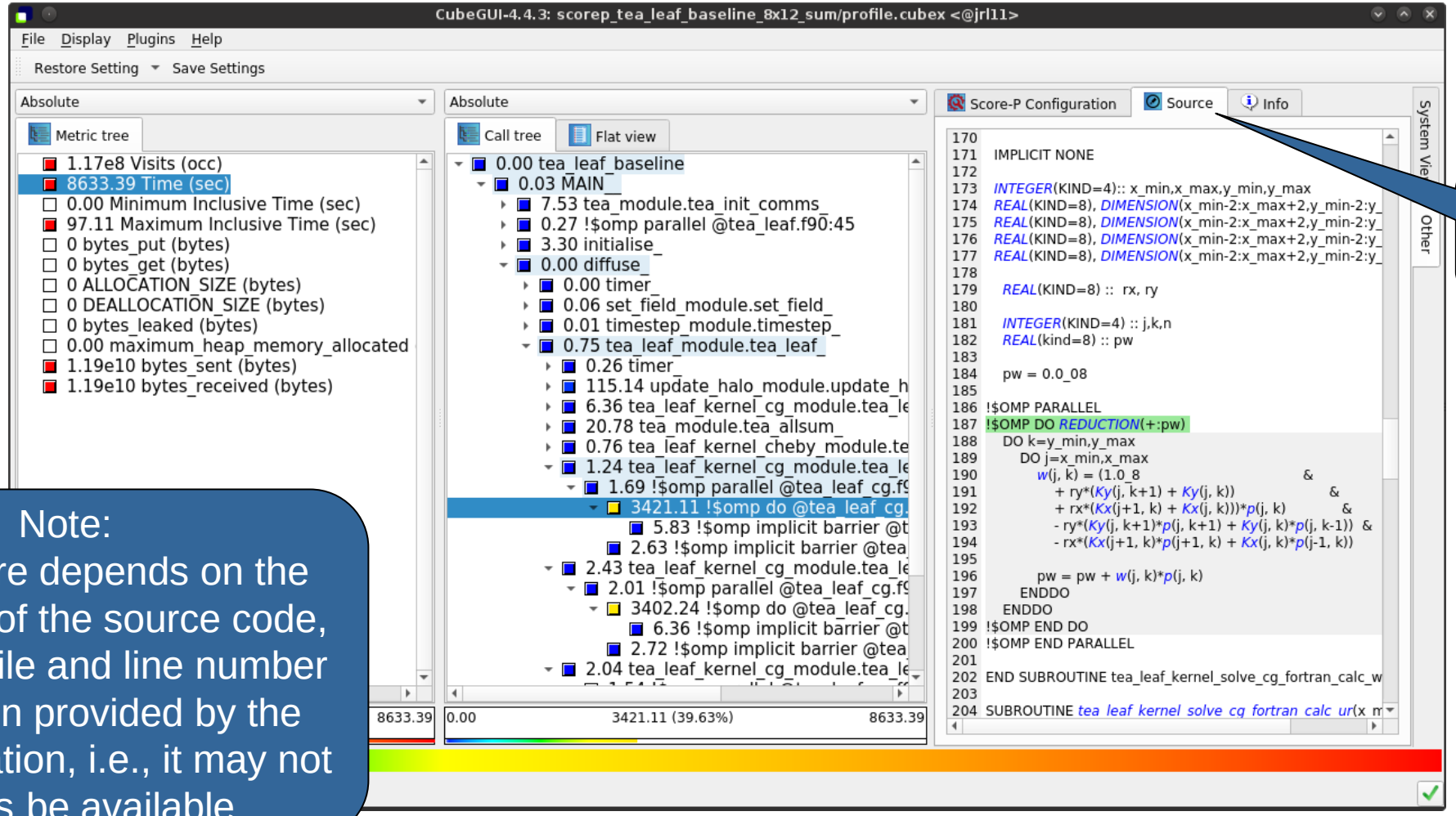
Important display modes

- Absolute
  - Absolute value shown in seconds/bytes/counts
- Selection percent
  - Value shown as percentage w.r.t. the selected node "on the left" (metric/call path)
- Peer percent (system tree only)
  - Value shown as percentage relative to the maximum peer value

Source-code view via context menu



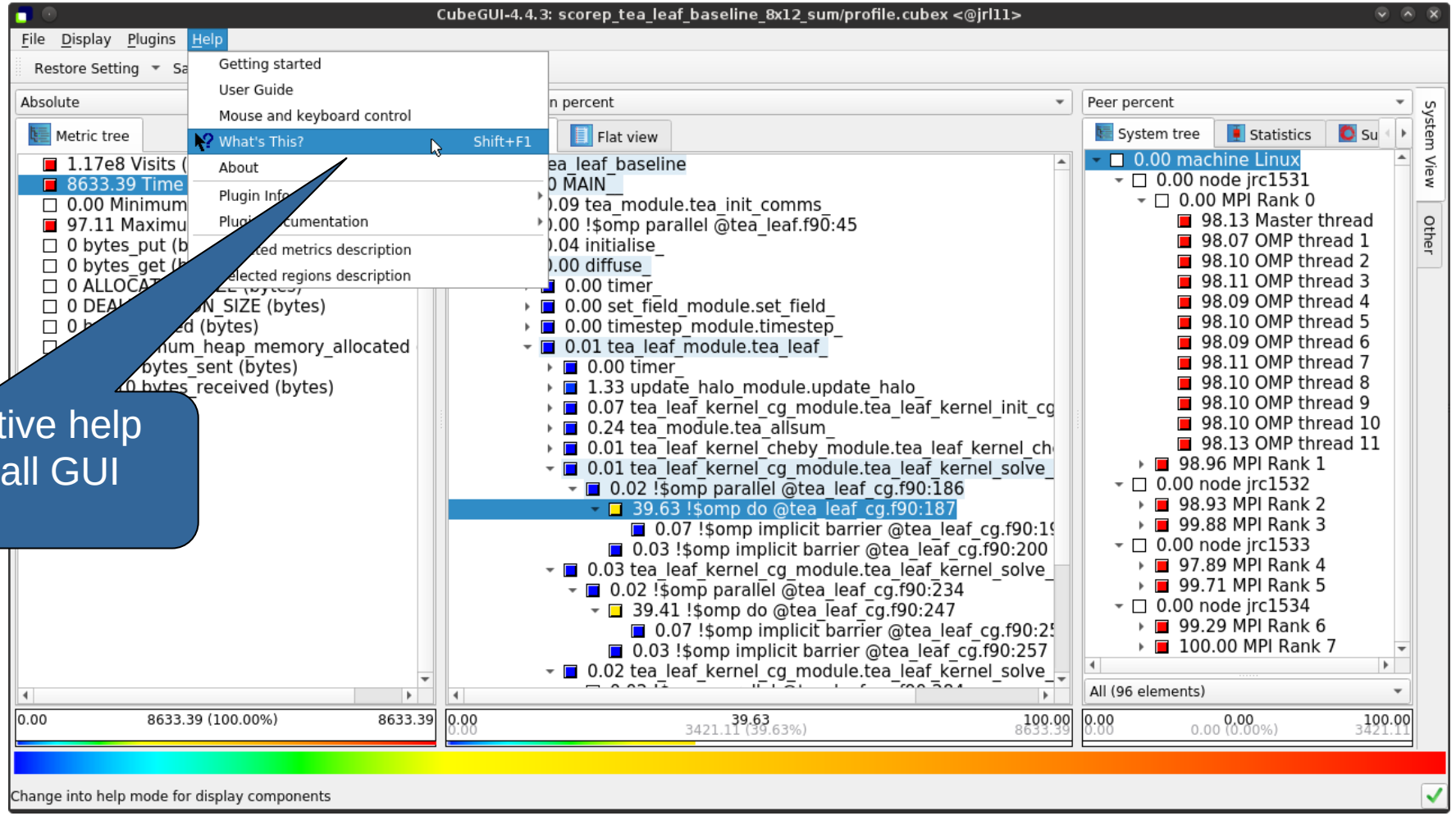
Source-code view



Select “Source” tab

Note:
This feature depends on the availability of the source code, as well as file and line number information provided by the instrumentation, i.e., it may not always be available

Context-sensitive help



Context-sensitive help available for all GUI items

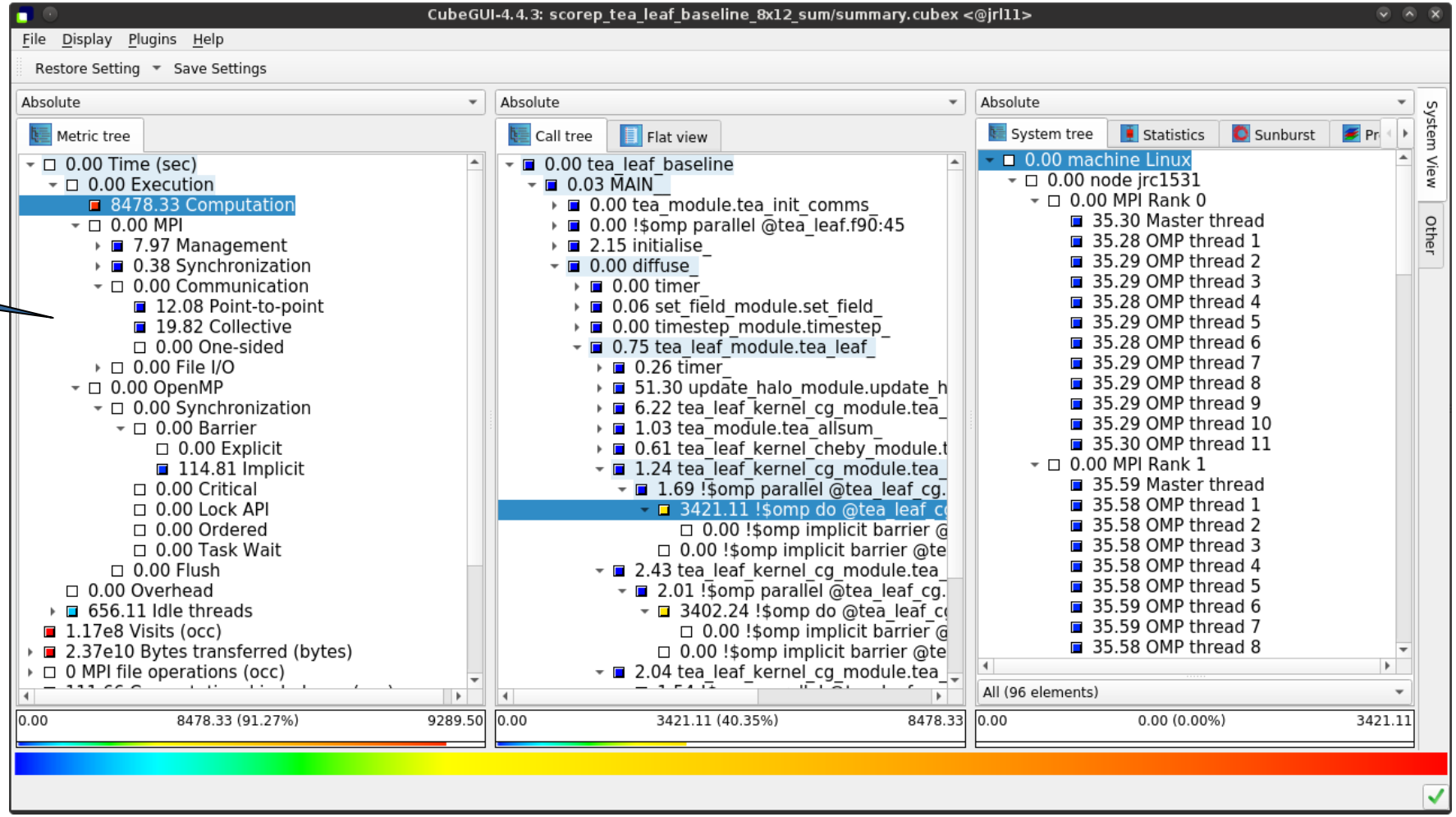
Scalasca report post-processing

- Scalasca's report post-processing derives additional metrics and generates a structured metric hierarchy
- Automatically run (if needed) when using the **square** convenience command:

```
% square scorep_tea_leaf_baseline_8x12_sum
INFO: Post-processing runtime summarization report (profile.cubex)...
INFO: Displaying ./scorep_tea_leaf_baseline_8x12_sum/summary.cubex...

                          [GUI showing post-processed summary analysis report]
```

Post-processed summary analysis report

Split base metrics into more specific metrics, e.g. computation vs parallelization costs

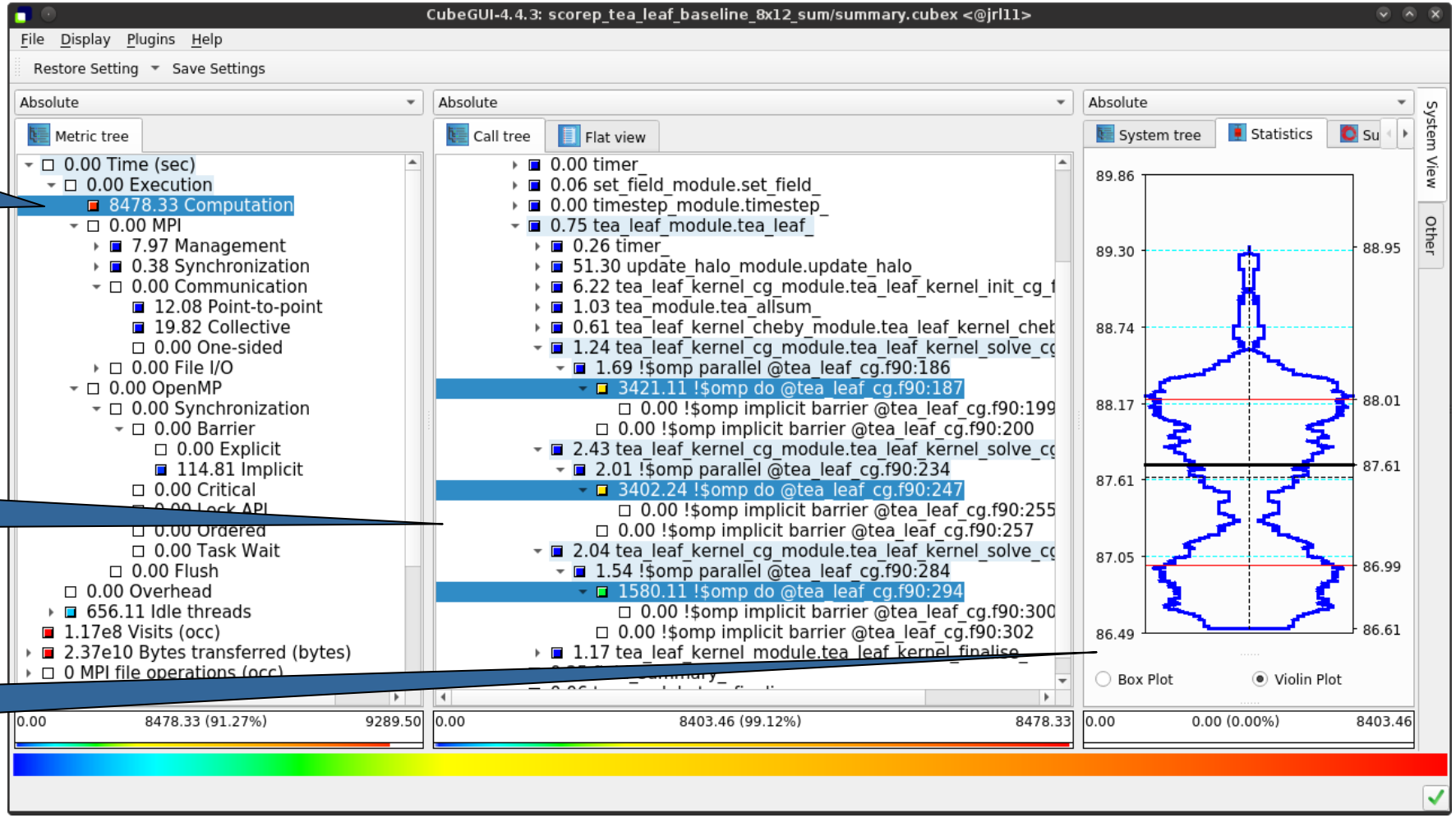


TeaLeaf summary report analysis (I)

91% of the execution time is computation…

…almost entirely spent in 3 OpenMP `do` loops…

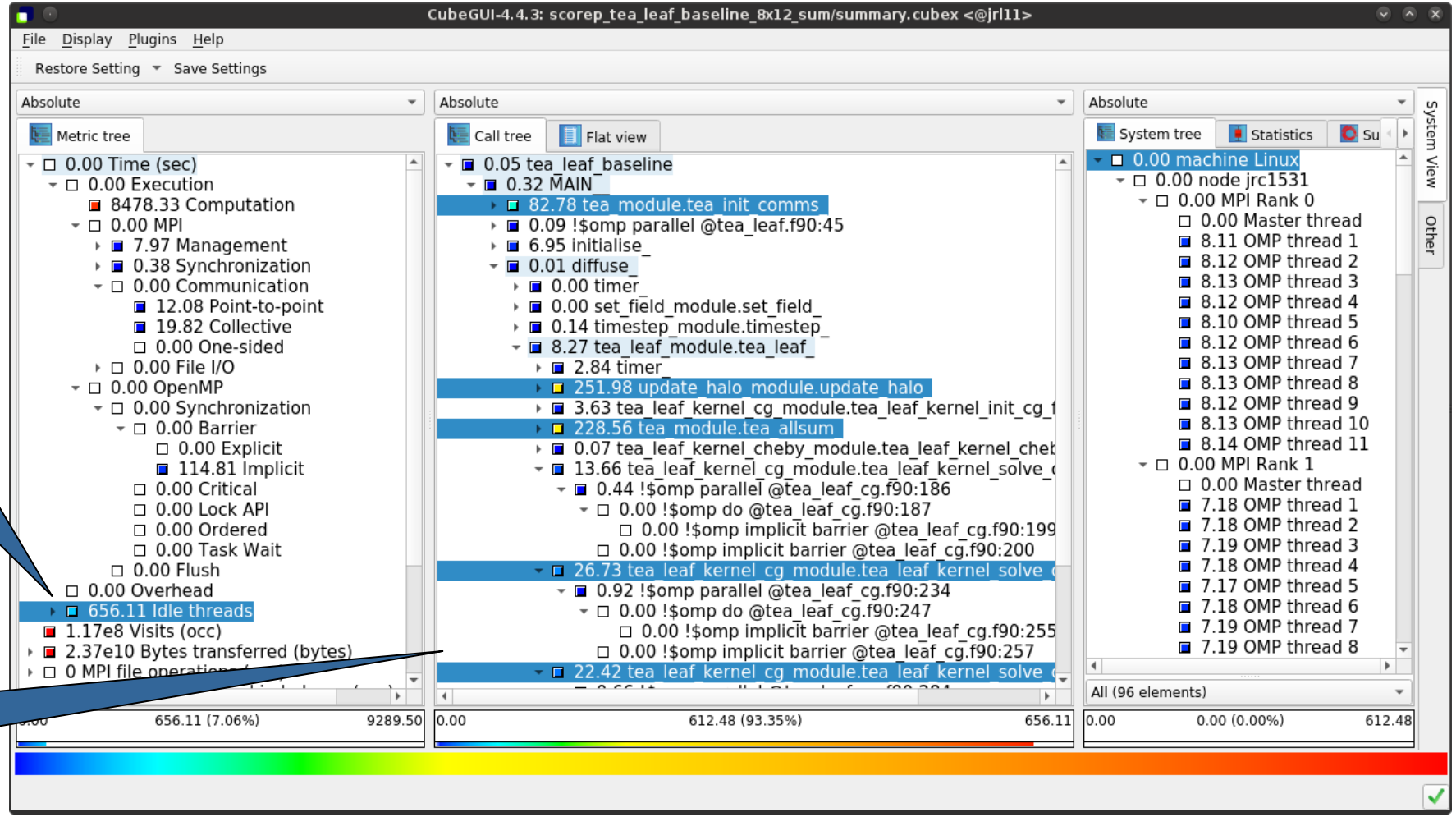
…with a slight imbalance across ranks & threads



TeaLeaf summary report analysis (II)

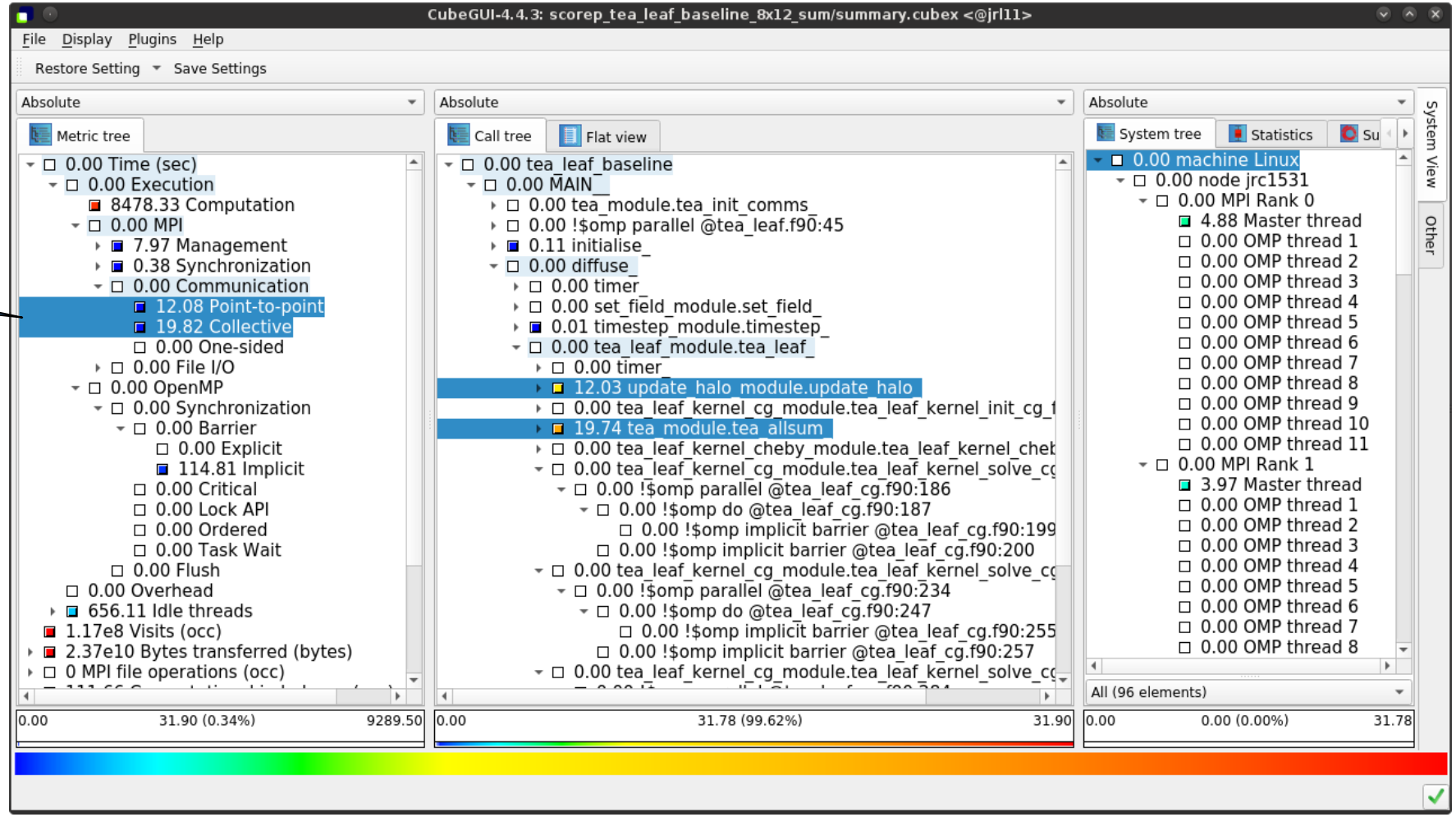
7% of the total CPU execution time is due due to "idle threads"…

… when not within OpenMP-parallelized code regions



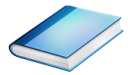
TeaLeaf summary report analysis (III)

MPI communication time is negligible (0.34%); but communication is only on the master threads (MPI_THREAD_FUNNELED)



Cube: Further information

- Parallel program analysis report exploration tools
  - Libraries for Cube report reading & writing
  - Algebra utilities for report processing
  - GUI for interactive analysis exploration
- Available under 3-clause BSD open-source license
- Documentation & sources:
  - https://www.scalasca.org
- User guide also part of installation:
  - <prefix>/share/doc/cubegui/CubeUserGuide.pdf
- Contact:
  - mailto: scalasca@fz-juelich.de

Reference material 

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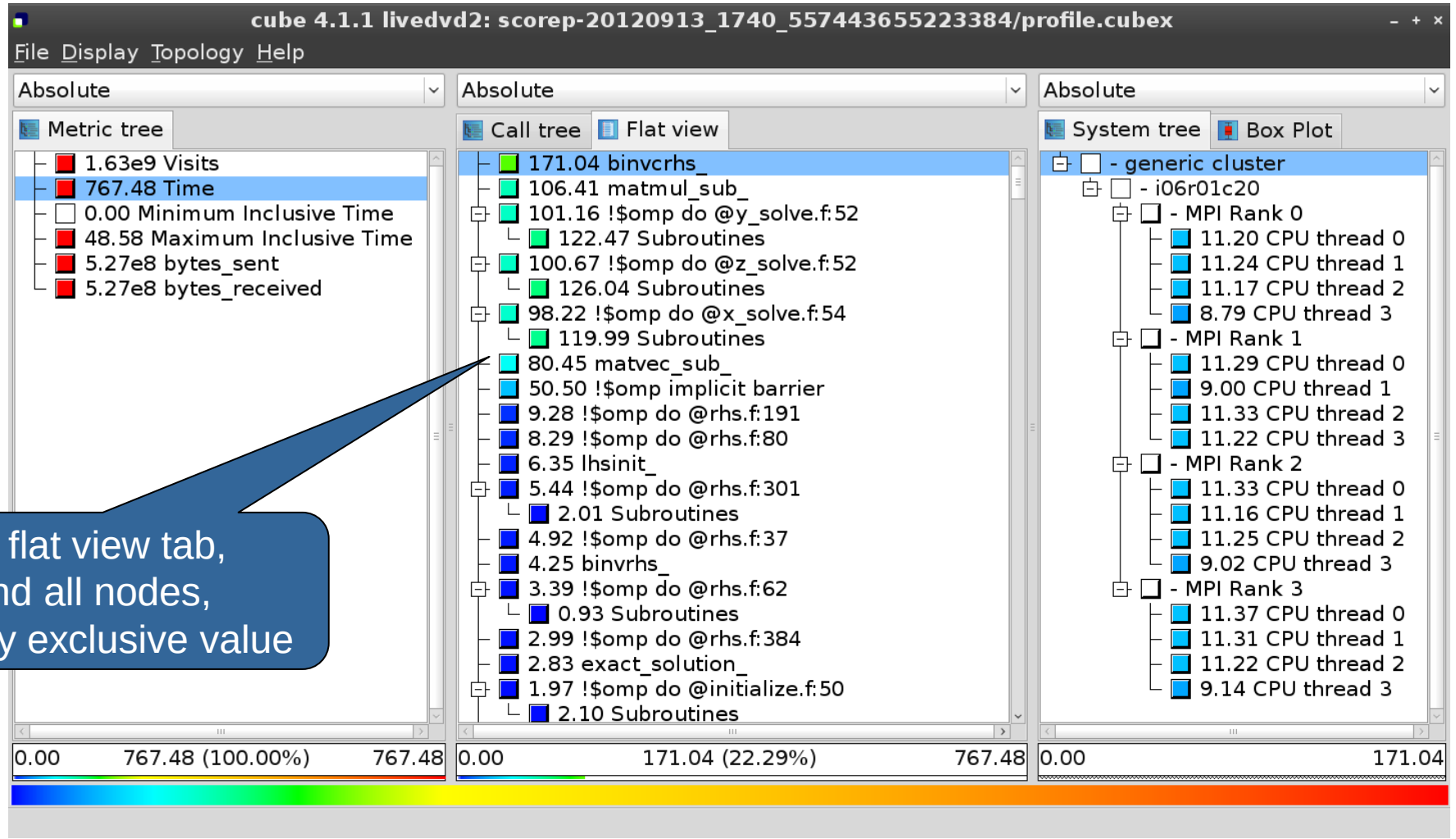
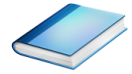
cube
scalasca

Flat profile view



Derived metrics



- Derived metrics are defined using CubePL expressions, e.g.:

metric::time(i)/metric::visits(e)

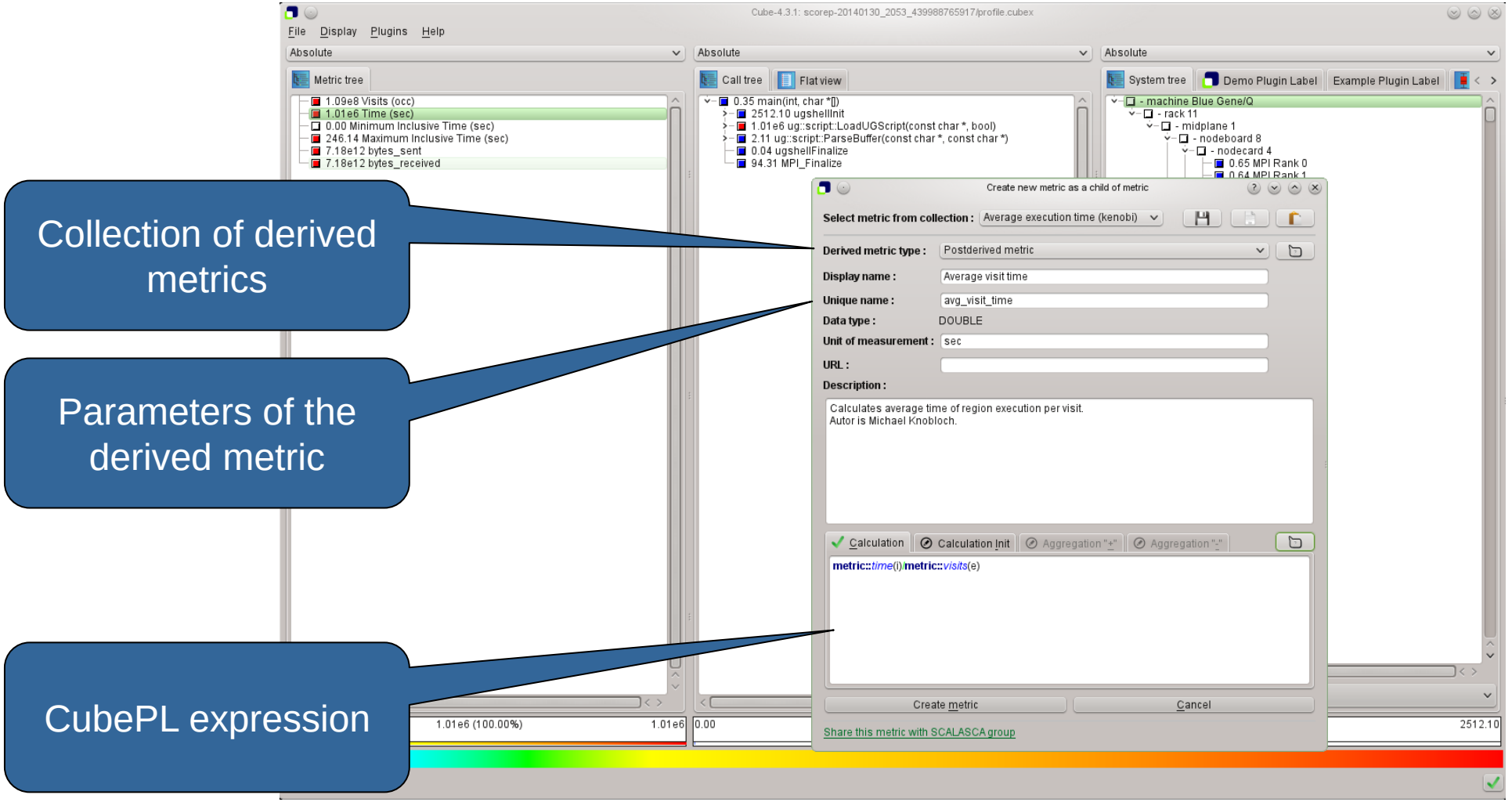
- Values of derived metrics are not stored, but calculated on-the-fly
- Types of derived metrics:
  - Prederived: evaluation of the CubePL expression is performed before aggregation
  - Postderived: evaluation of the CubePL expression is performed after aggregation

- Examples:
  - “Average execution time”: Postderived metric with expression

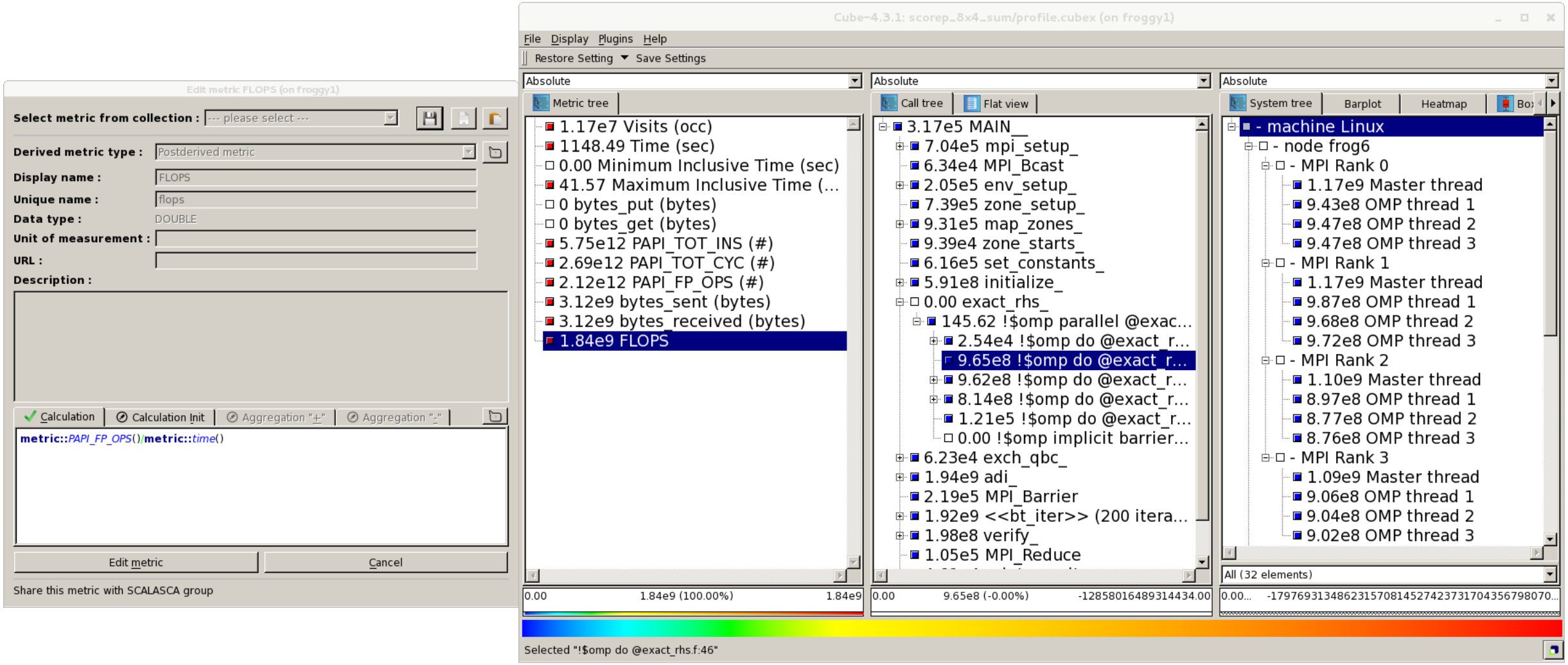
metric::time(i)/metric::visits(e)

  - “Number of FLOP per second”: Postderived metric with expression

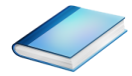
Derived metrics in Cube GUI



Example: FLOPS based on PAPI_FP_OPS and time



CUBE algebra utilities



- Extracting solver sub-tree from analysis report

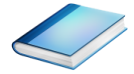
```
% cube_cut  -r '<<ITERATION>>'  scorep_bt-mz_C_32x4_sum/profile.cubex
Writing cut.cubex... done.
```

- Calculating difference of two reports

```
% cube_diff  scorep_bt-mz_C_32x4_sum/profile.cubex  cut.cubex
Writing diff.cubex... done.
```

- Additional utilities for merging, calculating mean, etc.
- Default output of cube_*utility* is a new report *utility*.cubex
- Further utilities for report scoring & statistics
- Run utility with `–h' (or no arguments) for brief usage info

Iteration profiling



- Show time dependent behavior by “unrolling” iterations
- Preparations:
  - Mark loop body by using Score-P instrumentation API in your source code

```
SCOREP_USER_REGION_DEFINE( scorep_bt_loop )
SCOREP_USER_REGION_BEGIN( scorep_bt_loop, "<<bt_iter>>", SCOREP_USER_REGION_TYPE_DYNAMIC )
SCOREP_USER_REGION_END( scorep_bt_loop )
```

- Result in the Cube profile:
  - Iterations shown as separate call trees

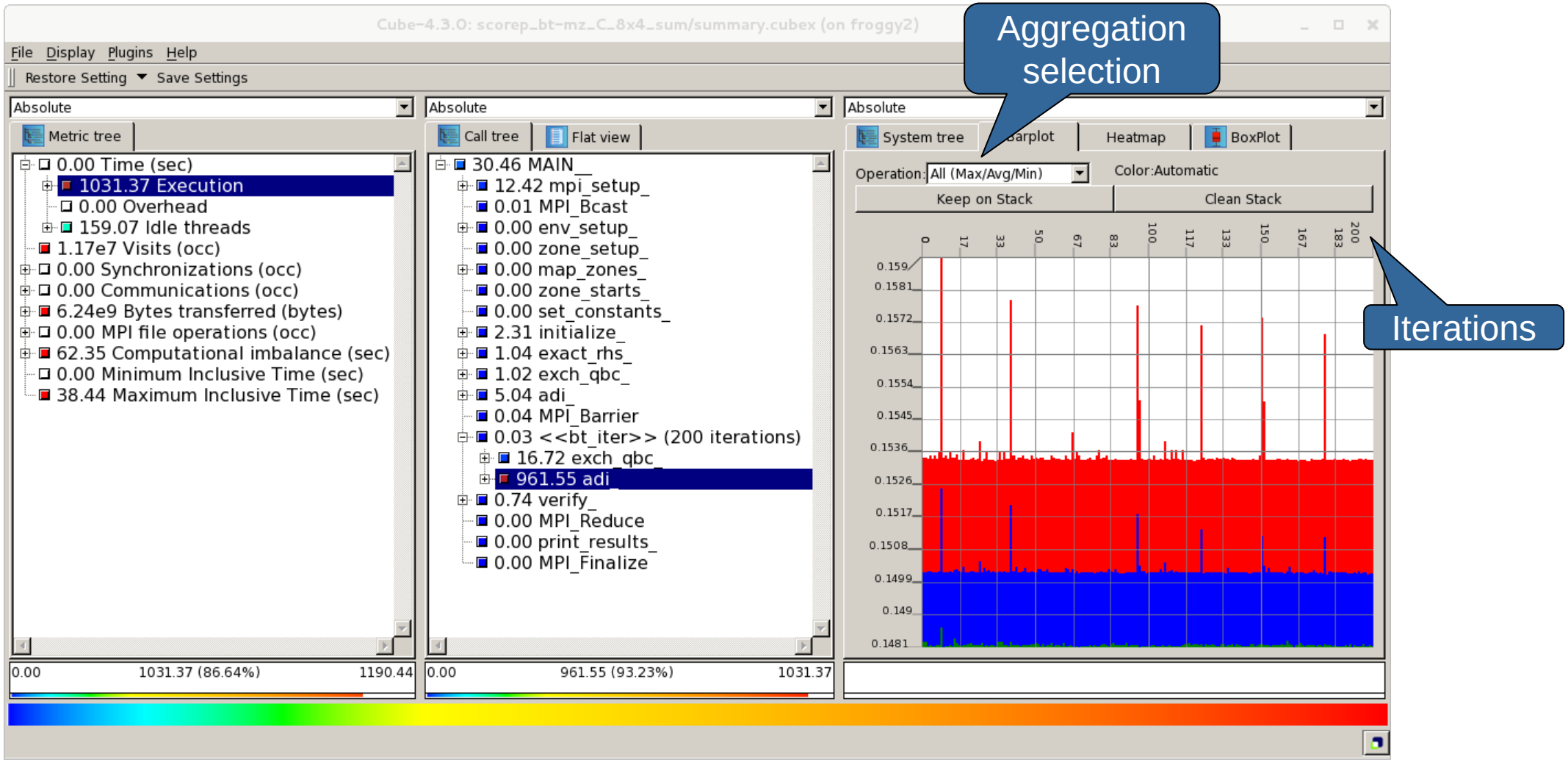
➢Useful for checking results for specific iterations

or

  - Select your user-instrumented region and mark it as loop
  - Choose “Hide iterations”

➢View the Barplot statistics or the (thread x iterations) Heatmap

Iteration profiling: Barplot



Iteration profiling: Heatmap