

Analysis report examination with Cube

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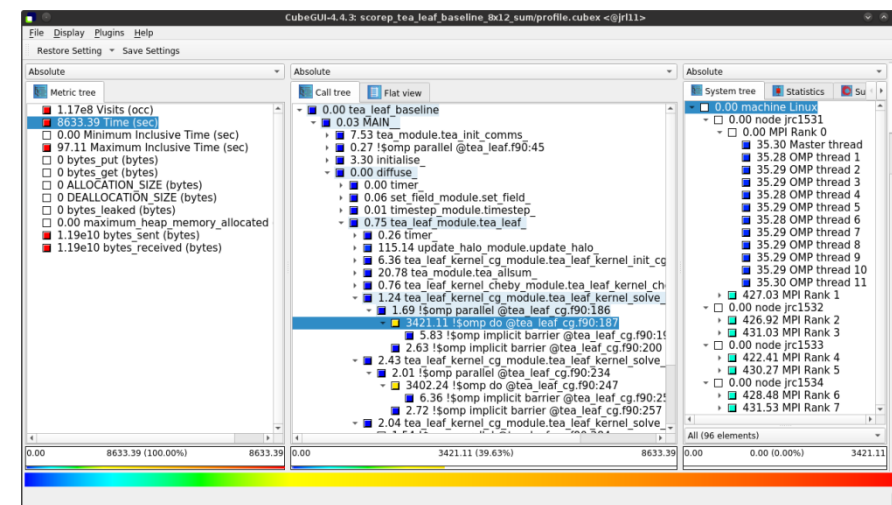


Cube

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 – Usage via Local Client

mailto: scalasca@fz-juelich.de

▪ Local Client Options:

- User installation from tarball
- **Running binary:**
 - win32 binary, Mac OS .dmg, Linux binary .AppImage
 - Example for the AppImage:

```
desk$ wget https://apps.fz-juelich.de/scalasca/releases/cube/4.9/dist/CubeGui-4.9.1.AppImage

desk$ chmod u+x CubeGui-4.9.1.AppImage
desk$ ./CubeGui-4.9.1.AppImage
```

- Available in Fedora distribution

▪ Accessing Cube files

- copy .cubex file (or entire scorep directory) to desktop from remote system via scp
- **locally mount remote filesystem via sshfs**

```
desk$ mkdir $HOME/mnt
desk$ sshfs <user>@glogin-p3.hpc.gwdg.de:/scratch/lustre-grete/projects/tr_20260831-vi-hps-tuning /$HOME/mnt
```

- Running a `cube_server` on the remote system and connect to it

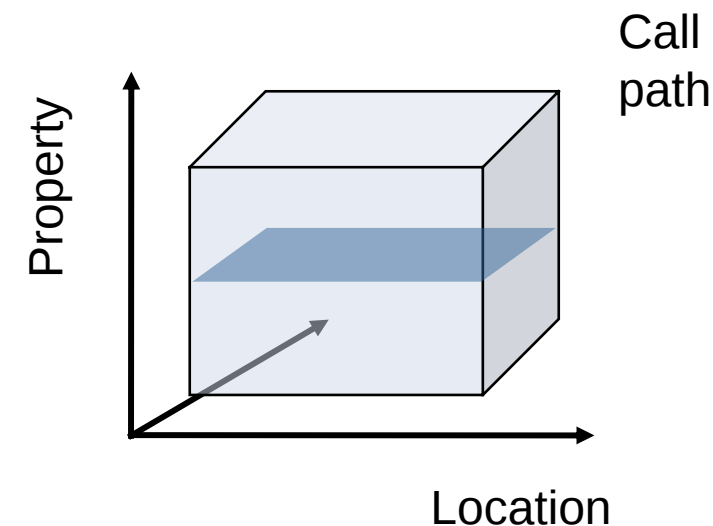
```
desk$ ssh -L 3300:localhost:3300 <user>@glogin-p3.hpc.gwdg.de
login$ module load cubelib/4.9.1
login$ cube_server
```

All download options:

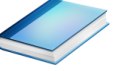
<https://www.scalasca.org/scalasca/software/cube-4.x/download.html>

Analysis presentation and exploration

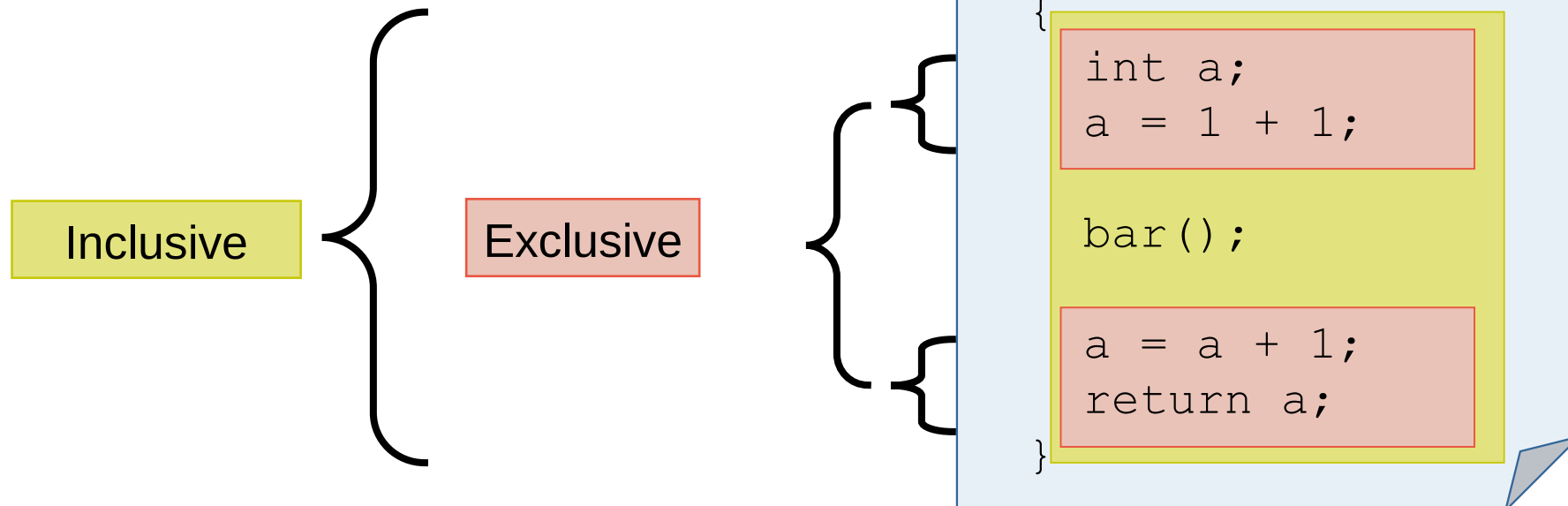
- Representation of values (severity matrix) on three hierarchical axes
 - Performance property (metric)
 - Call path (program location)
 - System location (process/thread)
- Three coupled tree browsers
- Cube displays severities
 - As *value*: for precise comparison
 - As *colour*: for easy identification 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



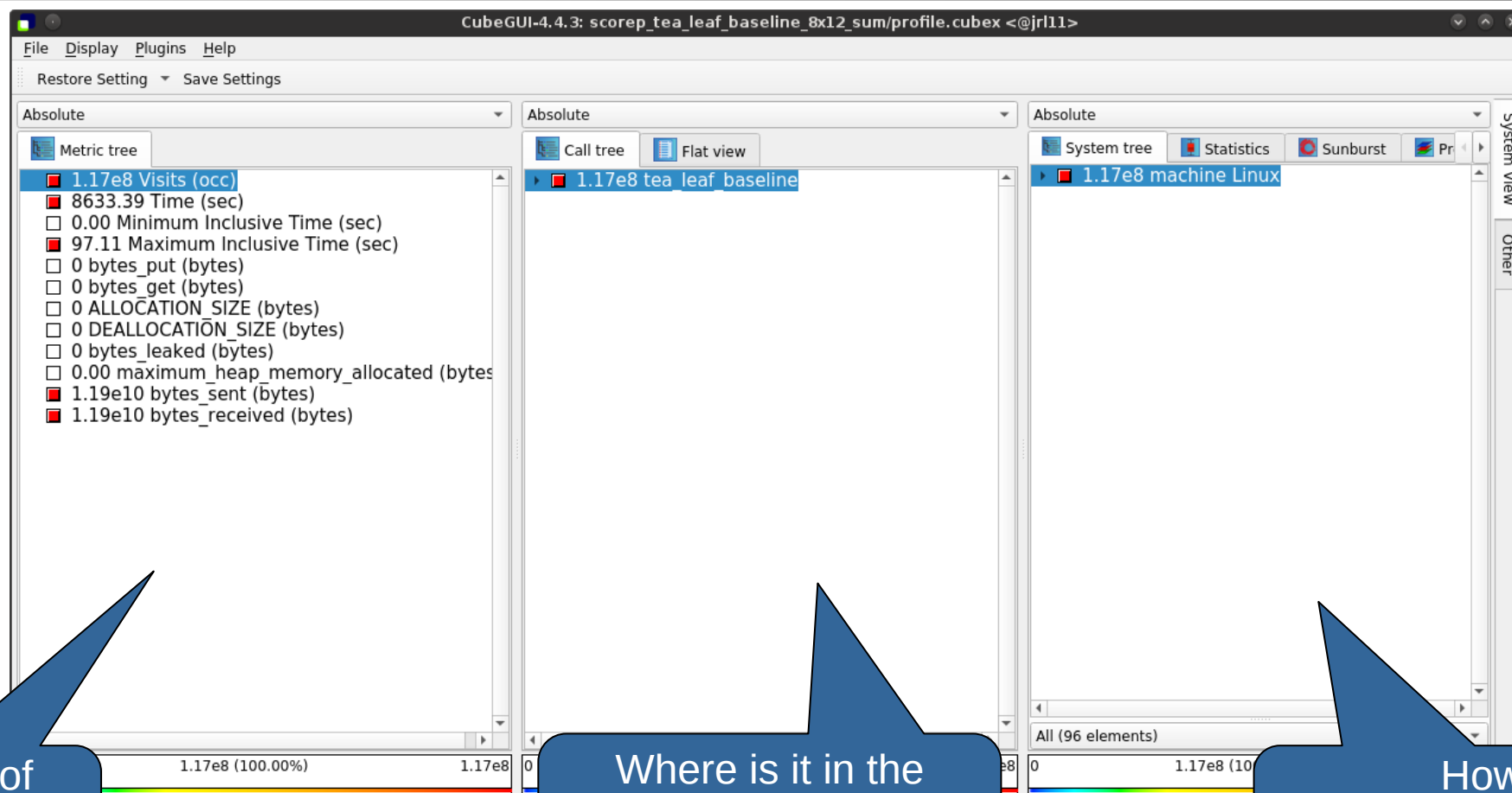
Case study: TeaLeaf

- 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)

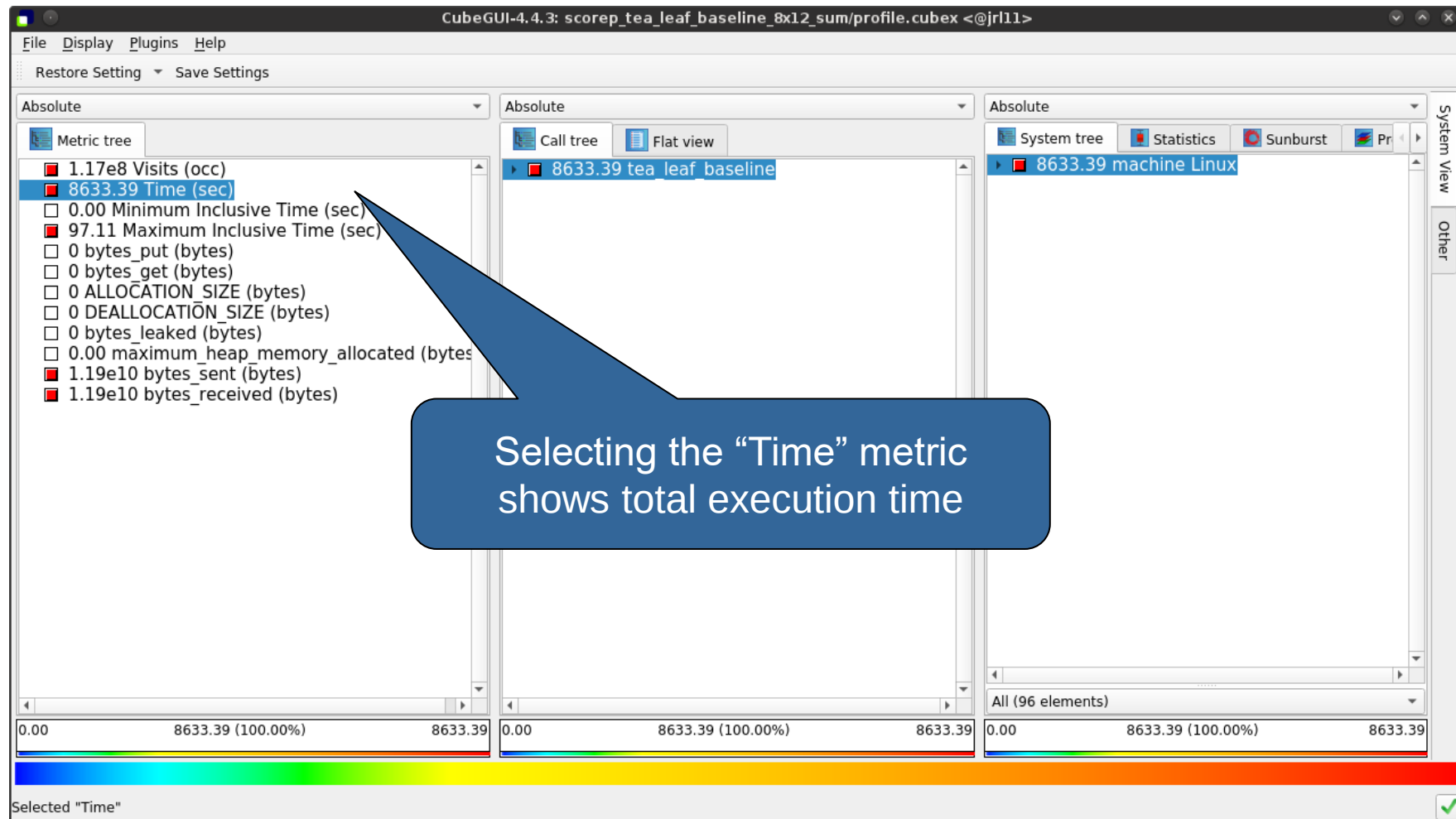


What kind of performance metric?

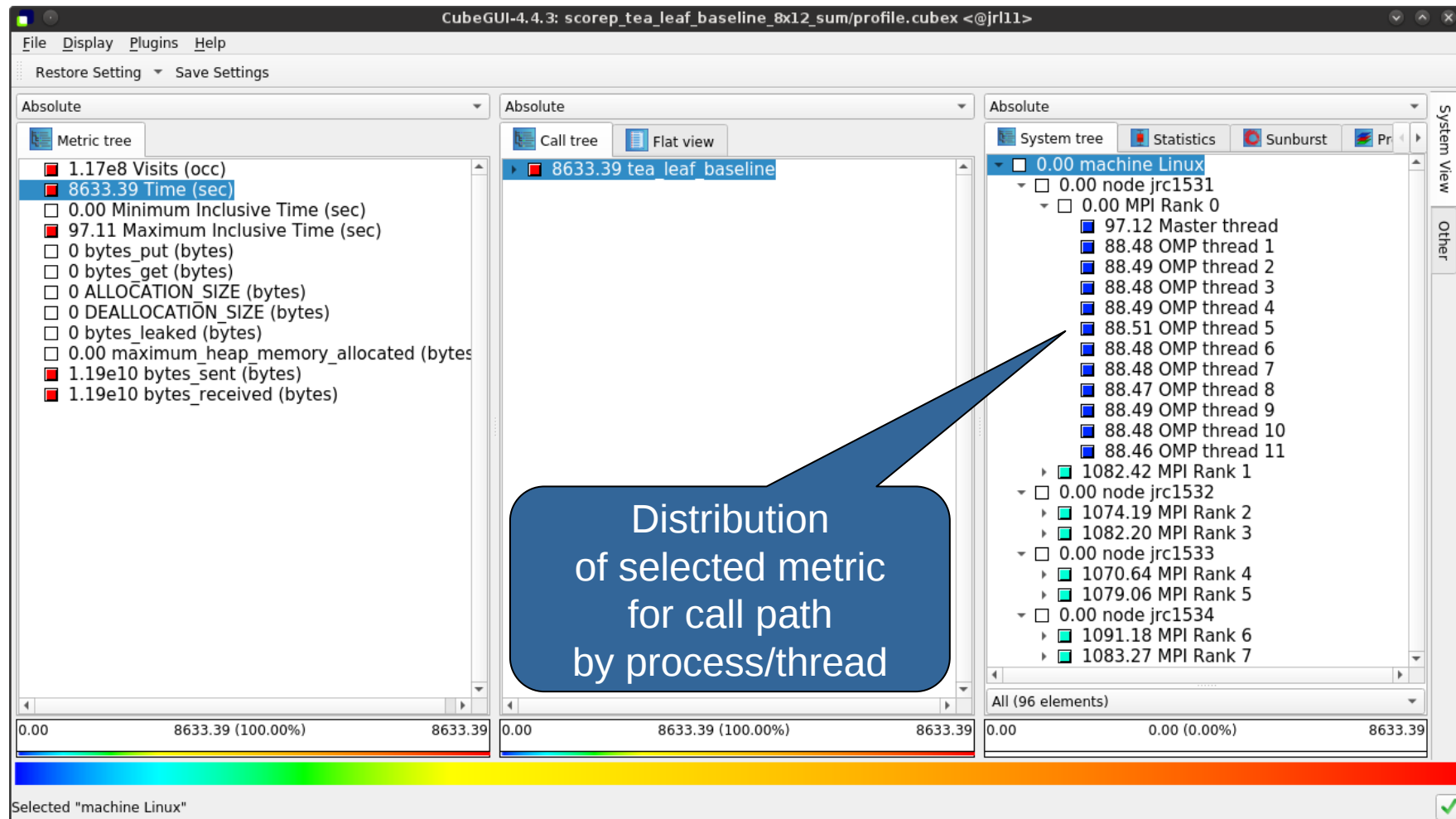
Where is it in the source code?
In what context?

How is it distributed across the processes/threads?

Metric selection

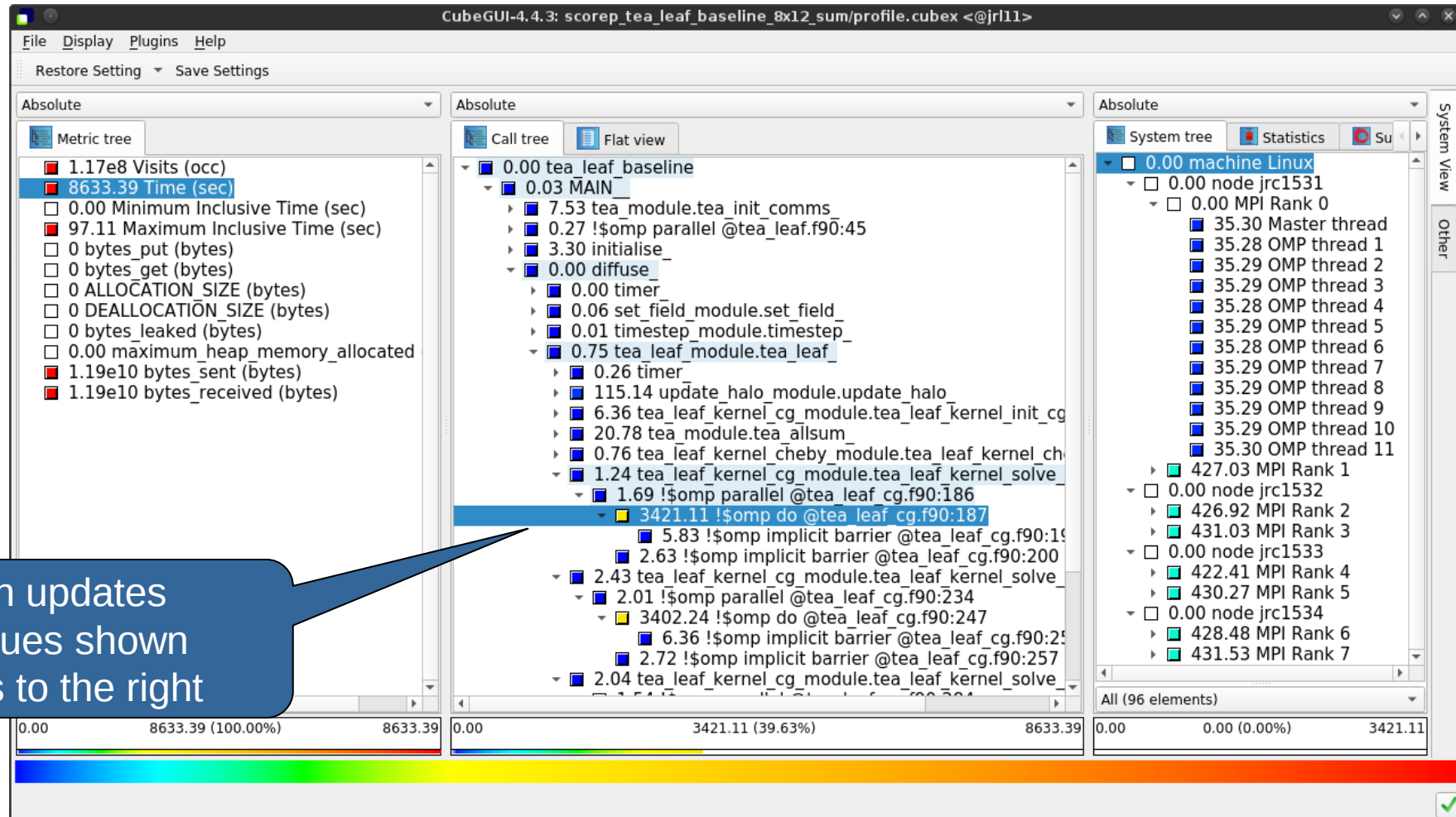


Expanding the system tree



Ready

Selecting a call path



Multiple selection

The screenshot displays the CubeGUI-4.4.3 interface with the title bar "CubeGUI-4.4.3: scorep_tea_leaf_baseline_8x12_sum/profile.cubex <@jrl11>". The interface is divided into three main panels: "Metric tree" on the left, "Call tree" in the center, and "System tree" on the right. The "Metric tree" panel shows a list of metrics, with "8633.39 Time (sec)" highlighted. The "Call tree" panel shows a hierarchical view of the program's execution, with several nodes selected. A blue callout bubble points to the selected nodes in the "Call tree" panel, containing the text "Select multiple nodes with Ctrl-click". The "System tree" panel shows a hierarchical view of the system's components, with "0.00 machine Linux" selected. The bottom of the interface features a progress bar and a status bar.

File Display Plugins Help

Restore Setting Save Settings

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
- 1.19e10 bytes_sent (bytes)
- 1.19e10 bytes_received (bytes)

Absolute

Call tree Flat view

- 0.00 timer
- 0.06 set_field_module.set_field_
- 0.01 timestep_module.timestep_
- 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
- 5.83 !\$omp implicit barrier @tea_leaf_cg.f90:19
- 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
- 6.36 !\$omp implicit barrier @tea_leaf_cg.f90:25
- 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.f90:3
- 3.24 !\$omp implicit barrier @tea_leaf_cg.f90:302
- 1.37 tea_leaf_kernel_module.tea_leaf_kernel_finalise
- 0.25 field_summary_

Absolute

System tree Statistics Su

- 0.00 machine Linux
- 0.00 node jrc1531
- 0.00 MPI Rank 0
- 86.98 Master thread
- 86.62 OMP thread 1
- 86.62 OMP thread 2
- 87.04 OMP thread 3
- 86.83 OMP thread 4
- 86.61 OMP thread 5
- 86.74 OMP thread 6
- 86.65 OMP thread 7
- 86.65 OMP thread 8
- 86.90 OMP thread 9
- 86.84 OMP thread 10
- 86.90 OMP thread 11
- 1054.35 MPI Rank 1
- 0.00 node jrc1532
- 1044.42 MPI Rank 2
- 1053.24 MPI Rank 3
- 0.00 node jrc1533
- 1042.13 MPI Rank 4
- 1051.65 MPI Rank 5
- 0.00 node jrc1534
- 1060.86 MPI Rank 6
- 1055.43 MPI Rank 7

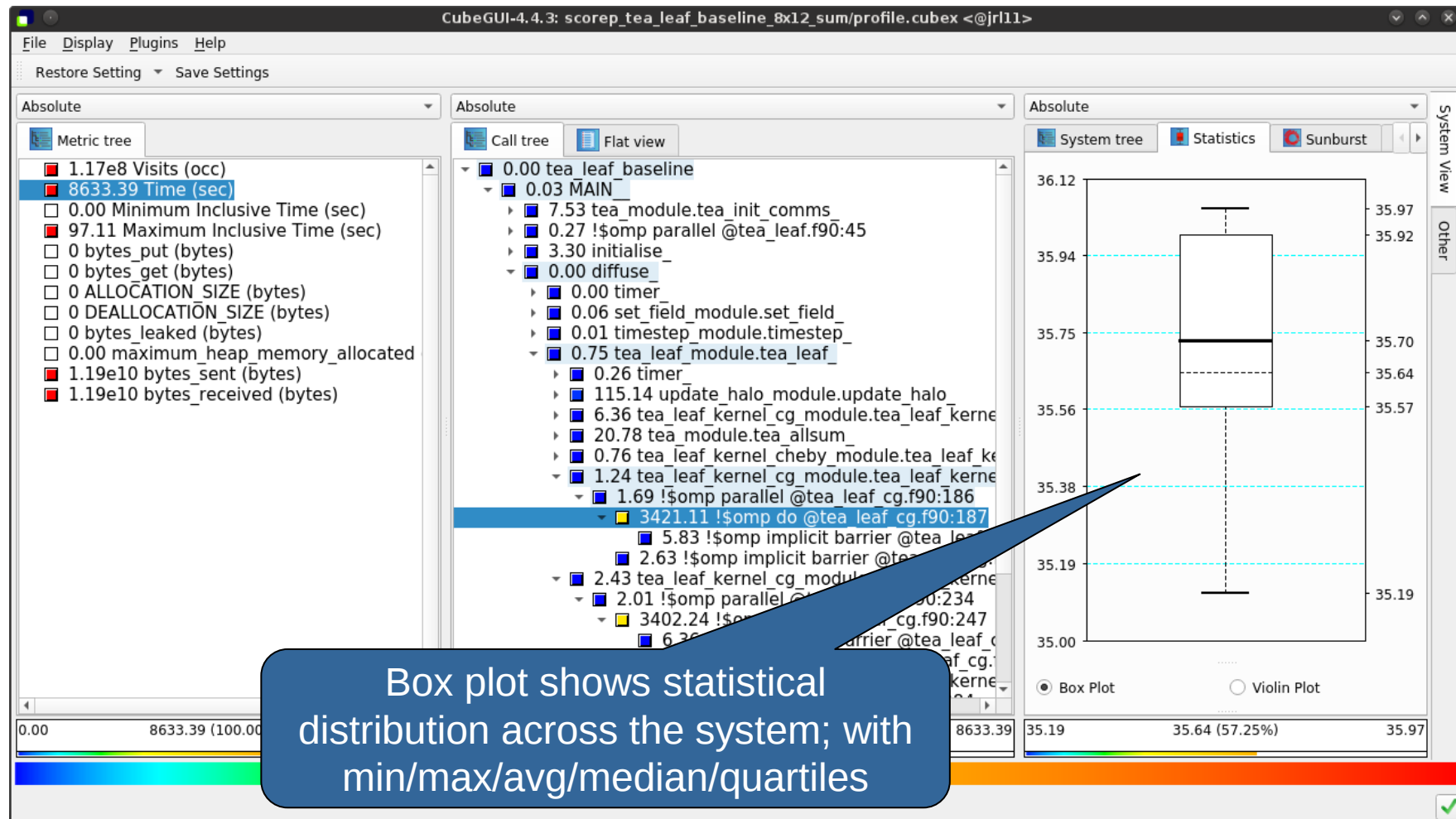
System View other

All (96 elements)

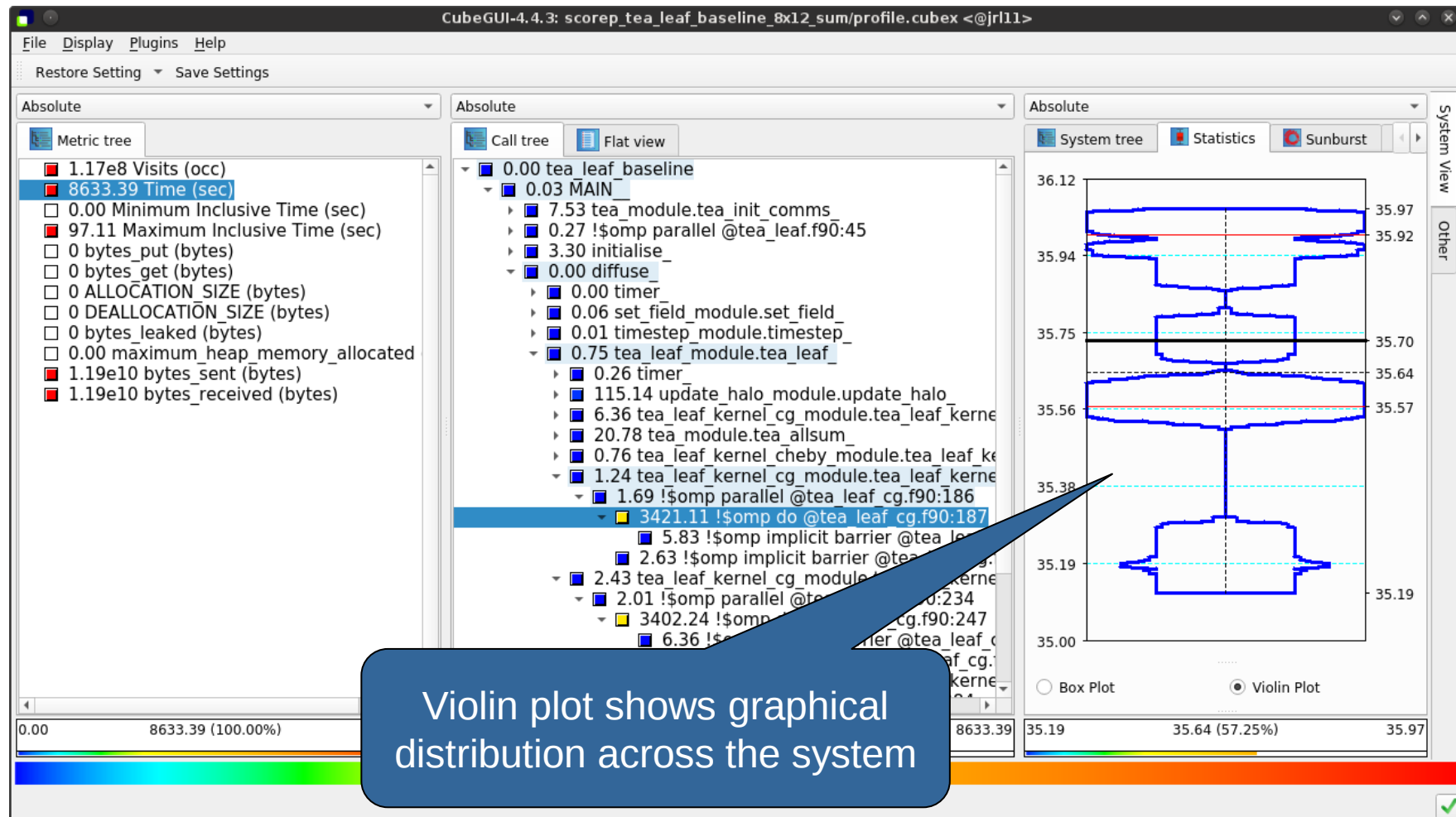
0.00 8633.39 (100.00%) 8633.39 0.00 8403.46 (97.34%) 8633.39 0.00 0.00 (0.00%) 8403.46

Select multiple nodes with Ctrl-click

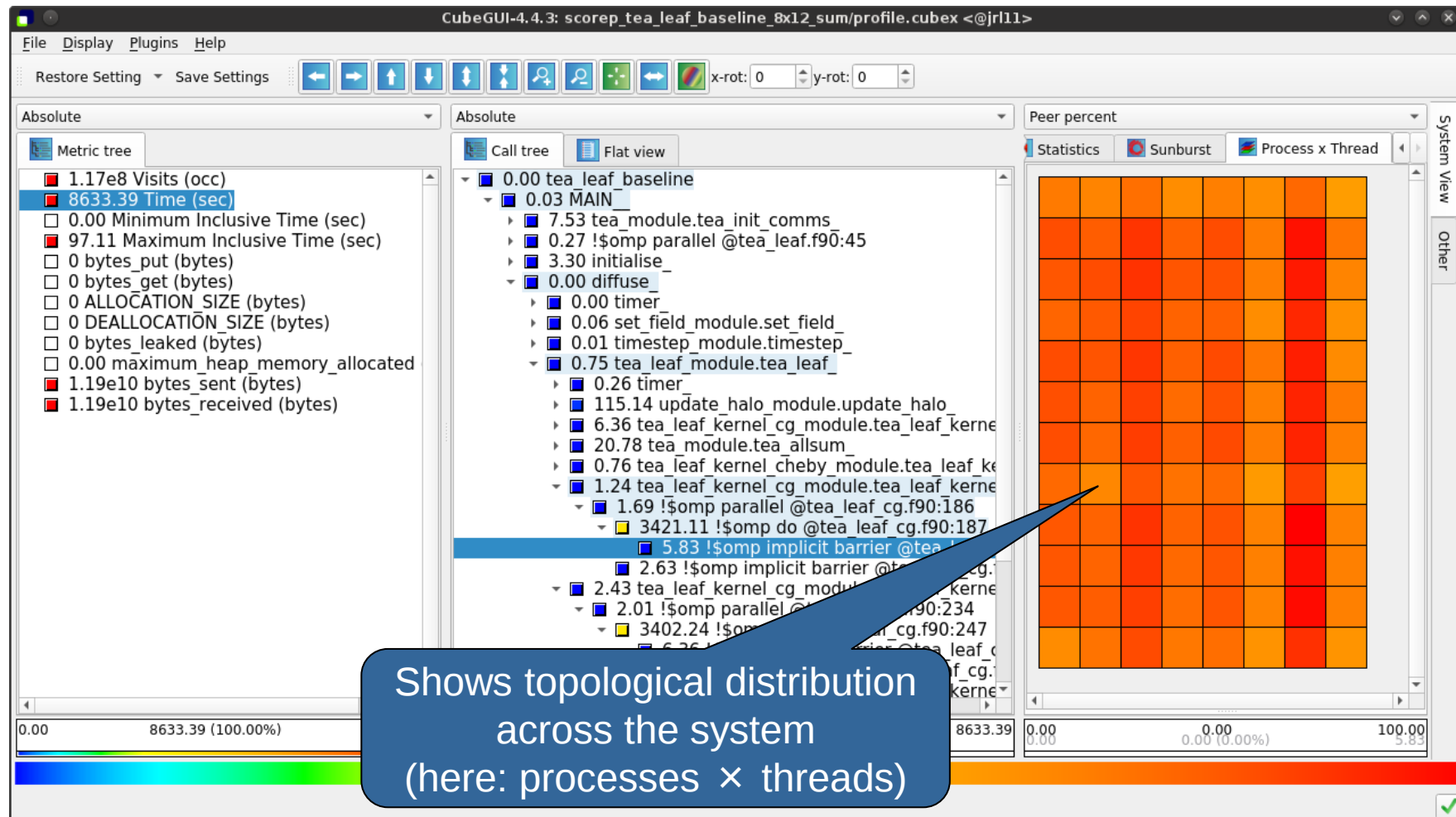
Box plot view



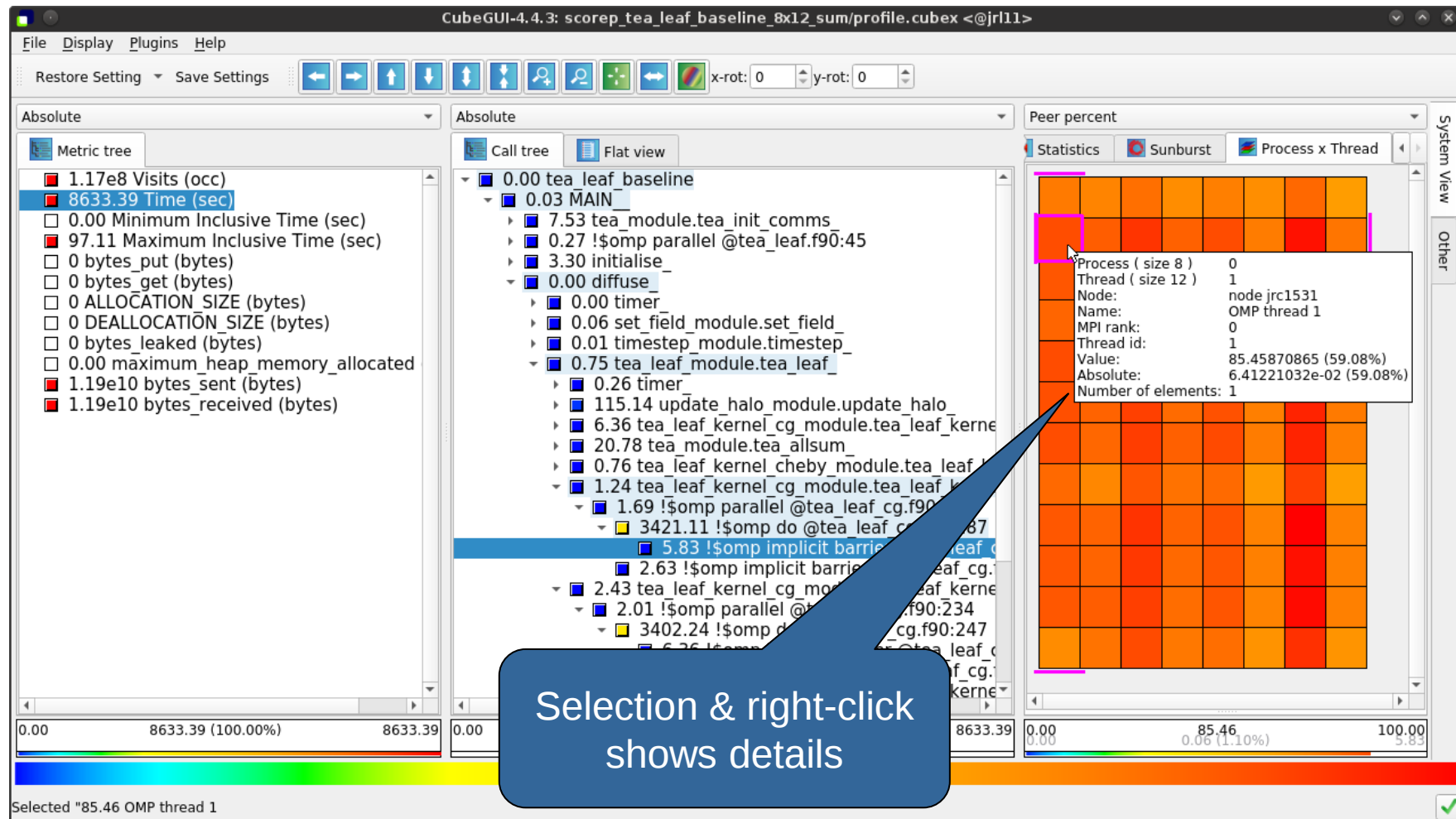
Violin plot view



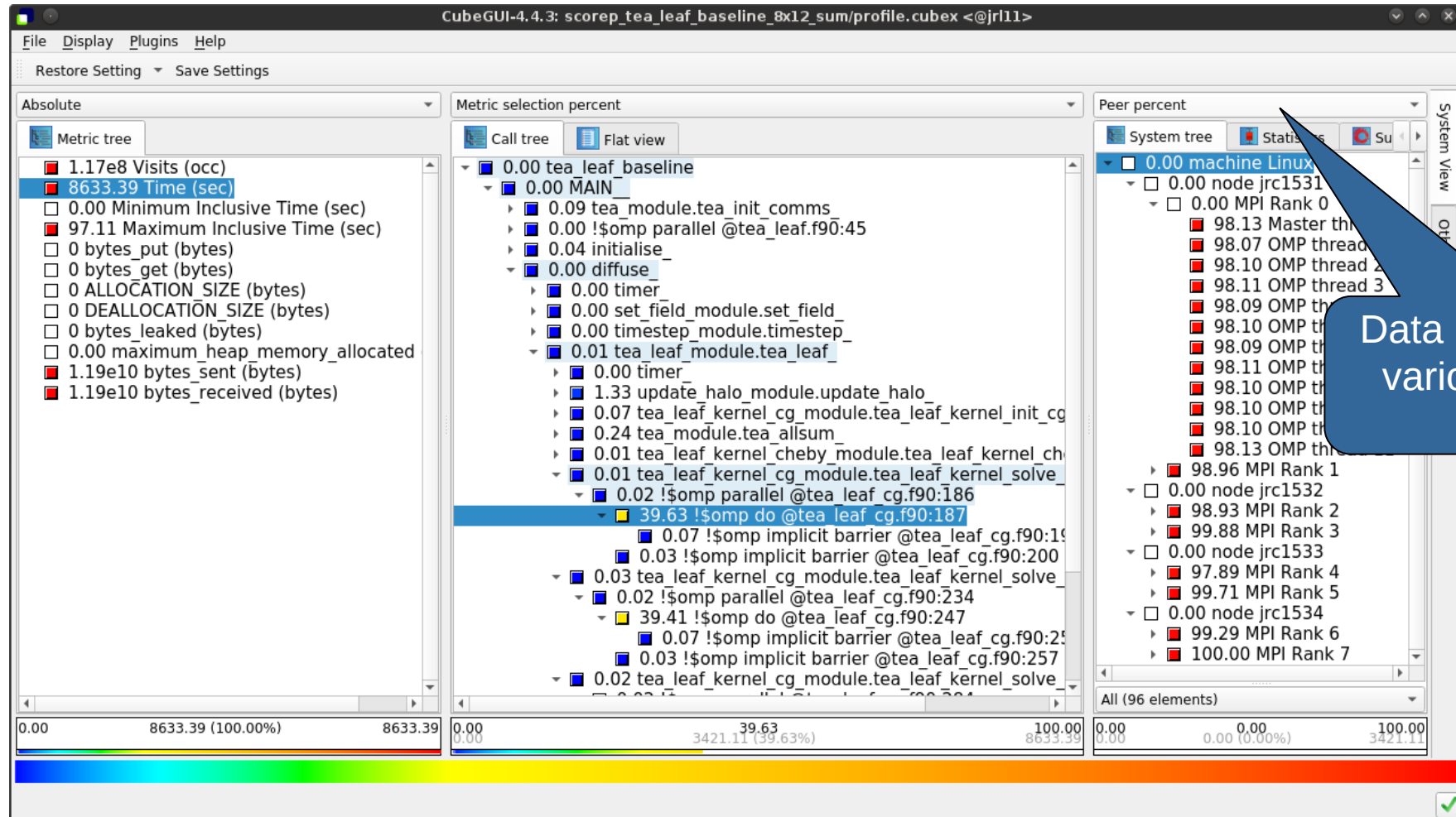
Topology view



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

The screenshot displays the CubeGUI-4.4.3 interface with three main panels: Metric tree, Call tree, and System tree. The Call tree panel is active, showing a hierarchical view of the execution. A right-click context menu is open over the selected item `3421.11 !$omp do @tea_leaf_cg.f90:186`. 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 points to the context menu with the text "Right-click opens context menu".

Right-click opens context menu

Shows a short description of the clicked item

Source-code view

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

File Display Plugins Help

Restore Setting Save Settings

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
- 1.19e10 bytes_sent (bytes)
- 1.19e10 bytes_received (bytes)

Absolute

Call tree Flat view

- 0.00 tea_leaf_baseline
 - 0.03 MAIN
 - 7.53 tea_module.tea_init_comms
 - 0.27 !\$omp parallel @tea_leaf.f90:45
 - 3.30 initialise
 - 0.00 diffuse
 - 0.00 timer
 - 0.06 set_field_module.set_field
 - 0.01 timestep_module.timestep
 - 0.75 tea_leaf_module.tea_leaf
 - 0.26 timer
 - 115.14 update_halo_module.update_h
 - 6.36 tea_leaf_kernel_cg_module.tea_le
 - 20.78 tea_module.tea_allsum
 - 0.76 tea_leaf_kernel_cheby_module.te
 - 1.24 tea_leaf_kernel_cg_module.tea_le
 - 1.69 !\$omp parallel @tea_leaf_cg.f90
 - 3421.11 !\$omp do @tea_leaf_cg.f90
 - 5.83 !\$omp implicit barrier @tea
 - 2.63 !\$omp implicit barrier @tea
 - 2.43 tea_leaf_kernel_cg_module.tea_le
 - 2.01 !\$omp parallel @tea_leaf_cg.f90
 - 3402.24 !\$omp do @tea_leaf_cg.f90
 - 6.36 !\$omp implicit barrier @tea
 - 2.72 !\$omp implicit barrier @tea
 - 2.04 tea_leaf_kernel_cg_module.tea_le

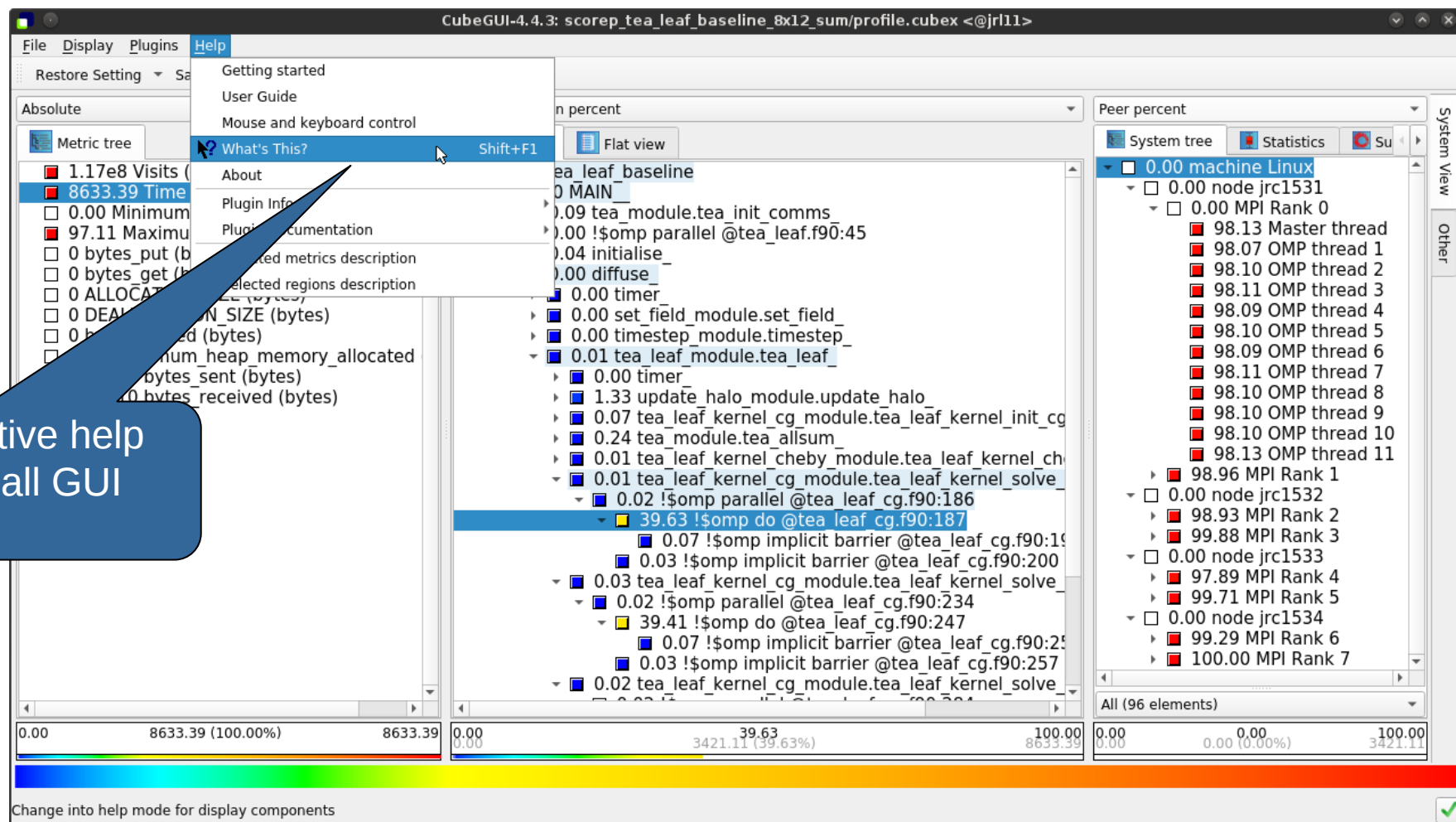
Score-P Configuration Source Info

```
170
171 IMPLICIT NONE
172
173 INTEGER(KIND=4):: x_min,x_max,y_min,y_max
174 REAL(KIND=8), DIMENSION(x_min-2:x_max+2,y_min-2:y
175 REAL(KIND=8), DIMENSION(x_min-2:x_max+2,y_min-2:y
176 REAL(KIND=8), DIMENSION(x_min-2:x_max+2,y_min-2:y
177 REAL(KIND=8), DIMENSION(x_min-2:x_max+2,y_min-2:y
178
179 REAL(KIND=8) :: rx, ry
180
181 INTEGER(KIND=4) :: j,k,n
182 REAL(kind=8) :: pw
183
184 pw = 0.0_08
185
186 !$OMP PARALLEL
187 !$OMP DO REDUCTION(+:pw)
188 DO k=y_min,y_max
189 DO j=x_min,x_max
190 w(j,k) = (1.0_8
191 + ry*(Ky(j,k+1) + Ky(j,k)) &
192 + rx*(Kx(j+1,k) + Kx(j,k))*p(j,k) &
193 - ry*(Ky(j,k+1)*p(j,k+1) + Ky(j,k)*p(j,k-1)) &
194 - rx*(Kx(j+1,k)*p(j+1,k) + Kx(j,k)*p(j-1,k))
195
196 pw = pw + w(j,k)*p(j,k)
197 ENDDO
198 ENDDO
199 !$OMP END DO
200 !$OMP END PARALLEL
201
202 END SUBROUTINE tea_leaf_kernel_solve_cg_fortran_calc_w
203
204 SUBROUTINE tea_leaf_kernel_solve_cg_fortran_calc_ur(x m
```

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



Scalasca report post-processing

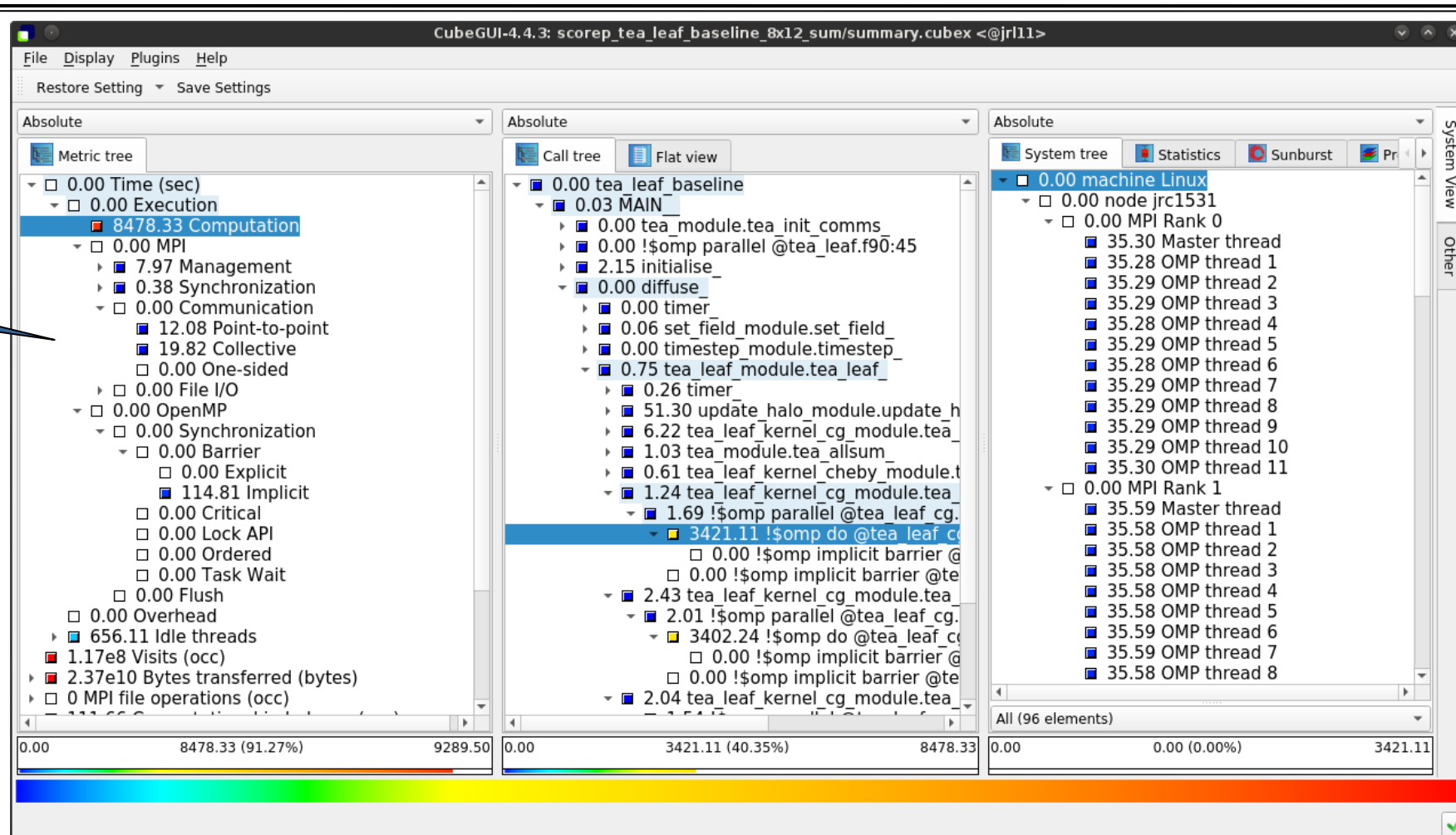
- Scalasca's report post-processing derives additional metrics and generates a structured metric hierarchy
- Automatically run (if needed) when using the **square** convenience command:

```
% 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

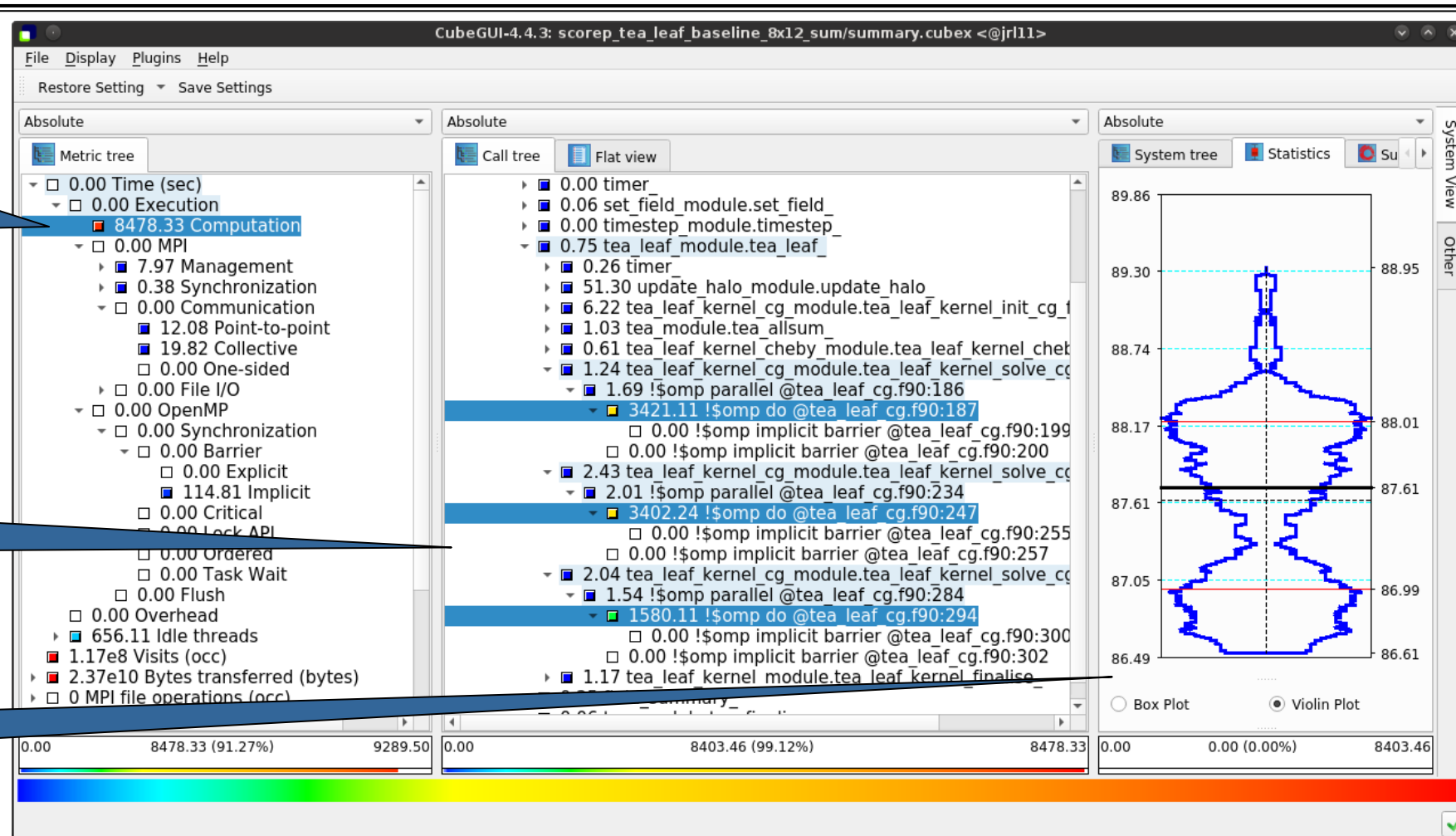


TeaLeaf summary report analysis (I)

91% of the execution time is computation...

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

...with a slight imbalance across ranks & threads



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

... when not within OpenMP-parallelized code regions

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

File Display Plugins Help

Restore Setting Save Settings

Absolute

Metric tree

- 0.00 Time (sec)
 - 0.00 Execution
 - 8478.33 Computation
 - 0.00 MPI
 - 7.97 Management
 - 0.38 Synchronization
 - 0.00 Communication
 - 12.08 Point-to-point
 - 19.82 Collective
 - 0.00 One-sided
 - 0.00 File I/O
 - 0.00 OpenMP
 - 0.00 Synchronization
 - 0.00 Barrier
 - 0.00 Explicit
 - 114.81 Implicit
 - 0.00 Critical
 - 0.00 Lock API
 - 0.00 Ordered
 - 0.00 Task Wait
 - 0.00 Flush
 - 0.00 Overhead
 - 656.11 Idle threads
 - 1.17e8 Visits (occ)
 - 2.37e10 Bytes transferred (bytes)
 - 0 MPI file operations

0.00 656.11 (7.06%) 9289.50

Absolute

Call tree Flat view

- 0.05 tea_leaf_baseline
 - 0.32 MAIN
 - 82.78 tea_module.tea_init_comms
 - 0.09 !\$omp parallel @tea_leaf.f90:45
 - 6.95 initialise_
 - 0.01 diffuse_
 - 0.00 timer_
 - 0.00 set_field_module.set_field_
 - 0.14 timestep_module.timestep_
 - 8.27 tea_leaf_module.tea_leaf_
 - 2.84 timer_
 - 251.98 update_halo_module.update_halo
 - 3.63 tea_leaf_kernel_cg_module.tea_leaf_kernel_init_cg_f
 - 228.56 tea_module.tea_allsum
 - 0.07 tea_leaf_kernel_cheby_module.tea_leaf_kernel_cheb
 - 13.66 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_c
 - 0.44 !\$omp parallel @tea_leaf_cg.f90:186
 - 0.00 !\$omp do @tea_leaf_cg.f90:187
 - 0.00 !\$omp implicit barrier @tea_leaf_cg.f90:199
 - 0.00 !\$omp implicit barrier @tea_leaf_cg.f90:200
 - 26.73 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_c
 - 0.92 !\$omp parallel @tea_leaf_cg.f90:234
 - 0.00 !\$omp do @tea_leaf_cg.f90:247
 - 0.00 !\$omp implicit barrier @tea_leaf_cg.f90:255
 - 0.00 !\$omp implicit barrier @tea_leaf_cg.f90:257
 - 22.42 tea_leaf_kernel_cg_module.tea_leaf_kernel_solve_c

0.00 612.48 (93.35%) 656.11

Absolute

System tree Statistics Su

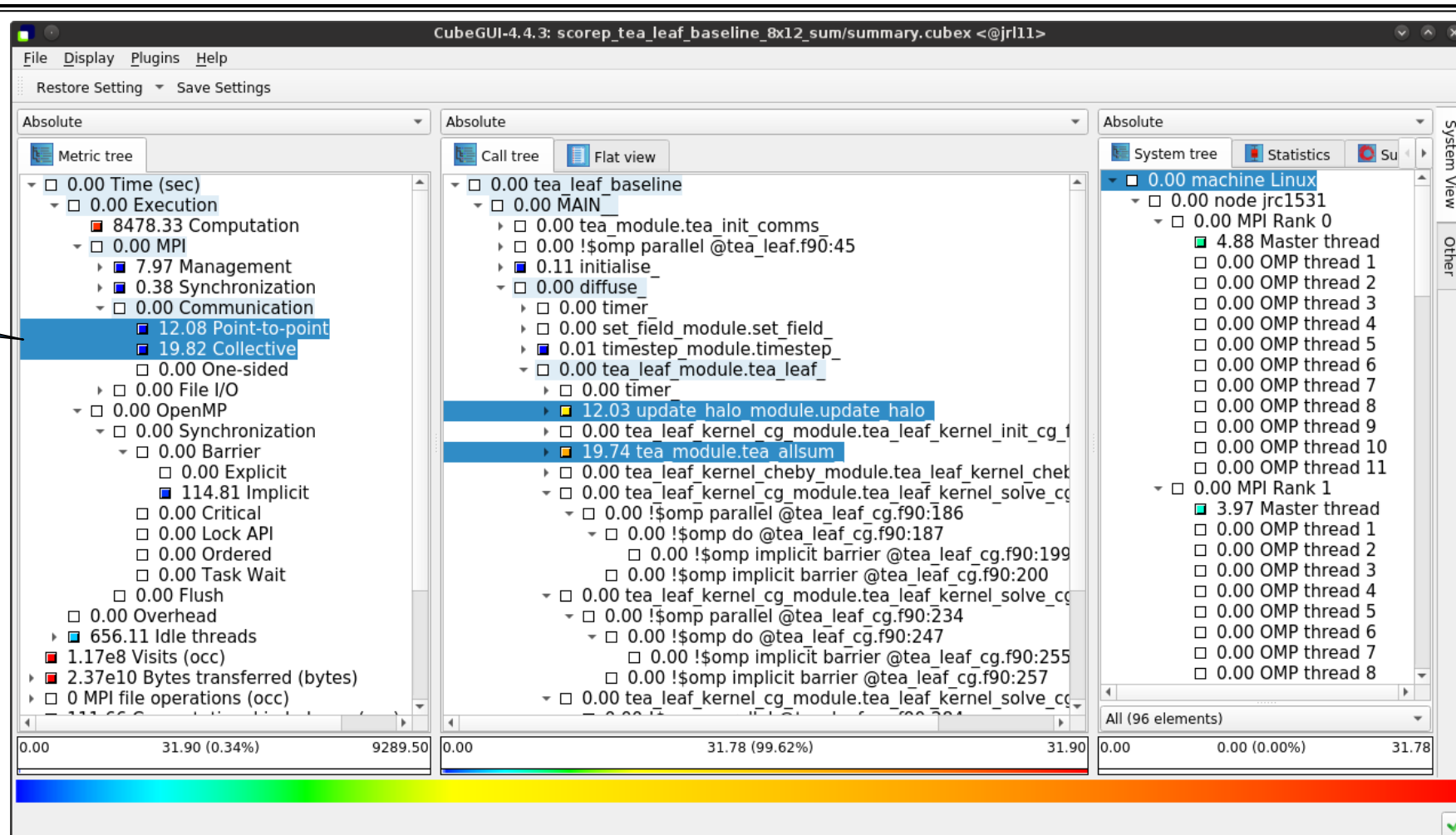
 - 0.00 machine Linux
 - 0.00 node jrc1531
 - 0.00 MPI Rank 0
 - 0.00 Master thread
 - 8.11 OMP thread 1
 - 8.12 OMP thread 2
 - 8.13 OMP thread 3
 - 8.12 OMP thread 4
 - 8.10 OMP thread 5
 - 8.12 OMP thread 6
 - 8.13 OMP thread 7
 - 8.13 OMP thread 8
 - 8.12 OMP thread 9
 - 8.13 OMP thread 10
 - 8.14 OMP thread 11
 - 0.00 MPI Rank 1
 - 0.00 Master thread
 - 7.18 OMP thread 1
 - 7.18 OMP thread 2
 - 7.19 OMP thread 3
 - 7.18 OMP thread 4
 - 7.17 OMP thread 5
 - 7.18 OMP thread 6
 - 7.19 OMP thread 7
 - 7.19 OMP thread 8

All (96 elements)

0.00 0.00 (0.00%) 612.48

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

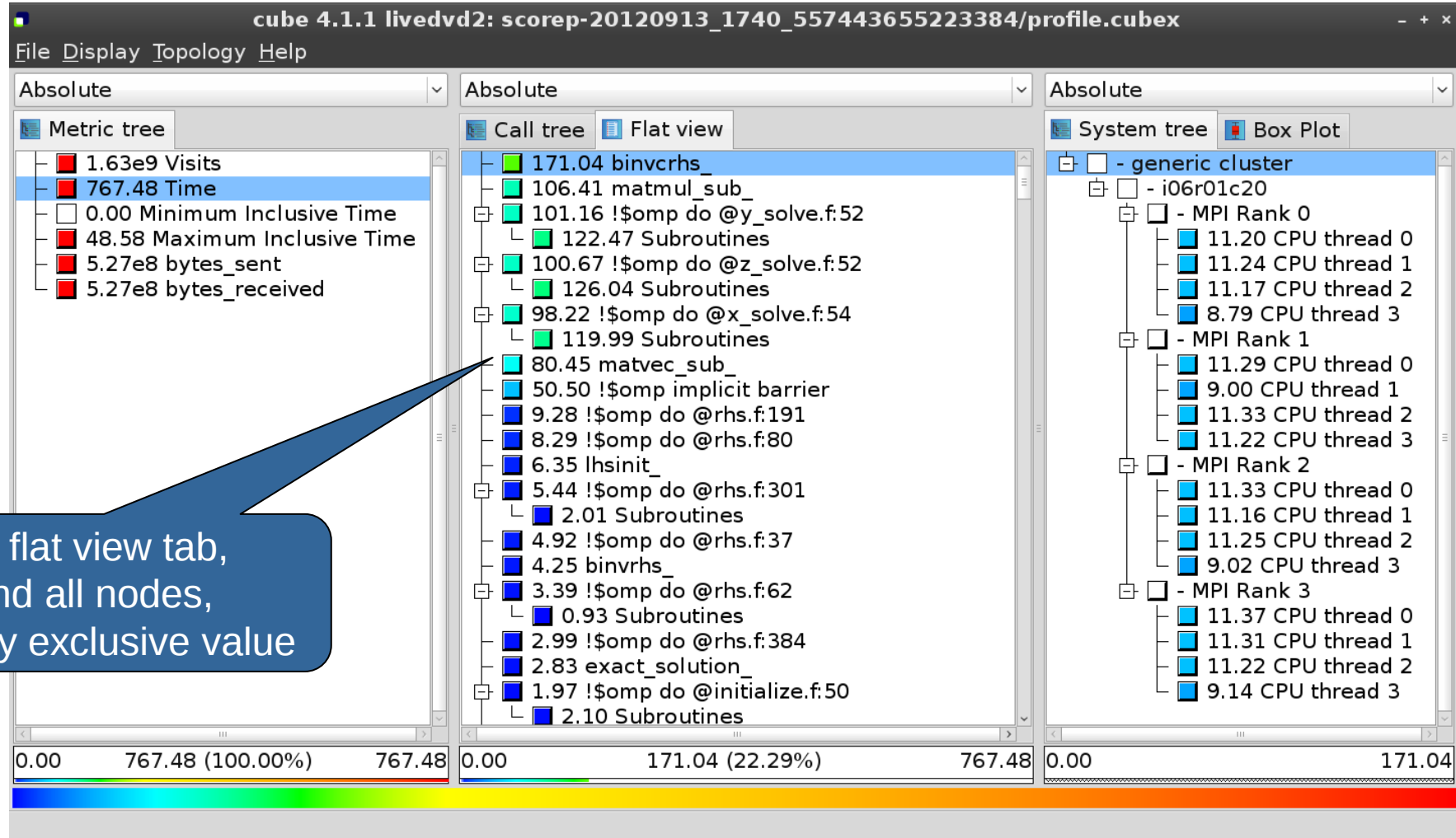
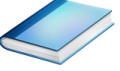
- Parallel program analysis report exploration tools
 - Libraries for Cube report reading & writing
 - Algebra utilities for report processing
 - GUI for interactive analysis exploration
- Available under 3-clause BSD open-source license
- Documentation & sources:
 - <https://www.scalasca.org>
- User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



Reference material



Flat profile view



Derived metrics



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

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

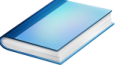
- Values of derived metrics are not stored, but calculated on-the-fly
- Types of derived metrics:
 - Prederived: evaluation of the CubePL expression is performed before aggregation
 - Postderived: evaluation of the CubePL expression is performed after aggregation
- Examples:
 - "Average execution time": Postderived metric with expression

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

- "Number of FLOP per second": Postderived metric with expression

`metric::FLOP()/metric::time()`

Derived metrics in Cube GUI



Collection of derived metrics

Parameters of the derived metric

CubePL expression

1.01e6 (100.00%) 1.01e6 0.00

2512.10

Example: FLOPS based on PAPI_FP_OPS and time



Example: FLOPS based on PAPI_FP_OPS and time

The image displays three screenshots from the Cube-4.3.1 software interface, illustrating the configuration and analysis of FLOPS metrics.

Left Screenshot: Edit metric FLOPS (on froggy1)

This window shows the configuration for a derived metric named "FLOPS".

- 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:**

The formula for the metric is defined as:

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

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

This window shows the "Metric tree" view. The selected metric is "1.84e9 FLOPS".

- 1.17e7 Visits (occ)**
- 1148.49 Time (sec)**
- 0.00 Minimum Inclusive Time (sec)**
- 41.57 Maximum Inclusive Time (sec)**
- 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**

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

This window shows the "System tree" view. The selected metric is "9.65e8 !\$omp do @exact_rhs.f:46".

- 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 @exact_rhs.f:46**
- 2.54e4 !\$omp do @exact_rhs.f:46**
- 9.65e8 !\$omp do @exact_rhs.f:46**
- 9.62e8 !\$omp do @exact_rhs.f:46**
- 8.14e8 !\$omp do @exact_rhs.f:46**
- 1.21e5 !\$omp do @exact_rhs.f:46**
- 0.00 !\$omp implicit barrier**
- 6.23e4 exch_qbc**
- 1.94e9 adi**
- 2.19e5 MPI_Barrier**
- 1.92e9 <<bt_iter>> (200 iterations)**
- 1.98e8 verify**
- 1.05e5 MPI_Reduce**

The bottom status bar indicates the selected metric: "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

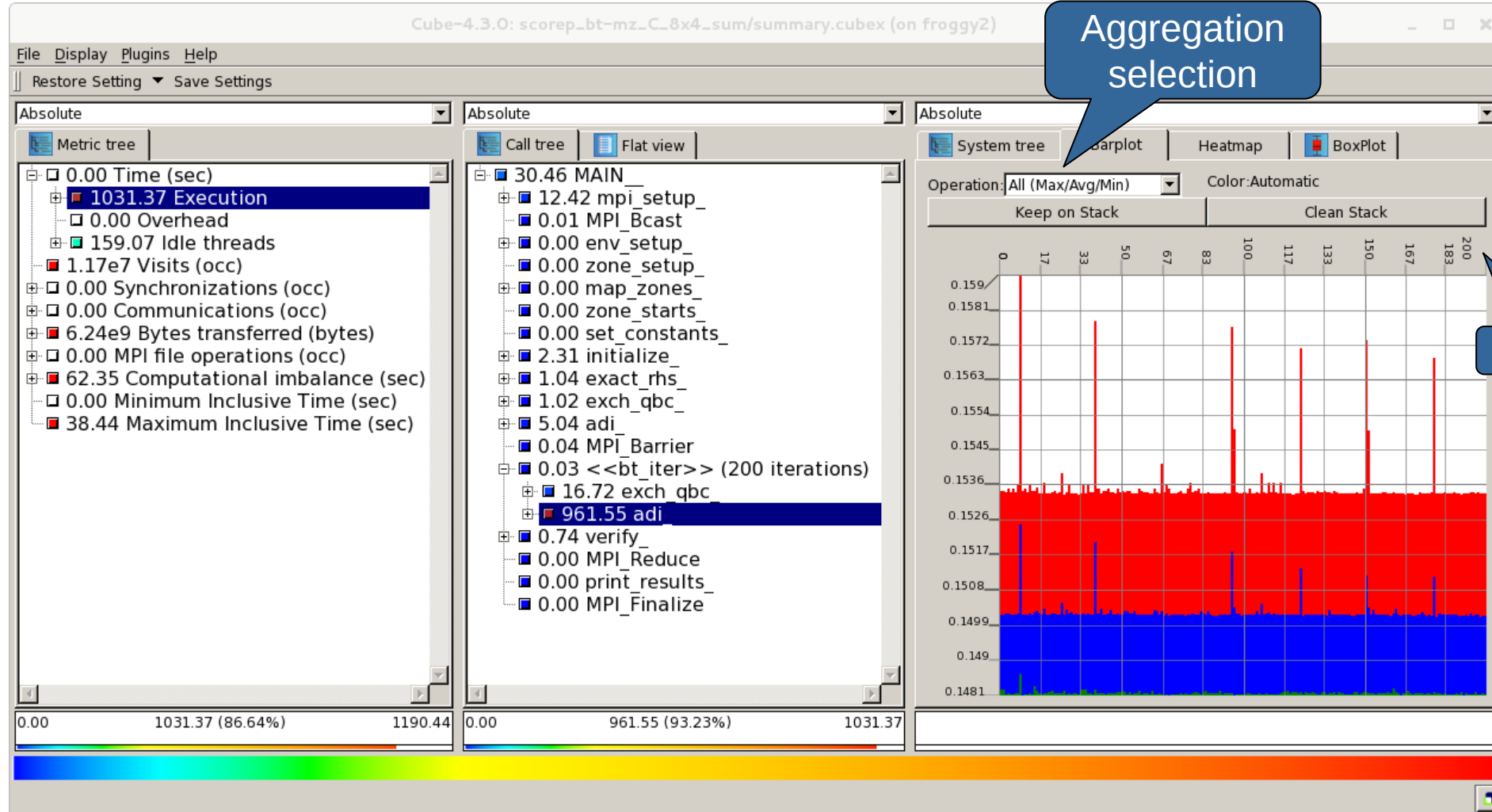
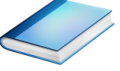


- Show time dependent behavior by “unrolling” iterations
- Preparations:
 - Mark loop body by using Score-P instrumentation API in your source code

```
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

