

Analysis report examination with Cube

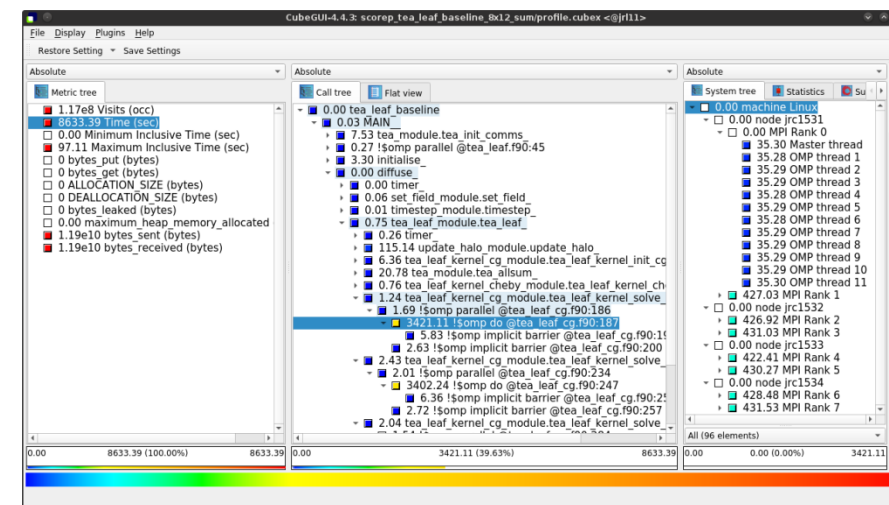
Ilya Zhukov
Jülich Supercomputing Centre



Cube

CubeLib DOI 10.5281/zenodo.7737408
CubeGUI DOI 10.5281/zenodo.7737411

- 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 \geq 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 v4.8.2 (Sept 2023)



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

- Run **remote** (*ssh*)
 - start X server (e.g., Xming) locally
 - connect to system with X forwarding enabled
 - load cube module and start cube remotely

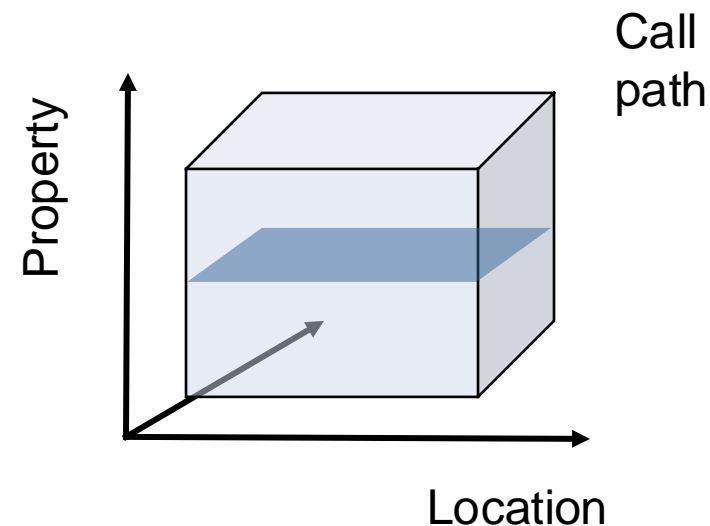
```
laptop$ ssh -X <yourid>@login.leonardo.cineca.it
Welcome to Leonardo ...
[leonardologin~]$ source /leonardo/pub/userexternal/\
/bwylie00/tools/nvmpi/setup.sh
[leonardologin~]$ cube ./scorep-*/profile.cubex
```

- Install & run **local**
 - Install Cube GUI locally on desktop
 - binary packages available for MacOS & Windows and externally provided by OpenHPC and various Linux distributions
 - source package available for Linux, requires Qt
 - configure/build/install manually or use your favourite framework (e.g. Spack or EasyBuild)
 - copy .cubex file (or entire scorep directory) to desktop from remote system **OR** locally mount remote filesystem
 - start cube locally

```
desk$ mkdir $HOME/mnt
desk$ sshfs [user@]remote.sys:[dir] $HOME/mnt
desk$ cd $HOME/mnt
desk$ cube ./scorep-*/profile.cubex
```

Analysis presentation and exploration

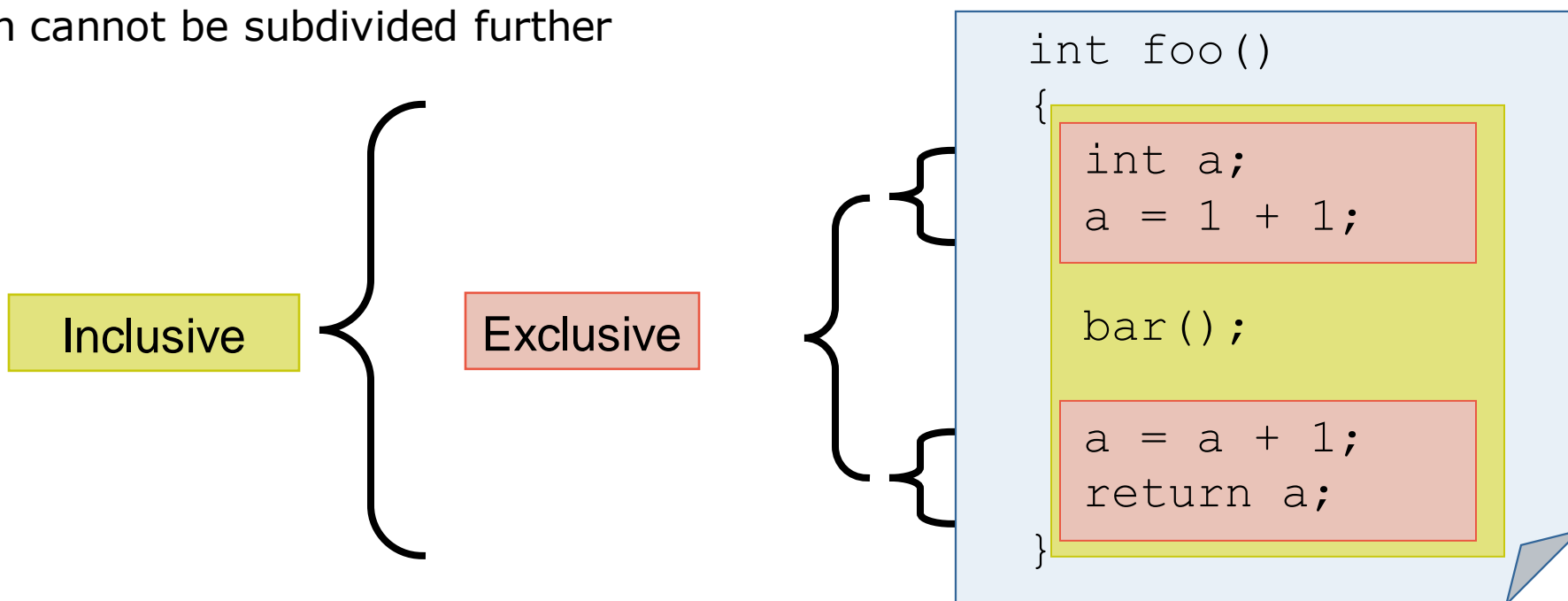
- Representation of values (severity matrix) on three hierarchical axes
 - Performance property (metric)
 - Call path (program location)
 - System location (process/thread)
- Three coupled tree browsers
- Cube displays severities
 - As *value*: for precise comparison
 - As *colour*: for easy identification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

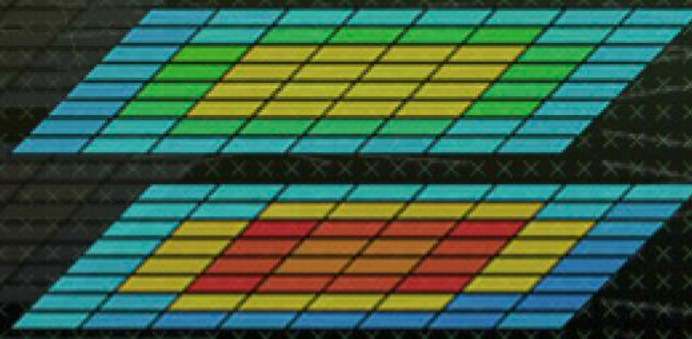


Inclusive vs. exclusive values



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





Demo: TeaLeaf case study



Case study: TeaLeaf

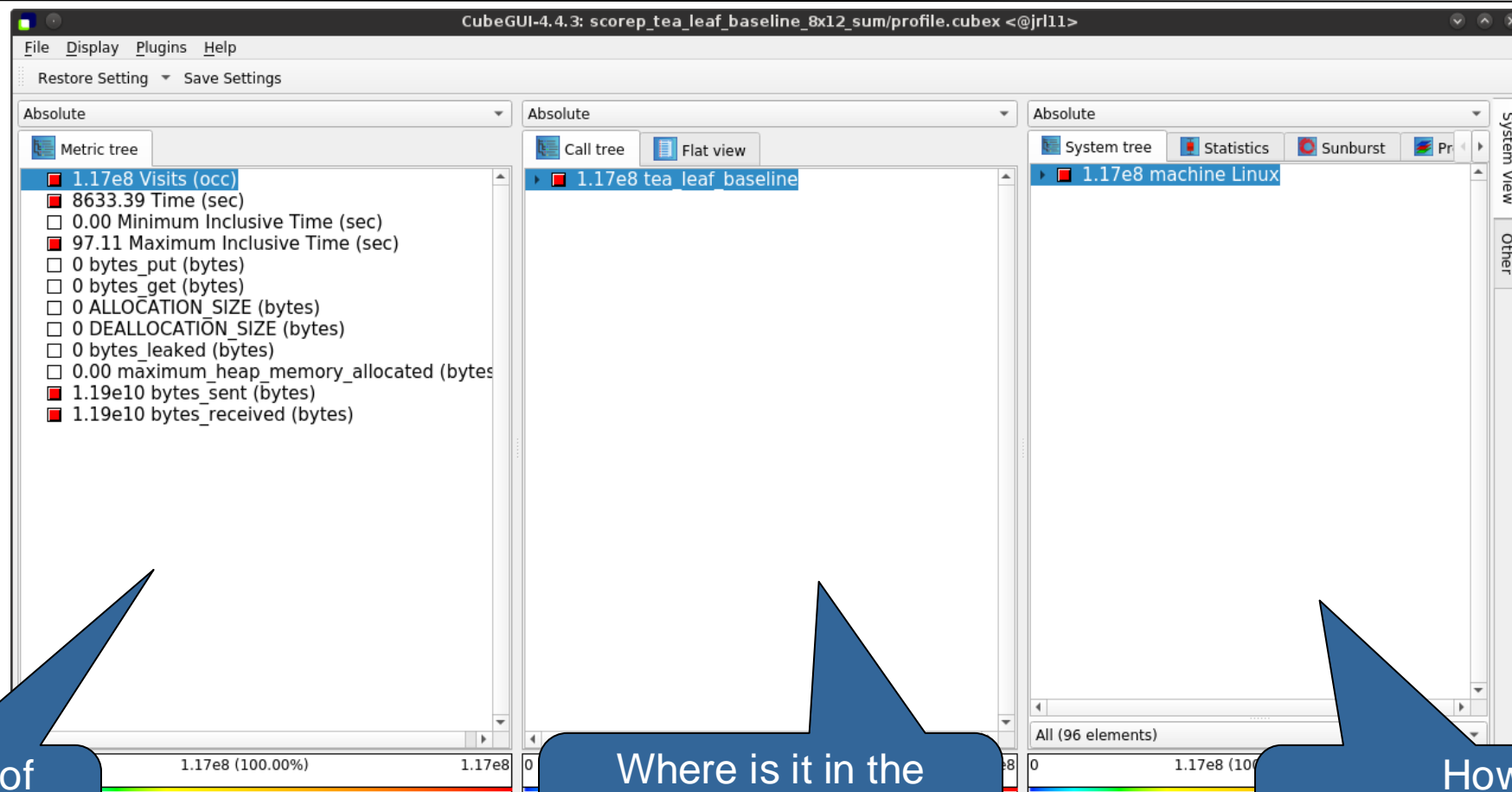
- HPC mini-app developed by the UK Mini-App Consortium
 - Solves the linear 2D heat conduction equation on a spatially decomposed regular grid using a 5 point stencil with implicit solvers
 - Part of the Mantevo 3.0 suite
 - Available on GitHub: <http://uk-mac.github.io/TeaLeaf/>

- 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)



What kind of performance metric?

Where is it in the source code?
In what context?

How is it distributed across the processes/threads?

Metric selection

CubeGUI-4.4.3: scorep_tea_leaf_baseline_8x12_sum/profile.cubex <@jrl11>

File Display Plugins Help

Restore Setting Save Settings

Absolute Absolute Absolute

Metric tree

- 1.17e8 Visits (occ)
- 8633.39 Time (sec)
- 0.00 Minimum Inclusive Time (sec)
- 97.11 Maximum Inclusive Time (sec)
- 0 bytes_put (bytes)
- 0 bytes_get (bytes)
- 0 ALLOCATION_SIZE (bytes)
- 0 DEALLOCATION_SIZE (bytes)
- 0 bytes_leaked (bytes)
- 0.00 maximum_heap_memory_allocated (bytes)
- 1.19e10 bytes_sent (bytes)
- 1.19e10 bytes_received (bytes)

Call tree Flat view

8633.39 tea leaf baseline

System tree Statistics Sunburst Pr

8633.39 machine Linux

System View Other

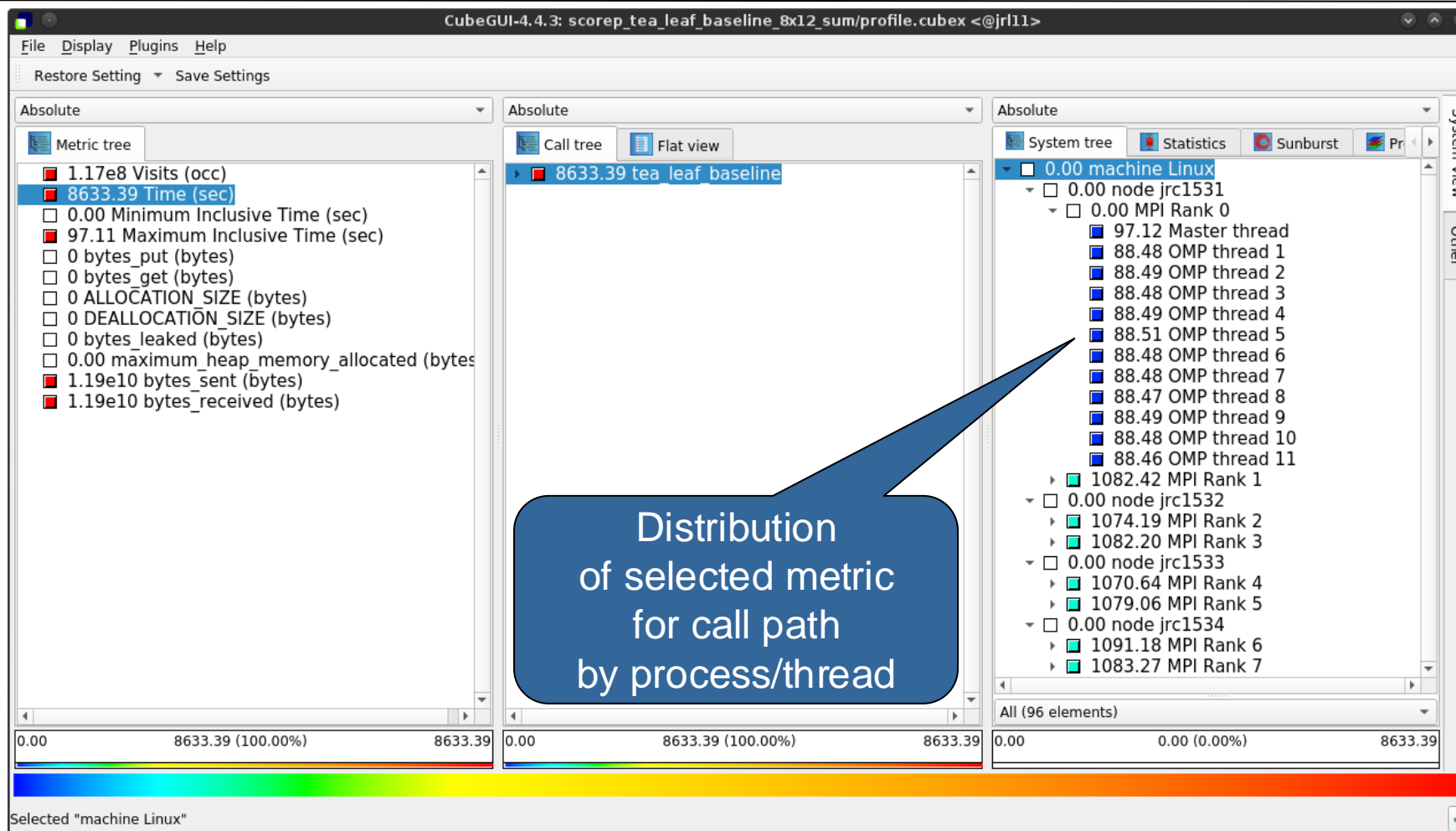
All (96 elements)

0.00 8633.39 (100.00%) 8633.39 0.00 8633.39 (100.00%) 8633.39 0.00 8633.39 (100.00%) 8633.39

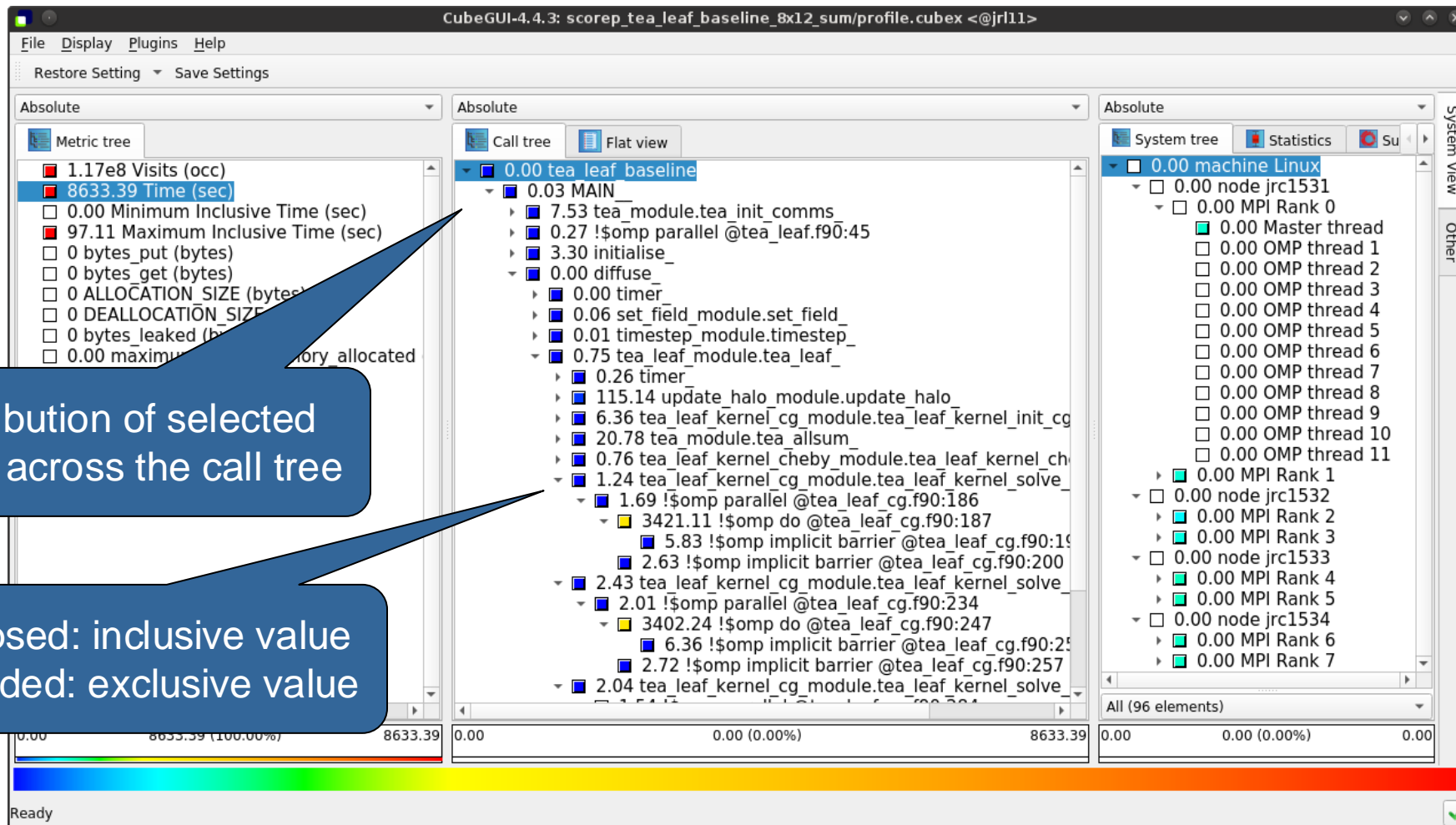
Selected "Time"

Selecting the "Time" metric shows total execution time

Expanding the system tree



Expanding the call tree



Selecting a call path

The screenshot displays the CubeGUI-4.4.3 interface for a performance profile. The main window is titled "CubeGUI-4.4.3: scorep_tea_leaf_baseline_8x12_sum/profile.cubex <@jrl11>". It features three main panels:

- Metric tree (left):** Lists various performance metrics. The "8633.39 Time (sec)" metric is highlighted in blue.
- Call tree (center):** Shows a hierarchical view of the application's execution. The path "0.03 MAIN_ > 0.27 !\$omp parallel @tea_leaf.f90:45 > 3.30 initialise_ > 0.00 diffuse_ > 0.75 tea_leaf_module.tea_leaf_ > 0.26 timer_ > 115.14 update_halo_module.update_halo_ > 6.36 tea_leaf_kernel_cg_module.tea_leaf_kernel_init_cg_ > 20.78 tea_module.tea_allsum_ > 0.76 tea_leaf_kernel_cheby_module.tea_leaf_kernel_ch_ > 1.24 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_ > 1.69 !\$omp parallel @tea_leaf_cg.f90:186 > 3421.11 !\$omp do @tea_leaf_cg.f90:187" is selected and highlighted in blue.
- System tree (right):** Shows the system's execution tree. The path "0.00 machine Linux > 0.00 node jrc1531 > 0.00 MPI Rank 0 > 35.30 Master thread > 35.28 OMP thread 1 > 35.29 OMP thread 2 > 35.29 OMP thread 3 > 35.28 OMP thread 4 > 35.29 OMP thread 5 > 35.28 OMP thread 6 > 35.29 OMP thread 7 > 35.29 OMP thread 8 > 35.29 OMP thread 9 > 35.29 OMP thread 10 > 35.30 OMP thread 11" is selected and highlighted in blue.

A callout box with a blue background and white text points to the selected call path in the Call tree. The text reads: "Selection updates metric values shown in columns to the right".

At the bottom of the interface, there are three columns of data corresponding to the selected paths in the Metric tree, Call tree, and System tree. Each column shows a value and a percentage relative to the total time (8633.39 seconds):

Metric	Value	Percentage
Time (sec)	8633.39	100.00%
tea_leaf_baseline	0.00	0.00%
tea_leaf_kernel_solve (selected)	3421.11	39.63%
OMP thread 11 (selected)	0.00	0.00%
OMP thread 11 (selected)	3421.11	39.63%

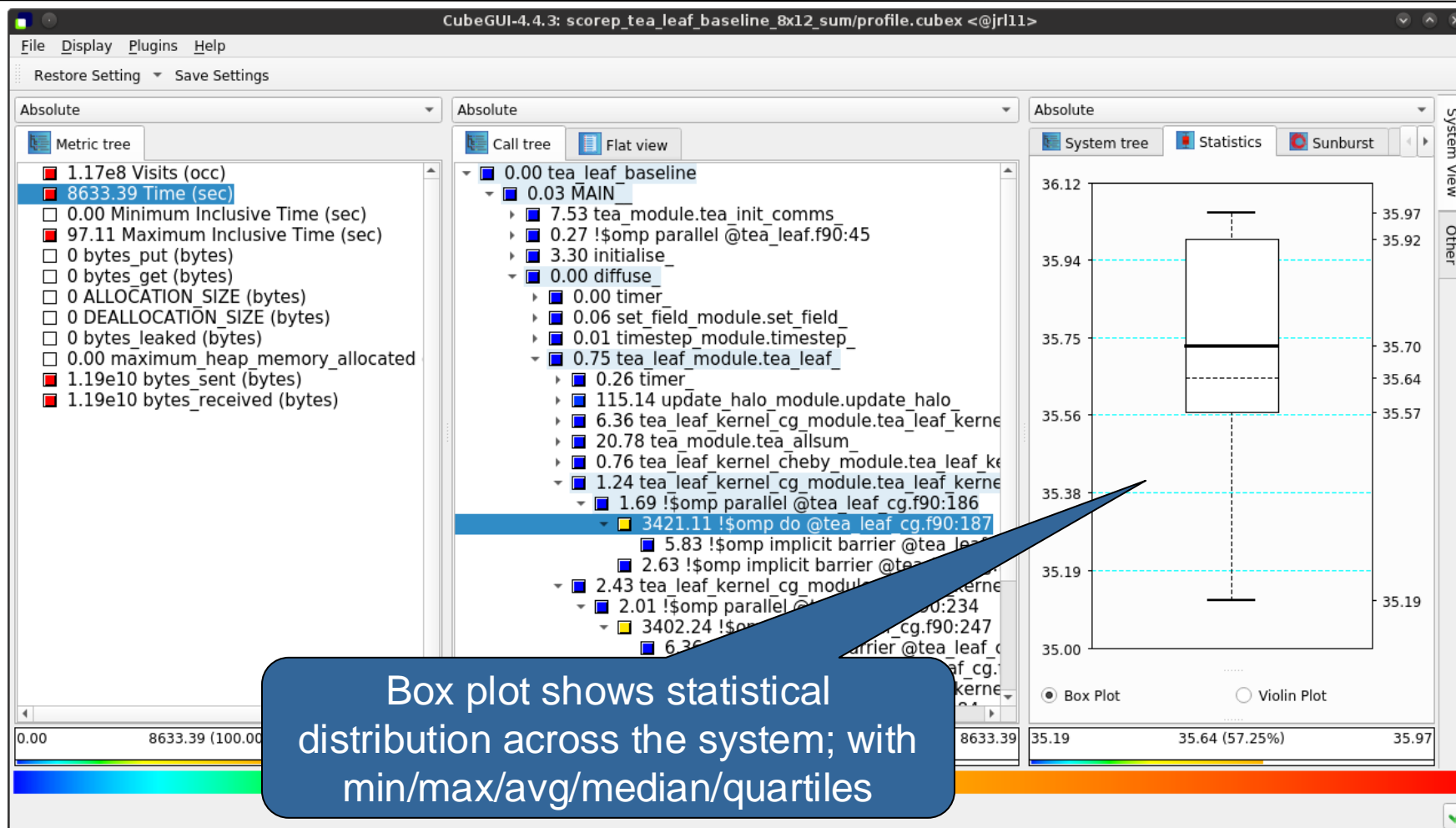
Multiple selection

The screenshot displays the CubeGUI-4.4.3 interface for the profile file `scorep_tea_leaf_baseline_8x12_sum/profile.cubex`. The interface is divided into three main panels:

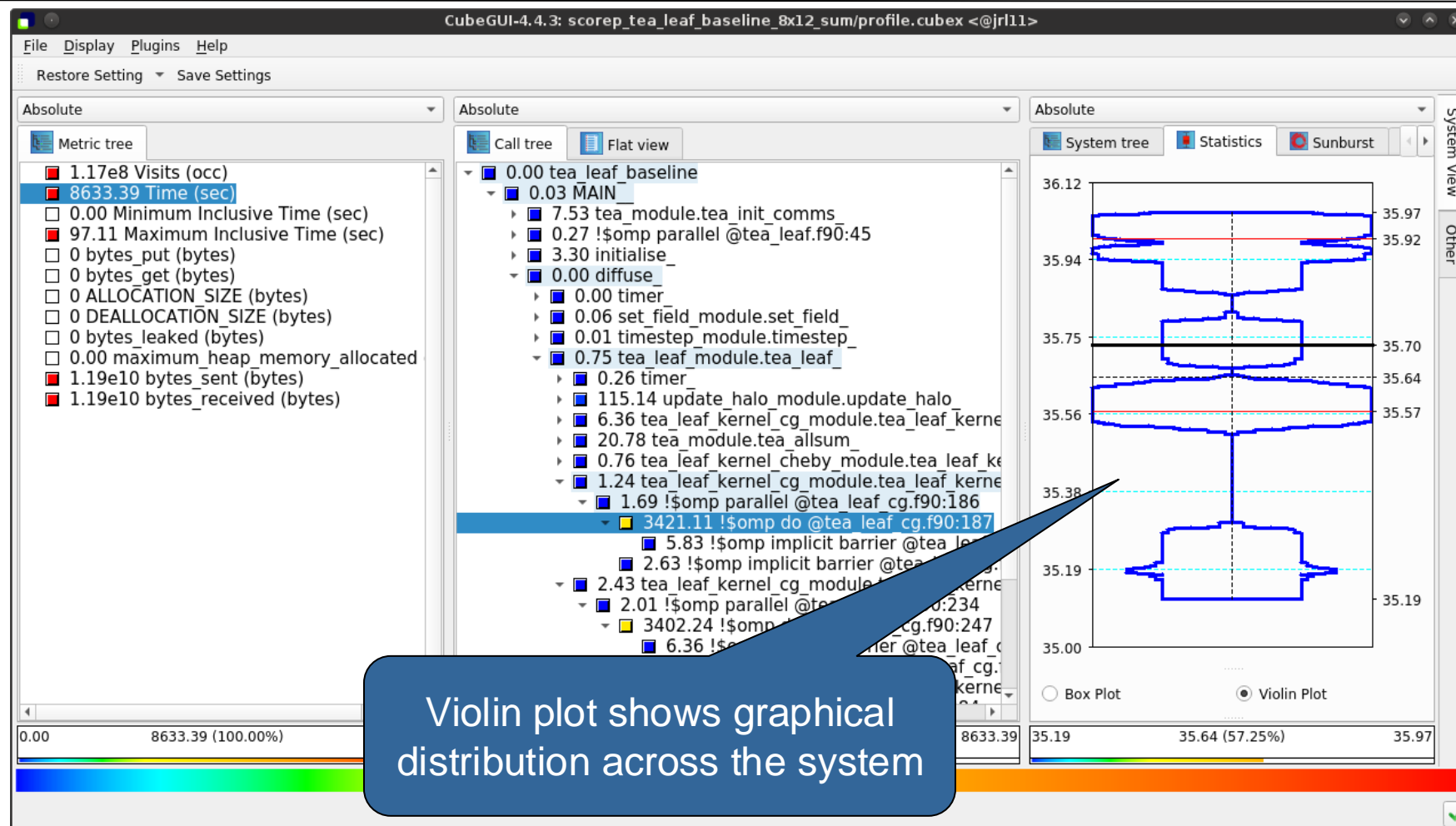
- Metric tree (left):** Shows various performance metrics. The `8633.39 Time (sec)` metric is highlighted in blue.
- Call tree (center):** Shows a hierarchical view of the application's execution. Several nodes are selected with blue highlights, including:
 - `0.75 tea_leaf_module.tea_leaf_`
 - `1.24 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_`
 - `1.69 !$omp parallel @tea leaf cg.f90:186`
 - `3421.11 !$omp do @tea leaf cg.f90:187`
 - `2.63 !$omp implicit barrier @tea leaf cg.f90:200`
 - `2.43 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_`
 - `2.01 !$omp parallel @tea leaf cg.f90:234`
 - `3402.24 !$omp do @tea leaf cg.f90:247`
 - `2.72 !$omp implicit barrier @tea leaf cg.f90:257`
 - `2.04 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_`
 - `1.54 !$omp parallel @tea leaf cg.f90:284`
 - `1580.11 !$omp do @tea leaf cg.f90:294`
 - `40.82 !$omp implicit barrier @tea leaf cg.f90:302`
 - `3.24 !$omp implicit barrier @tea leaf cg.f90:302`
- System tree (right):** Shows the system hierarchy, including the machine `Linux`, nodes `jrc1531` through `jrc1534`, and MPI Ranks 0 through 7. The `0.00 machine Linux` node is selected.

A blue callout box with a white border and a pointer to the selected nodes in the Call tree contains the text: **Select multiple nodes with Ctrl-click**.

Box plot view

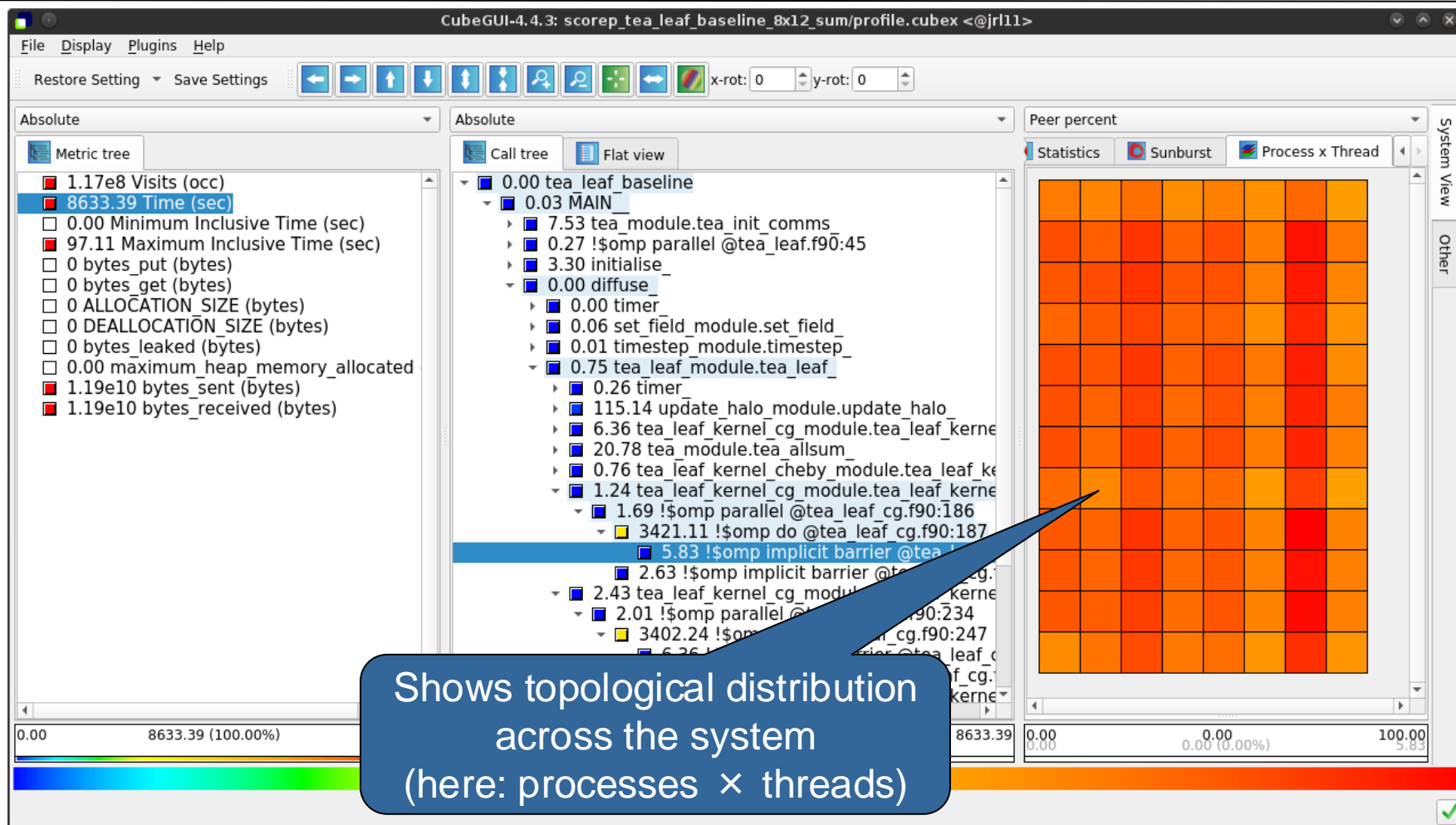


Violin plot view

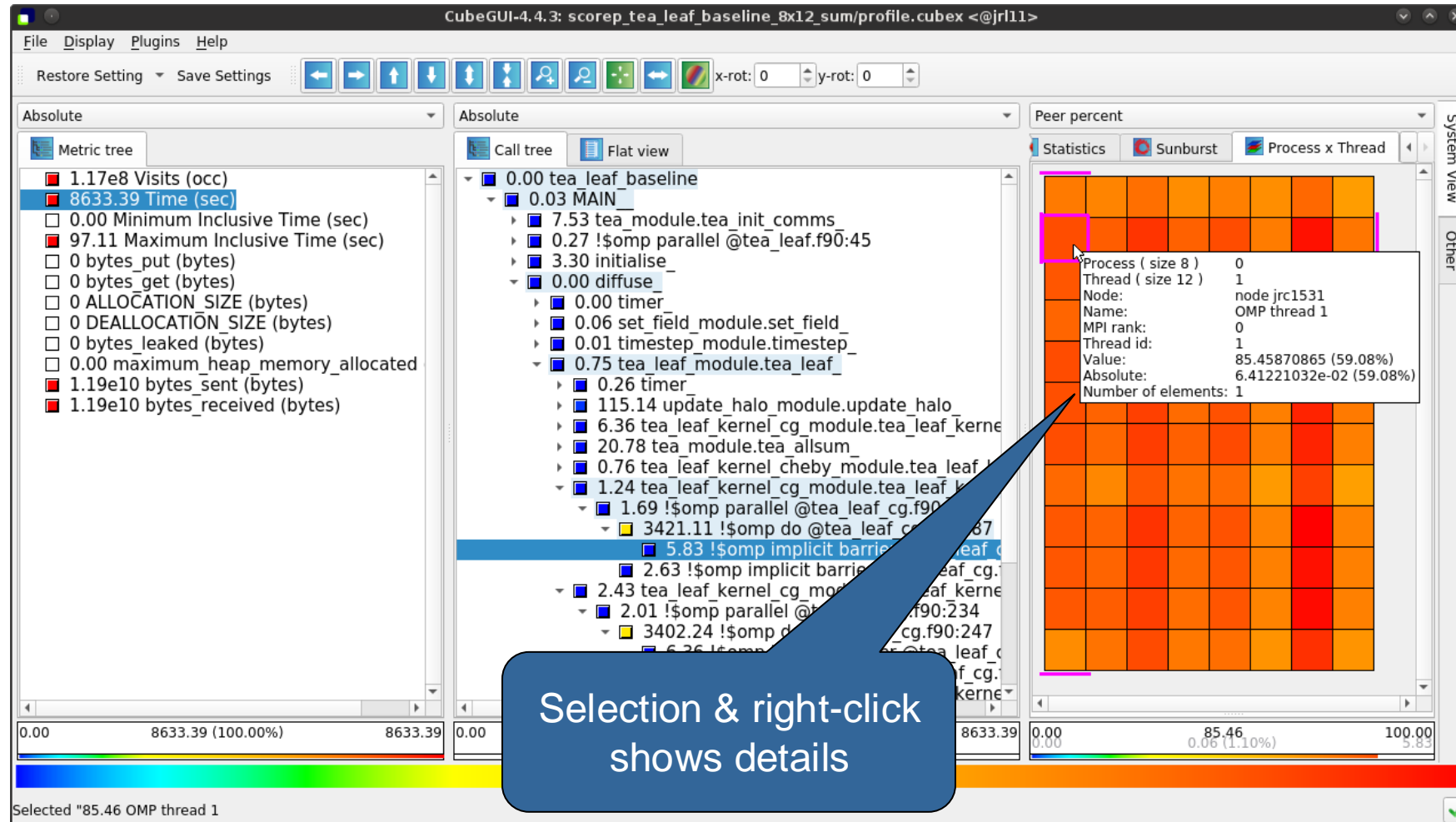


Violin plot shows graphical distribution across the system

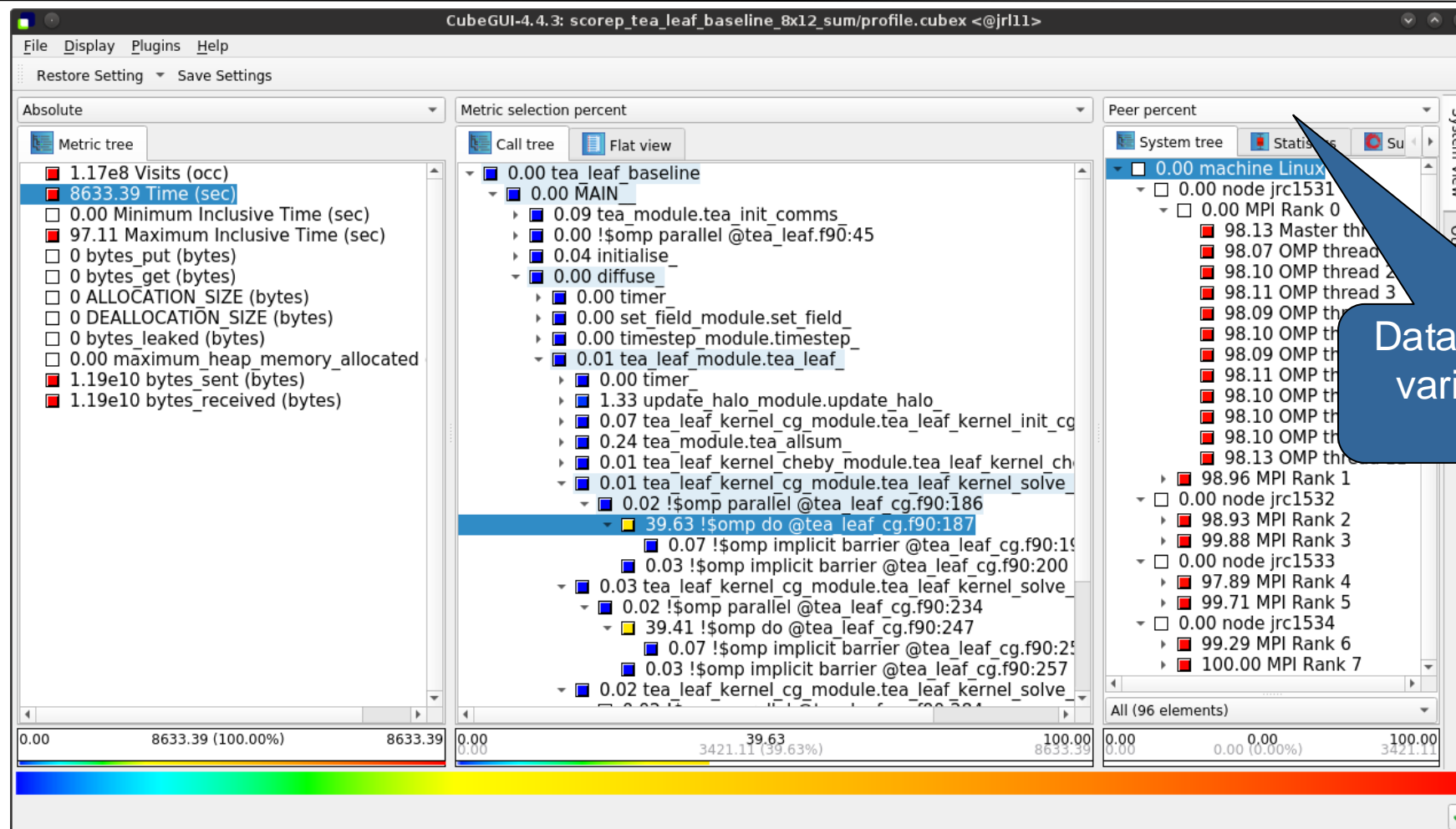
Topology view



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

The screenshot displays the CubeGUI-4.4.3 interface with three main panels: Metric tree, Call tree, and System tree. The Call tree panel shows a hierarchical view of execution metrics. A context menu is open over the item `3421.11 !$omp do @tea leaf cg.f90:18`. The menu options include: Info, Documentation, Set as loop, Expand/collapse, Hiding, Cut call tree, Find items, Clear found items, Sort tree items..., Min/max values, Copy to clipboard, Show max severity information, and Mark this item. A blue callout box with a white border and a pointer to the context menu contains the text: "Right-click opens context menu".

Right-click opens context menu

Source-code view

The screenshot shows the CubeGUI-4.4.3 interface with the following components:

- Metric tree (Left):** Displays various performance metrics such as '1.17e8 Visits (occ)', '8633.39 Time (sec)', and '97.11 Maximum Inclusive Time (sec)'.
- Call tree (Center):** Shows a hierarchical view of the execution flow, including '0.00 tea_leaf_baseline', '0.03 MAIN_', and '0.75 tea_leaf_module.tea_leaf_'. The '3421.11 !\$omp do @tea_leaf_cg' node is highlighted.
- Source code (Right):** Displays the Fortran source code for the 'tea_leaf_kernel_solve_cg_fortran_calc' subroutine. The 'Source' tab is selected, and the code is shown with line numbers from 170 to 204. A blue callout box points to the 'Source' tab with the text '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

The screenshot displays the CubeGUI-4.4.3 interface. The 'Help' menu is open, with 'What's This?' selected. A blue callout box points to this menu item, containing the text: 'Context-sensitive help available for all GUI items'. The main window shows a 'Metric tree' on the left, a central 'Flat view' of the metric hierarchy, and a 'System tree' on the right. The 'Flat view' shows a tree of metrics, with '39.63 !\$omp do @tea_leaf_cg.f90:187' selected. The 'System tree' shows a hierarchy of nodes and MPI ranks. At the bottom, there are three progress bars and a status bar that reads 'Change into help mode for display components'.

File Display Plugins Help

Restore Setting Sa

Absolute

Metric tree

1.17e8 Visits (

8633.39 Time

0.00 Minimum

97.11 Maximum

0 bytes_put (b

0 bytes_get (b

0 ALLOCAT

0 DEAL

0 IN_SIZE (bytes)

0 h

0 num_heap_memory_allocated

0 bytes_sent (bytes)

0 bytes_received (bytes)

Getting started

User Guide

Mouse and keyboard control

What's This? Shift+F1

About

Plugin Info

Plugin Documentation

Selected metrics description

Selected regions description

tea_leaf_baseline

0 MAIN_

0.09 tea_module.tea_init_comms

0.00 !\$omp parallel @tea_leaf.f90:45

0.04 initialise_

0.00 diffuse_

0.00 timer_

0.00 set_field_module.set_field_

0.00 timestep_module.timestep_

0.01 tea_leaf_module.tea_leaf_

0.00 timer_

1.33 update_halo_module.update_halo_

0.07 tea_leaf_kernel_cg_module.tea_leaf_kernel_init_cg_

0.24 tea_module.tea_allsum_

0.01 tea_leaf_kernel_cheby_module.tea_leaf_kernel_ch_

0.01 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_

0.02 !\$omp parallel @tea_leaf_cg.f90:186

39.63 !\$omp do @tea_leaf_cg.f90:187

0.07 !\$omp implicit barrier @tea_leaf_cg.f90:19

0.03 !\$omp implicit barrier @tea_leaf_cg.f90:200

0.03 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_

0.02 !\$omp parallel @tea_leaf_cg.f90:234

39.41 !\$omp do @tea_leaf_cg.f90:247

0.07 !\$omp implicit barrier @tea_leaf_cg.f90:25

0.03 !\$omp implicit barrier @tea_leaf_cg.f90:257

0.02 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_

Peer percent

System tree

Statistics

Su

System View

Other

0.00 machine Linux

0.00 node jrc1531

0.00 MPI Rank 0

98.13 Master thread

98.07 OMP thread 1

98.10 OMP thread 2

98.11 OMP thread 3

98.09 OMP thread 4

98.10 OMP thread 5

98.09 OMP thread 6

98.11 OMP thread 7

98.10 OMP thread 8

98.10 OMP thread 9

98.10 OMP thread 10

98.13 OMP thread 11

98.96 MPI Rank 1

0.00 node jrc1532

98.93 MPI Rank 2

99.88 MPI Rank 3

0.00 node jrc1533

97.89 MPI Rank 4

99.71 MPI Rank 5

0.00 node jrc1534

99.29 MPI Rank 6

100.00 MPI Rank 7

All (96 elements)

0.00 8633.39 (100.00%) 8633.39

0.00 3421.11 (39.63%) 100.00

0.00 0.00 (0.00%) 3421.11

Change into help mode for display components

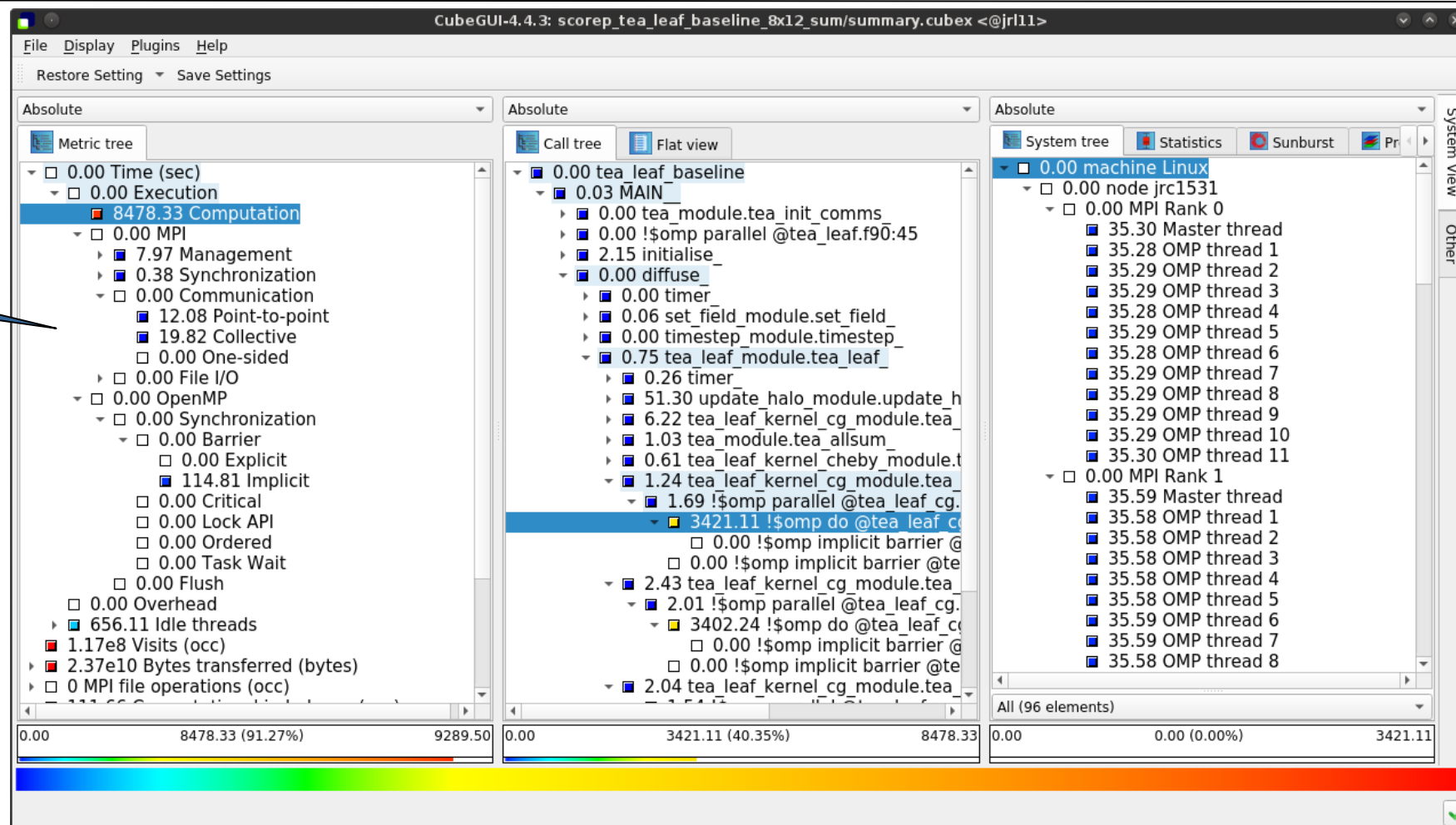
Scalasca report post-processing

- 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

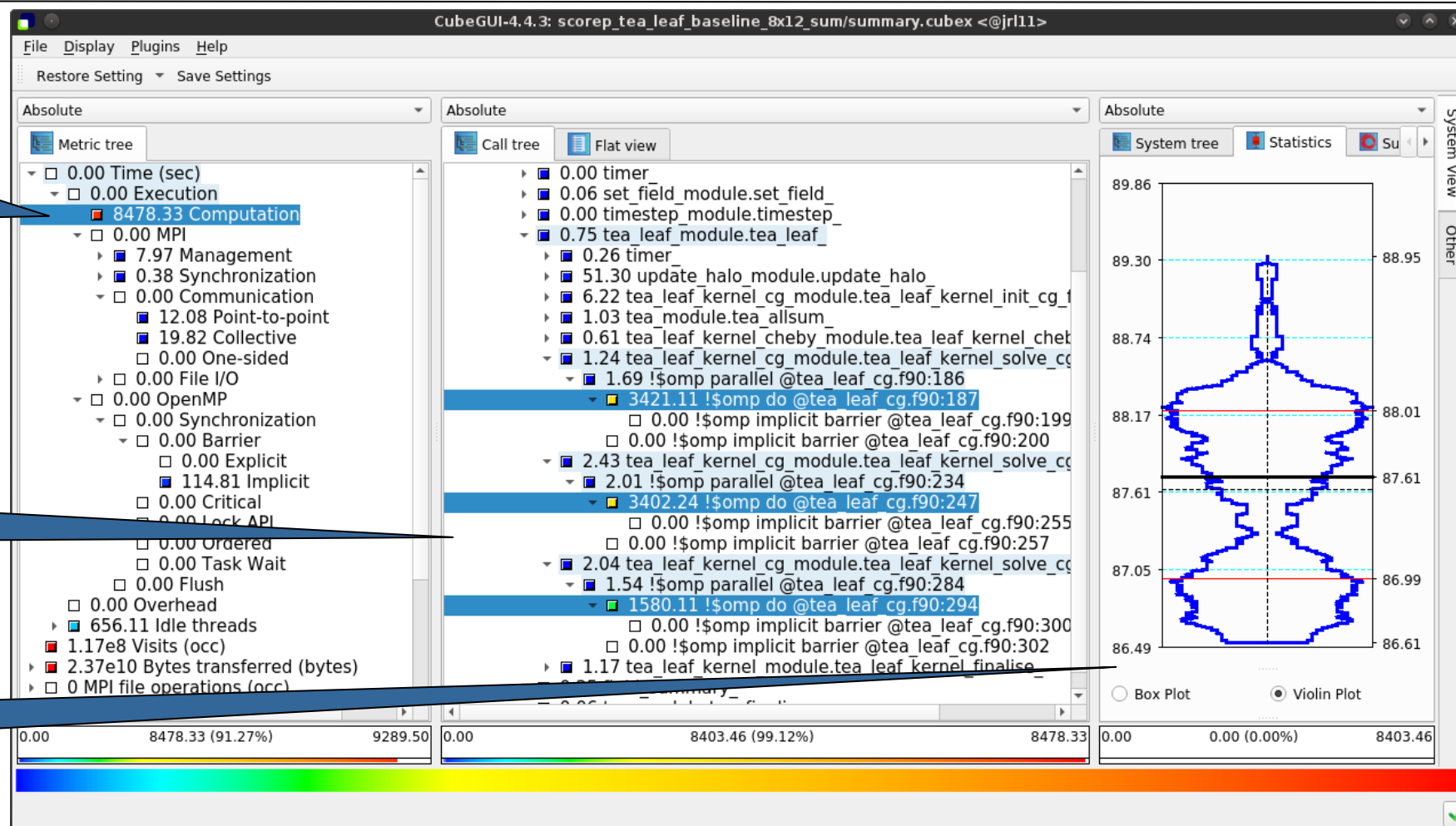


TeaLeaf summary report analysis (I)

91% of the execution time is computation...

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

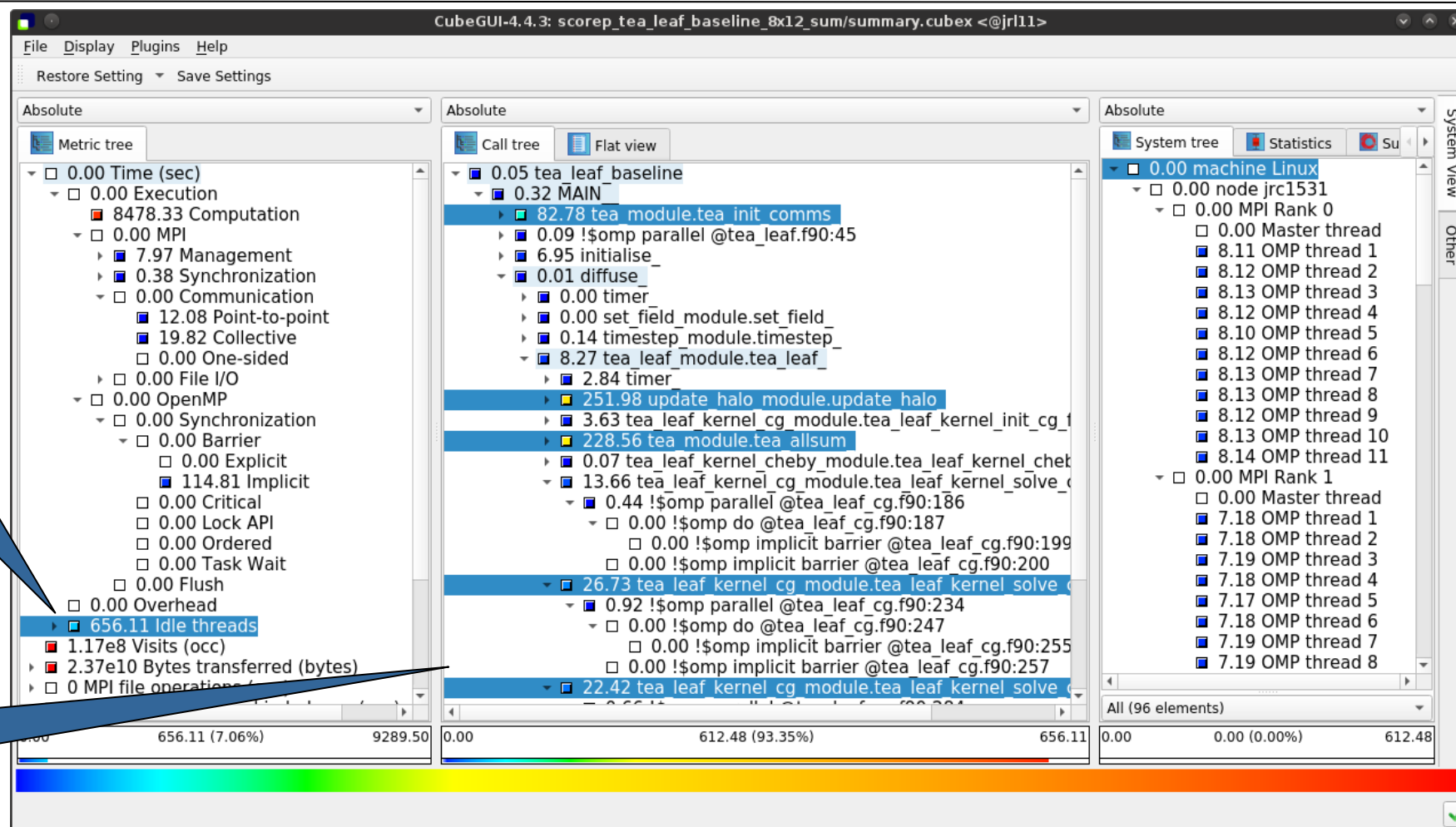
...with a slight imbalance across ranks & threads



TeaLeaf summary report analysis (II)

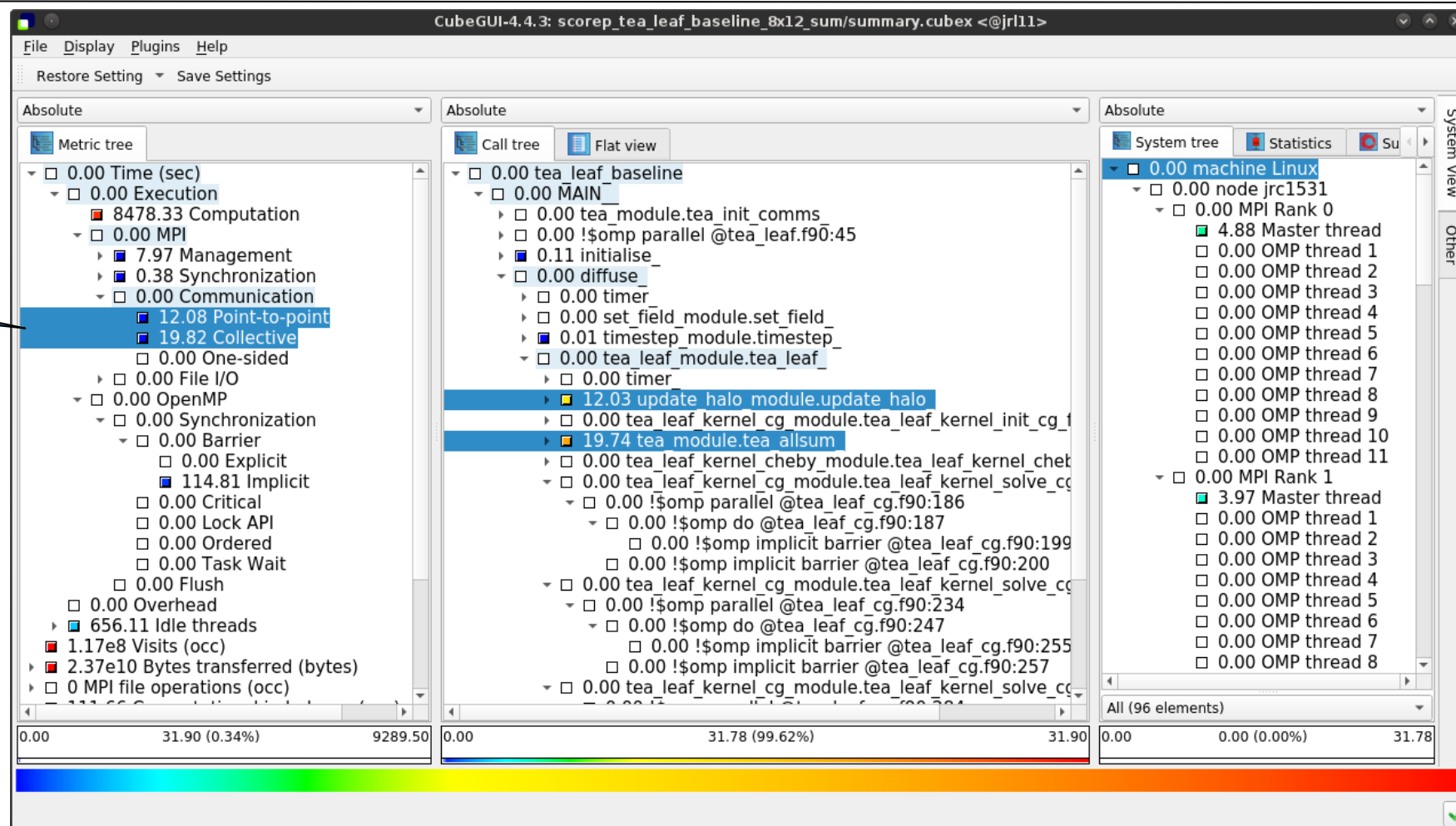
7% of the total CPU execution time is due due to "idle threads"...

... when not within OpenMP-parallelized code regions



TeaLeaf summary report analysis (III)

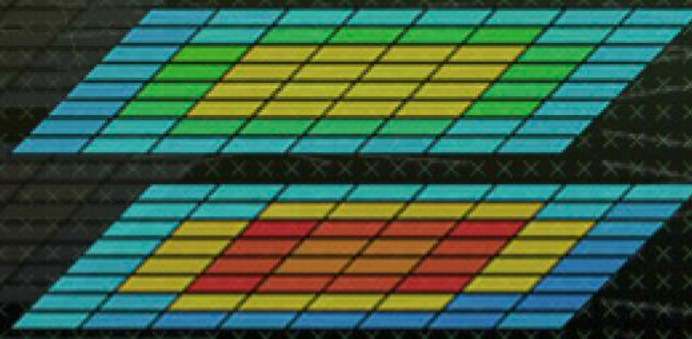
MPI communication time is negligible (0.34%); but communication is only on the master threads (MPI_THREAD_FUNNELED)



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](mailto:scalasca@fz-juelich.de)

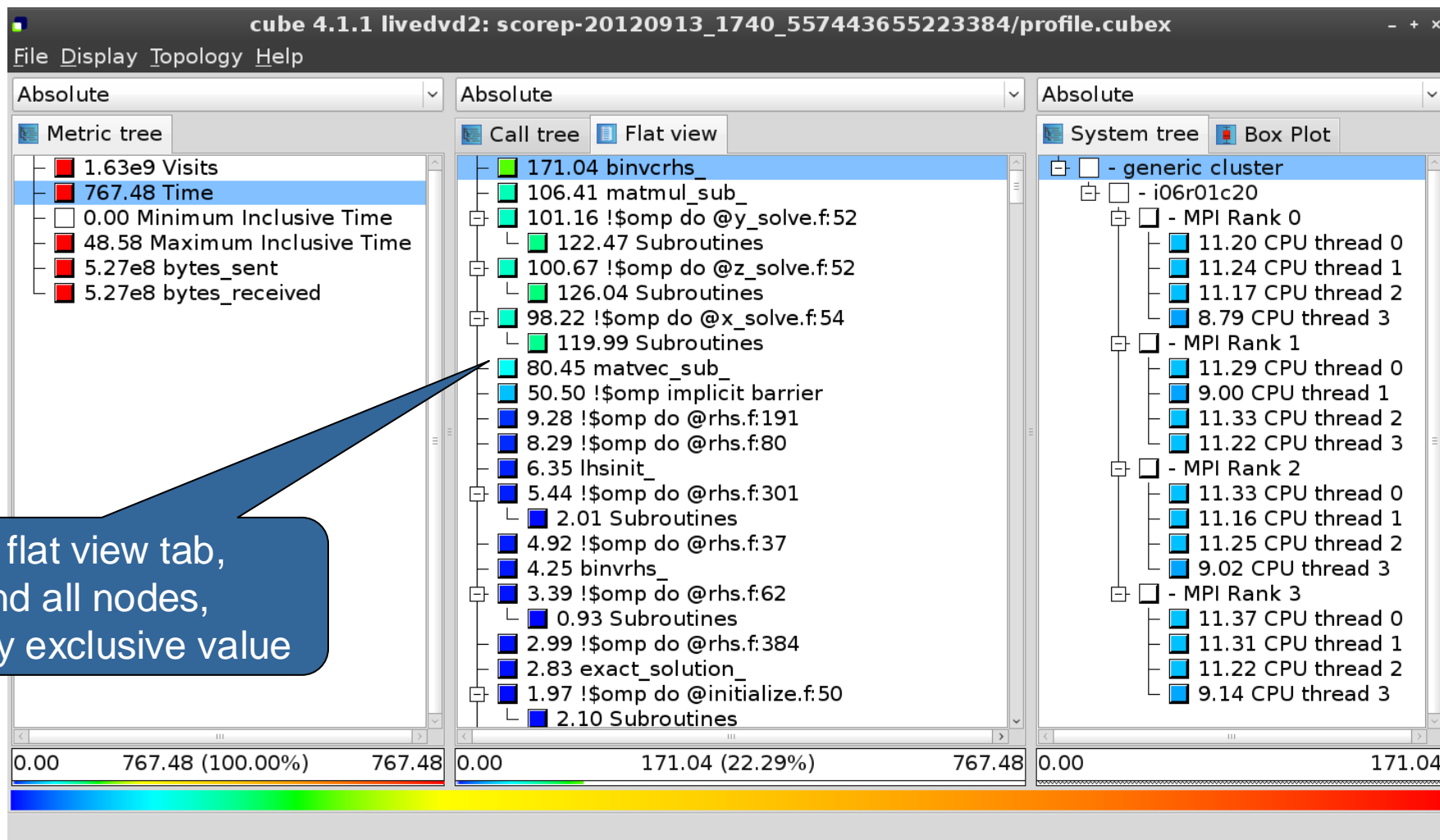




Reference material



Flat profile view



Select flat view tab,
expand all nodes,
and sort by exclusive value

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)

Derived metrics in Cube GUI



Collection of derived metrics

Parameters of the derived metric

CubePL expression

The screenshot shows the Cube GUI interface with a dialog box for creating a new derived metric. The dialog is titled "Create new metric as a child of metric". It features several input fields and a description area. The "Select metric from collection" dropdown is set to "Average execution time (kenobi)". The "Derived metric type" is "Postderived metric". The "Display name" is "Average visit time", the "Unique name" is "avg_visit_time", the "Data type" is "DOUBLE", and the "Unit of measurement" is "sec". The "Description" field contains the text: "Calculates average time of region execution per visit. Autor is Michael Knobloch." Below the description, there are radio buttons for "Calculation", "Calculation Init", "Aggregation '*'", and "Aggregation '**'", with "Calculation" selected. The "Calculation" section contains the CubePL expression: `metric::time()/metric::visits(e)`. At the bottom of the dialog, there are "Create metric" and "Cancel" buttons, and a link to "Share this metric with SCALASCA group".

Example: FLOPS based on PAPI_FP_OPS and time



Cube-4.3.1: scorep_8x4_sum/profile.cubex (on froggy1)

File Display Plugins Help
Restore Setting Save Settings

Edit metric FLOPS (on froggy1)

Select metric from collection: --- please select ---

Derived metric type: Postderived metric

Display name: FLOPS

Unique name: flops

Data type: DOUBLE

Unit of measurement:

URL:

Description:

Calculation Calculation Init Aggregation "+" Aggregation "-"

`metric::PAPI_FP_OPS()/metric::time()`

Edit metric Cancel

Share this metric with SCALASCA group

Absolute

Metric tree

- 1.17e7 Visits (occ)
- 1148.49 Time (sec)
- 0.00 Minimum Inclusive Time (sec)
- 41.57 Maximum Inclusive Time (...)
- 0 bytes_put (bytes)
- 0 bytes_get (bytes)
- 5.75e12 PAPI_TOT_INS (#)
- 2.69e12 PAPI_TOT_CYC (#)
- 2.12e12 PAPI_FP_OPS (#)
- 3.12e9 bytes_sent (bytes)
- 3.12e9 bytes_received (bytes)
- 1.84e9 FLOPS**

Absolute

Call tree Flat view

- 3.17e5 MAIN_
 - 7.04e5 mpi_setup_
 - 6.34e4 MPI_Bcast
 - 2.05e5 env_setup_
 - 7.39e5 zone_setup_
 - 9.31e5 map_zones_
 - 9.39e4 zone_starts_
 - 6.16e5 set_constants_
 - 5.91e8 initialize_
 - 0.00 exact_rhs_
 - 145.62 !\$omp parallel @exac...
 - 2.54e4 !\$omp do @exact_r...
 - 9.65e8 !\$omp do @exact_r...**
 - 9.62e8 !\$omp do @exact_r...
 - 8.14e8 !\$omp do @exact_r...
 - 1.21e5 !\$omp do @exact_r...
 - 0.00 !\$omp implicit barrier...
 - 6.23e4 exch_qbc_
 - 1.94e9 adi_
 - 2.19e5 MPI_Barrier
 - 1.92e9 <<bt_iter>> (200 itera...
 - 1.98e8 verify_
 - 1.05e5 MPI_Reduce

Absolute

System tree Barplot Heatmap

 - machine Linux
 - node frog6
 - MPI Rank 0
 - 1.17e9 Master thread
 - 9.43e8 OMP thread 1
 - 9.47e8 OMP thread 2
 - 9.47e8 OMP thread 3
 - MPI Rank 1
 - 1.17e9 Master thread
 - 9.87e8 OMP thread 1
 - 9.68e8 OMP thread 2
 - 9.72e8 OMP thread 3
 - MPI Rank 2
 - 1.10e9 Master thread
 - 8.97e8 OMP thread 1
 - 8.77e8 OMP thread 2
 - 8.76e8 OMP thread 3
 - MPI Rank 3
 - 1.09e9 Master thread
 - 9.06e8 OMP thread 1
 - 9.04e8 OMP thread 2
 - 9.02e8 OMP thread 3

All (32 elements)

0.00 1.84e9 (100.00%) 1.84e9 0.00 9.65e8 (-0.00%) -12858016489314434.00 0.00... -179769313486231570814527423731704356798070...

Selected "\$!omp do @exact_rhs.f:46"

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

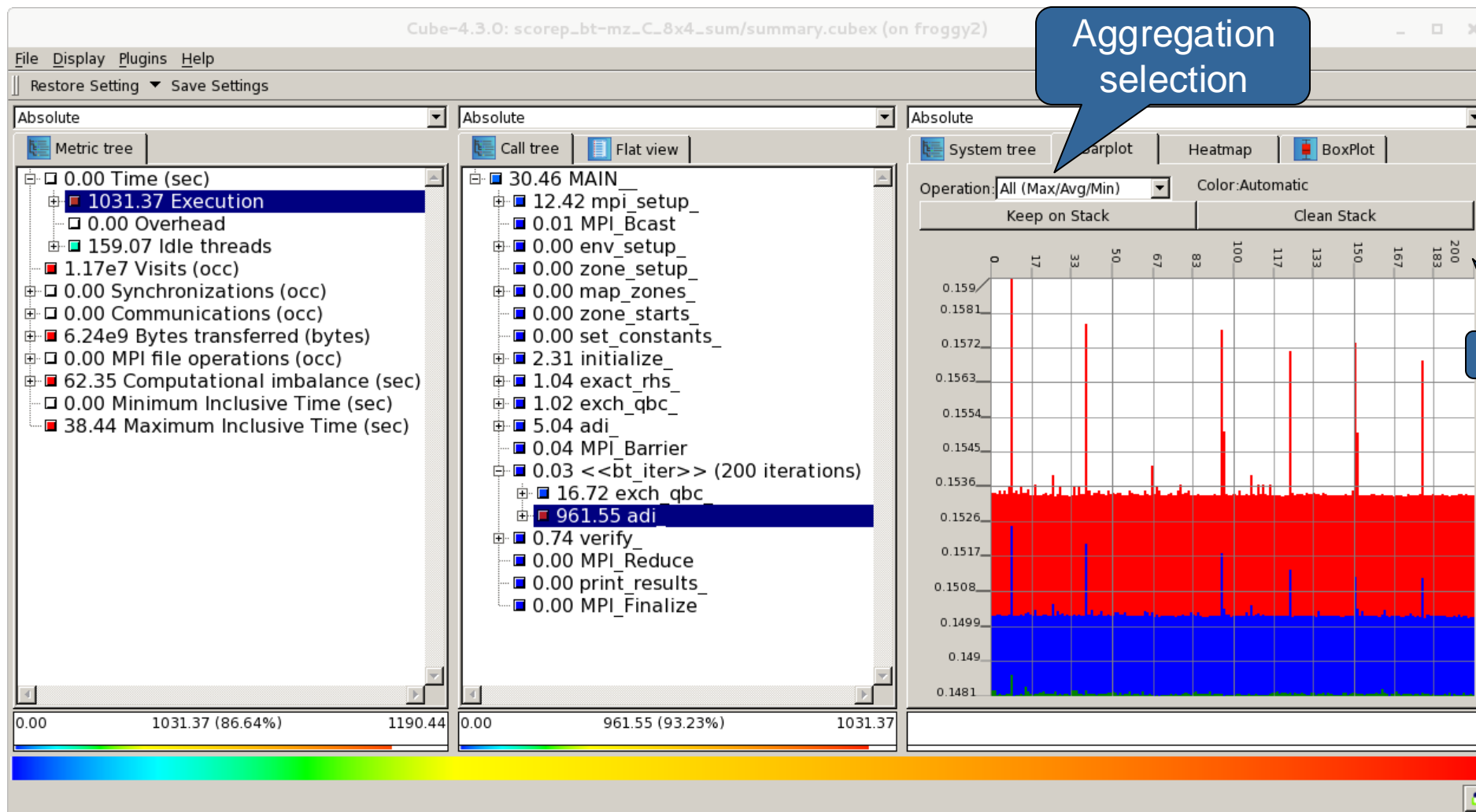


- Show time dependent behavior by “unrolling” iterations
- Preparations:
 - Mark loop body by using Score-P instrumentation API in your source code

```
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

