

# Analysis report examination with Cube

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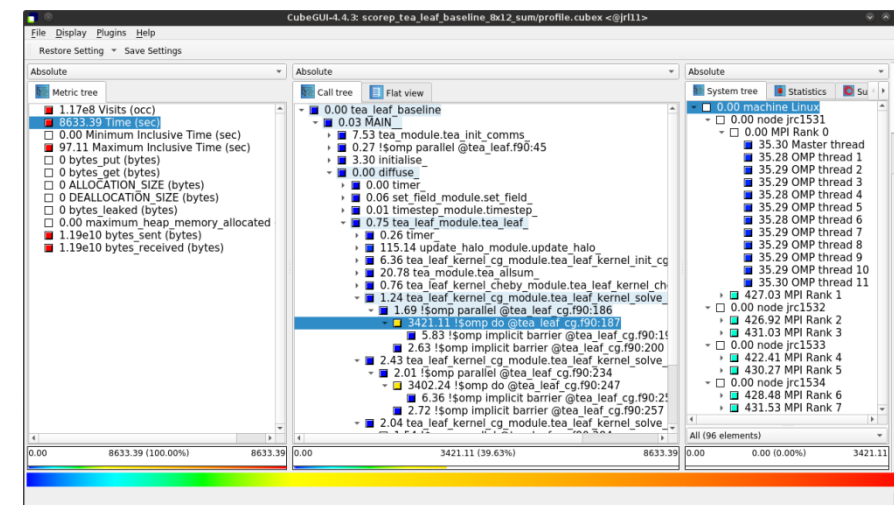


# Cube

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  $\geq 5$
- 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 v4.9.1 (December 2025)



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

# Cube GUI – Usage via Local Client

mailto: [scalasca@fz-juelich.de](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>@transfer1.bsc.es:/gpfs/scratch/nct_362 $HOME/mnt
```

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

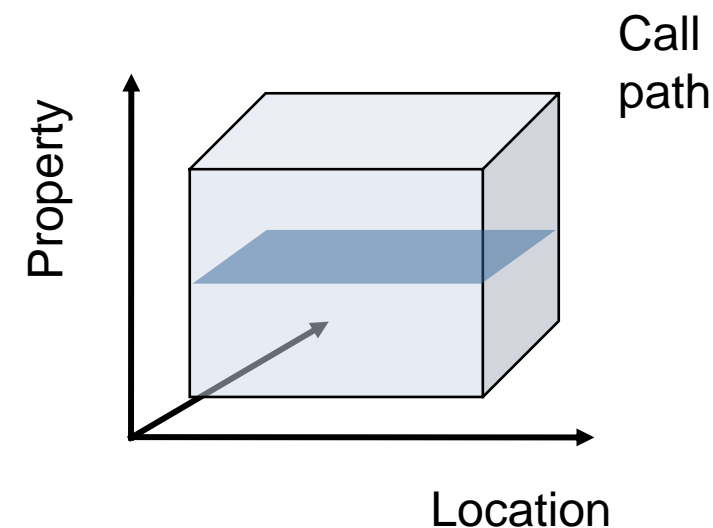
```
desk$ ssh -L 3300:localhost:3300 <user>@glogin1.bsc.es
login$ module load cubelib/4.9.1
login$ cube_server
```

All download options:

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

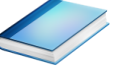
# Analysis presentation and exploration

- 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*

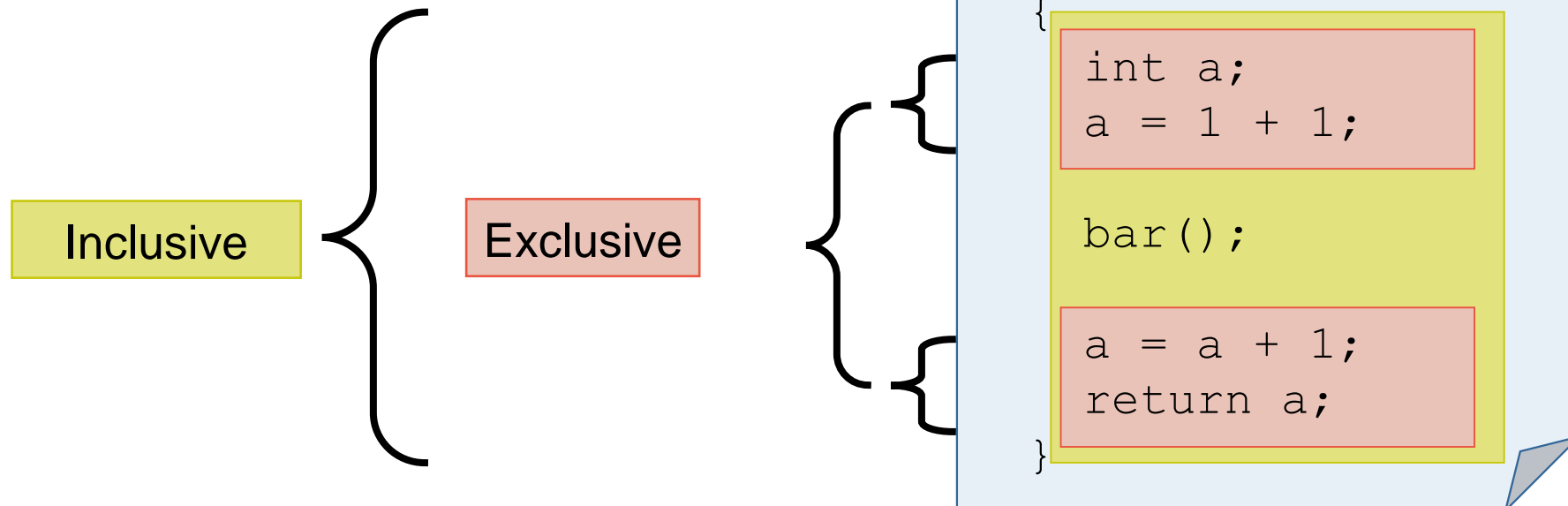




# Inclusive vs. exclusive values



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



# Demo: TeaLeaf case study

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## Case study: TeaLeaf

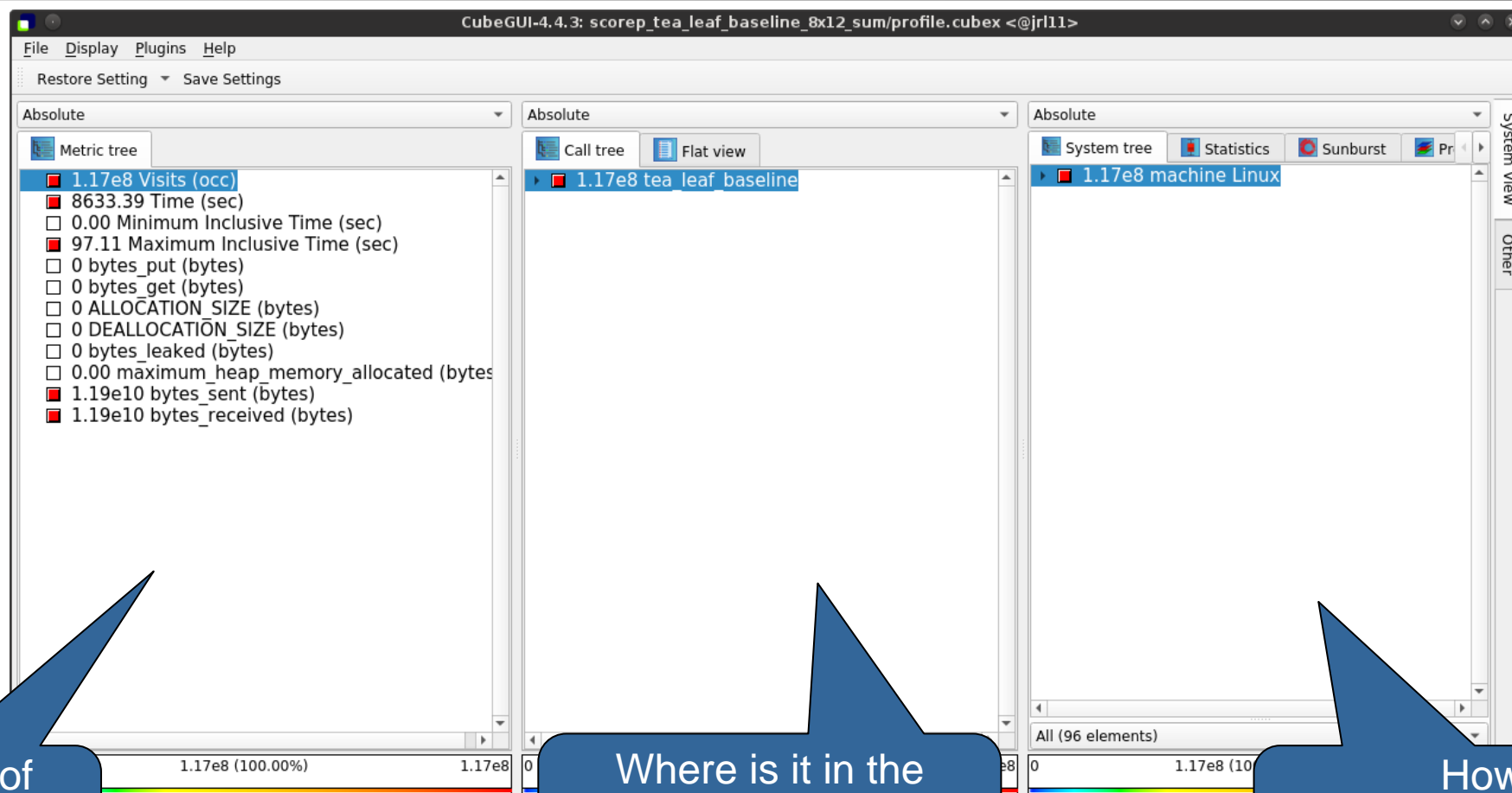
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- HPC mini-app developed by the UK Mini-App Consortium
  - Solves the linear 2D heat conduction equation on a spatially decomposed regular grid using a 5 point stencil with implicit solvers
  - Part of the Mantevo 3.0 suite
  - Available on GitHub: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



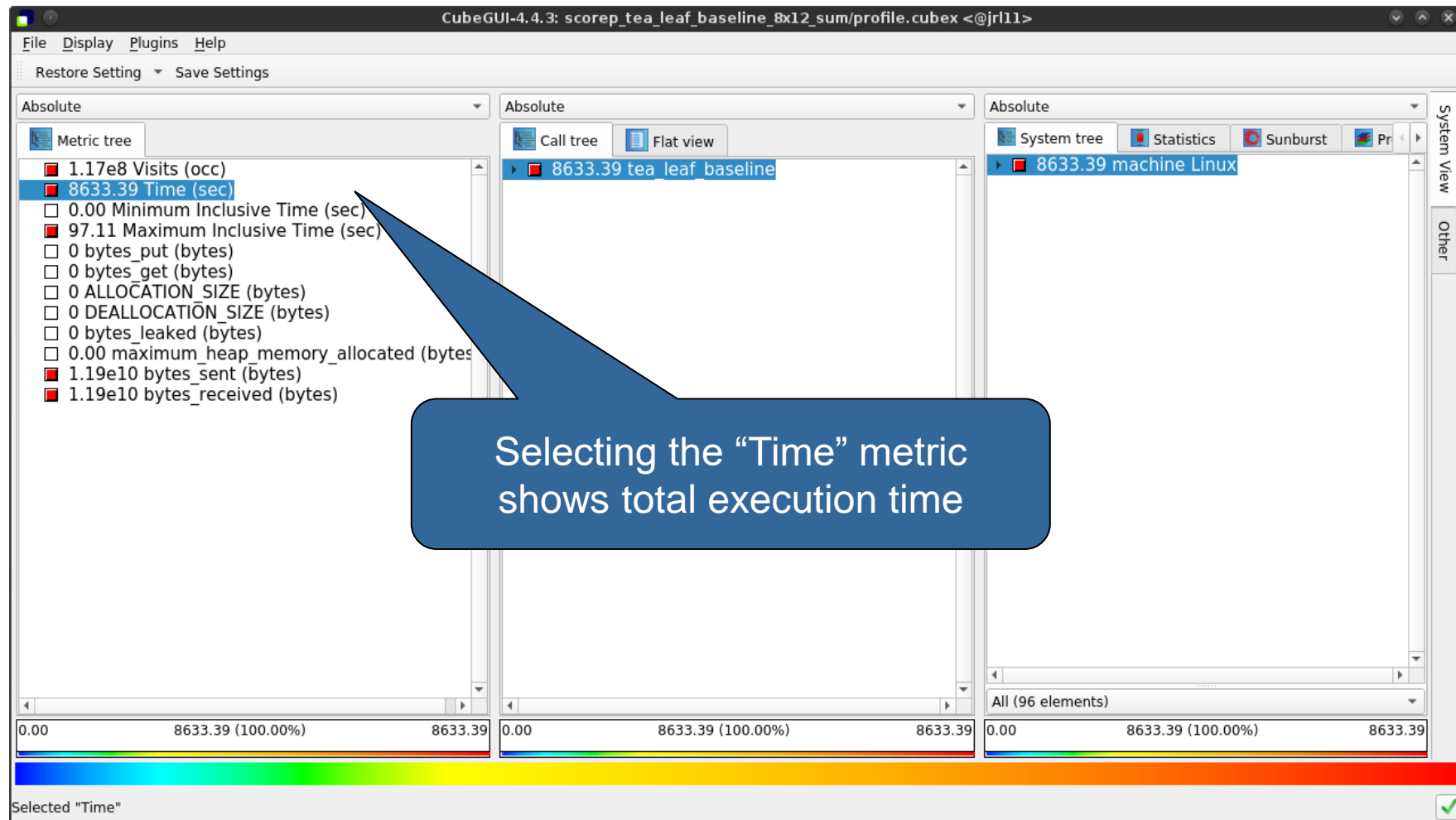
What kind of performance metric?

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

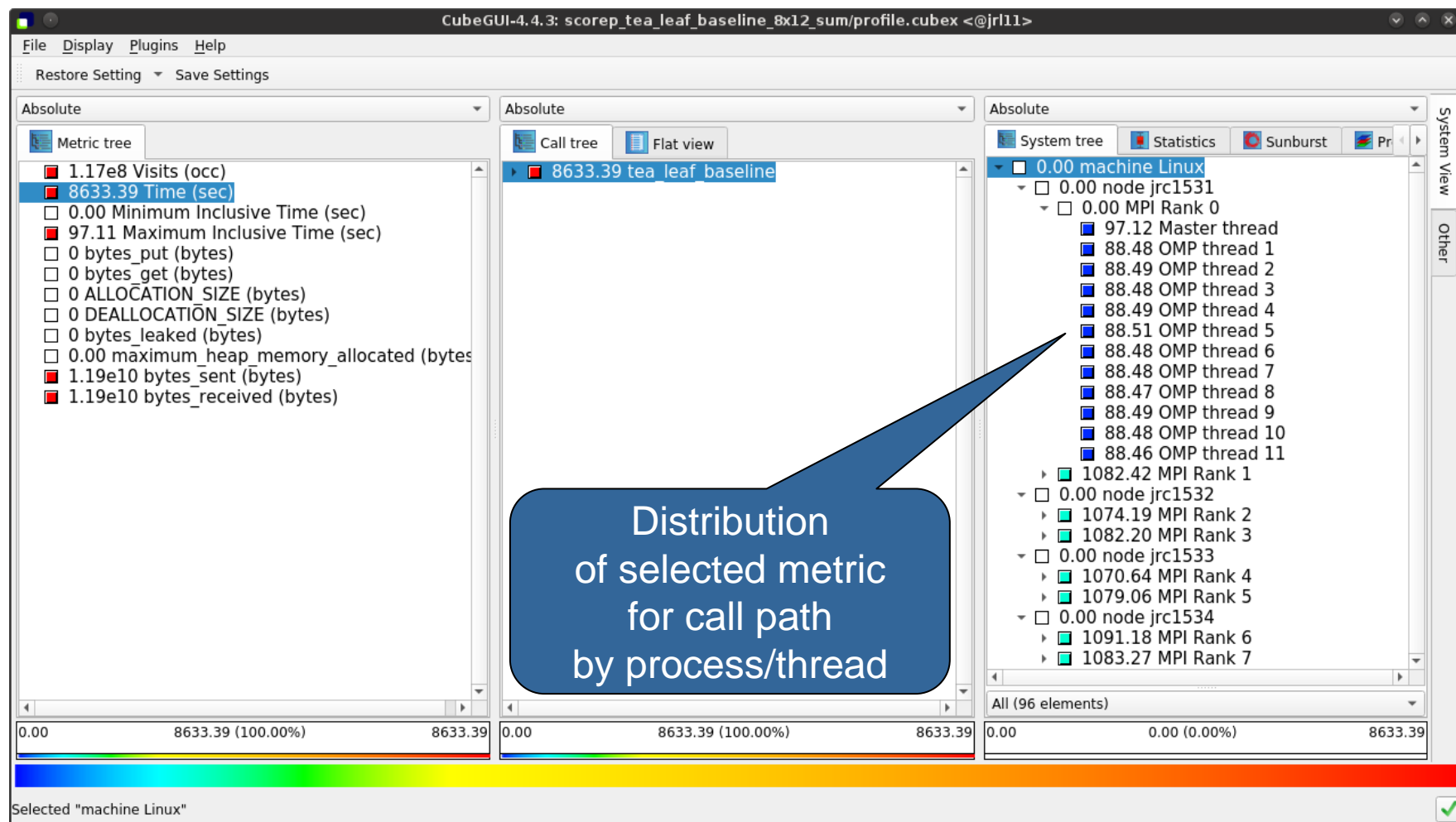
How is it distributed across the processes/threads?



# Metric selection



# Expanding the system tree



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 memory allocated

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\_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

Absolute

System tree Statistics Su

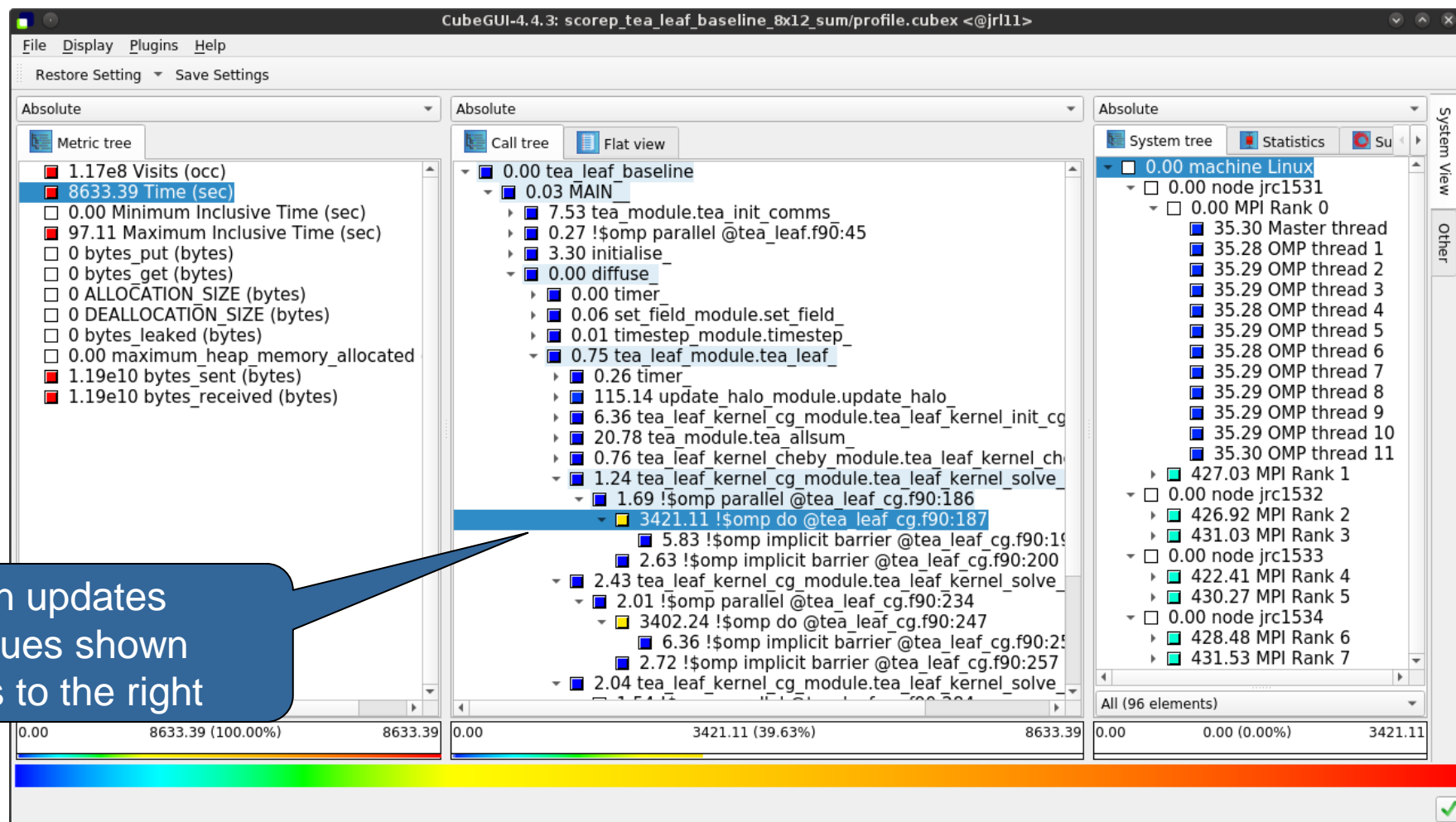
  - 0.00 machine Linux
    - 0.00 node jrc1531
      - 0.00 MPI Rank 0
        - 0.00 Master thread
        - 0.00 OMP thread 1
        - 0.00 OMP thread 2
        - 0.00 OMP thread 3
        - 0.00 OMP thread 4
        - 0.00 OMP thread 5
        - 0.00 OMP thread 6
        - 0.00 OMP thread 7
        - 0.00 OMP thread 8
        - 0.00 OMP thread 9
        - 0.00 OMP thread 10
        - 0.00 OMP thread 11
      - 0.00 MPI Rank 1
      - 0.00 MPI Rank 2
      - 0.00 MPI Rank 3
      - 0.00 node jrc1532
        - 0.00 MPI Rank 4
        - 0.00 MPI Rank 5
      - 0.00 node jrc1534
        - 0.00 MPI Rank 6
        - 0.00 MPI Rank 7

All (96 elements)

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

Ready

# Selecting a call path





# Multiple selection

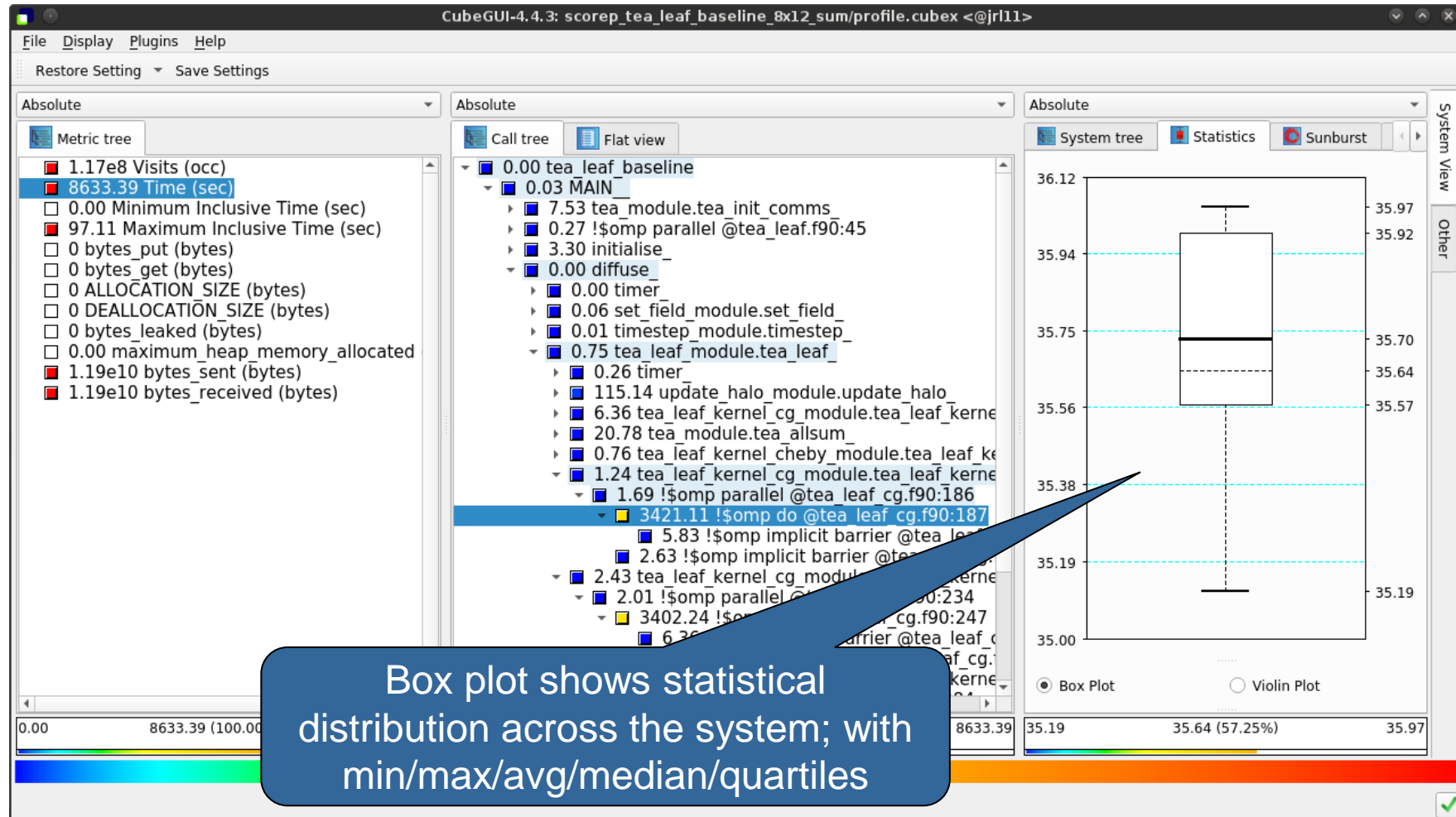
The screenshot displays the CubeGUI-4.4.3 interface with the title bar "CubeGUI-4.4.3: scorep\_tea\_leaf\_baseline\_8x12\_sum/profile.cubex <@jrl11>". The interface is divided into three main panels: "Metric tree", "Call tree", and "System tree".

- Metric tree:** Shows a list of metrics under the "Absolute" view. The "8633.39 Time (sec)" metric is highlighted in blue.
- Call tree:** Shows a hierarchical view of the call stack. The "0.75 tea\_leaf\_module.tea\_leaf\_" node is expanded, and several sub-nodes are highlighted in blue, including "3421.11 !\$omp do @tea\_leaf\_cg.f90:187", "3402.24 !\$omp do @tea\_leaf\_cg.f90:247", and "1580.11 !\$omp do @tea\_leaf\_cg.f90:294".
- System tree:** Shows a hierarchical view of the system components. The "0.00 machine Linux" node is expanded, and several sub-nodes are highlighted in blue, including "0.00 node jrc1531", "0.00 MPI Rank 0", and "1054.35 MPI Rank 1".

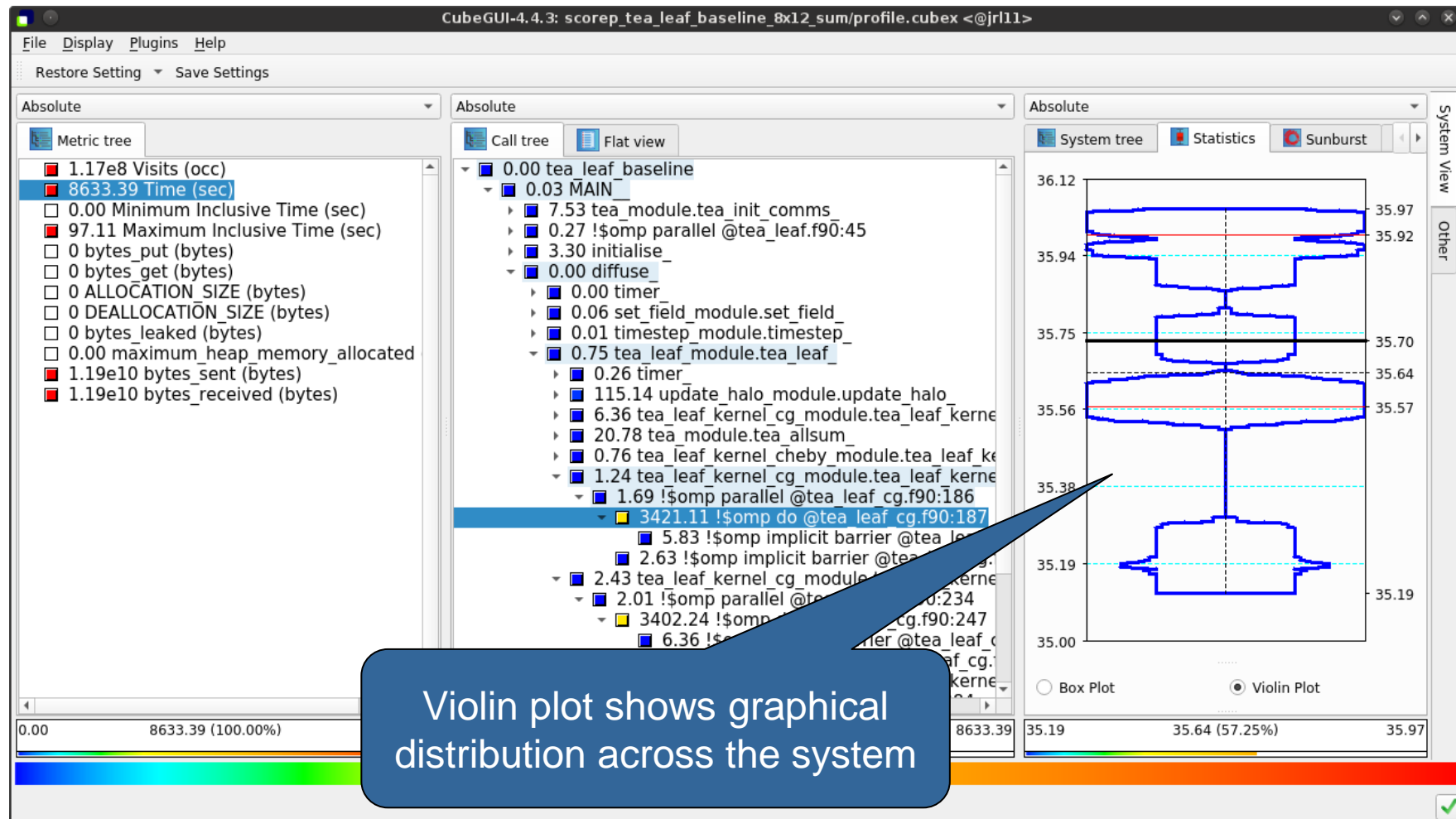
A blue callout box with a speech bubble points to the "System tree" panel, containing the text: "Select multiple nodes with Ctrl-click".

At the bottom of the interface, there are three progress bars showing the percentage of nodes selected. The first bar shows "0.00 8633.39 (100.00%) 8633.39", the second bar shows "0.00 8403.46 (97.34%) 8633.39", and the third bar shows "0.00 0.00 (0.00%) 8403.46".

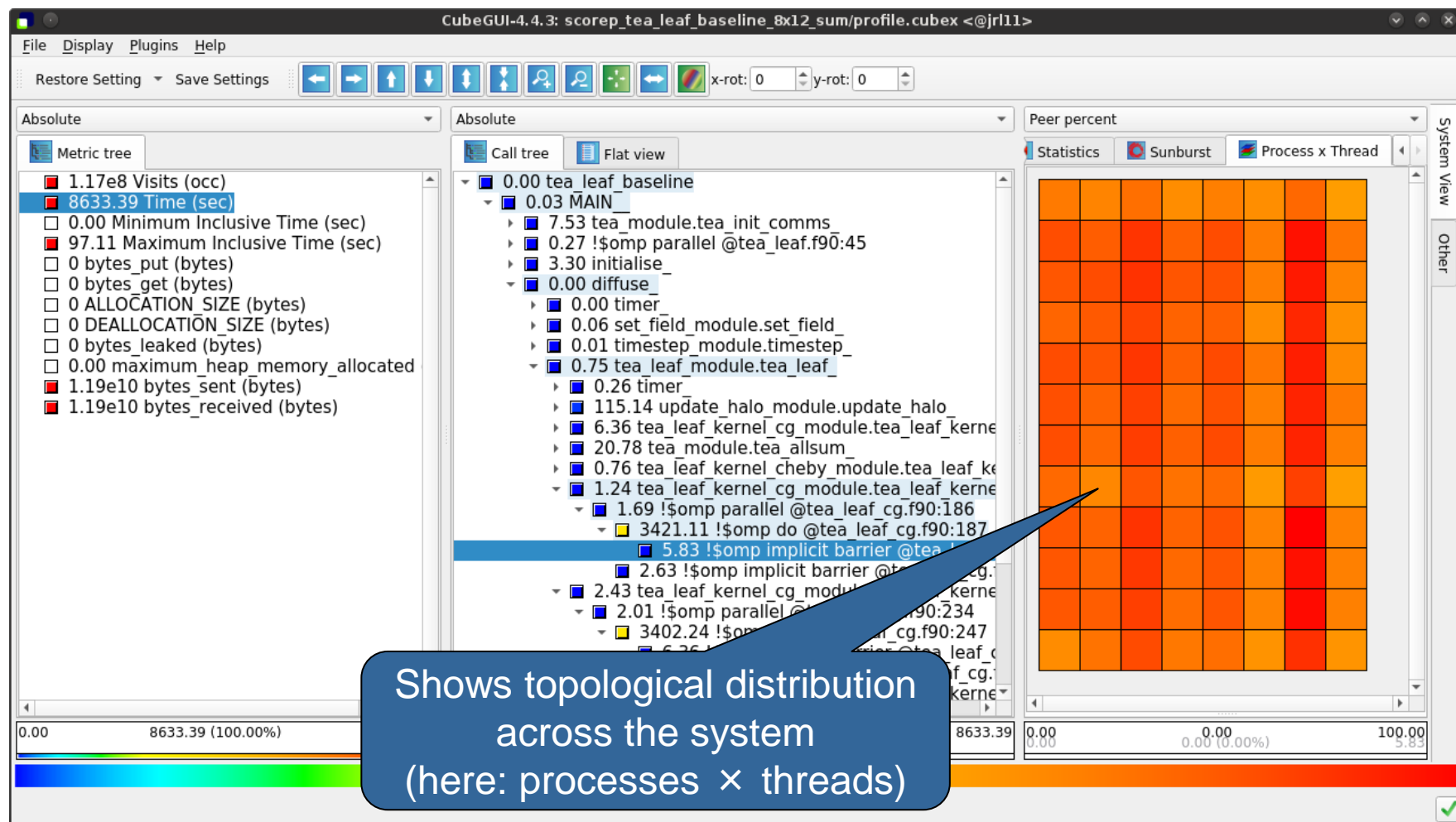
# Box plot view



# Violin plot view



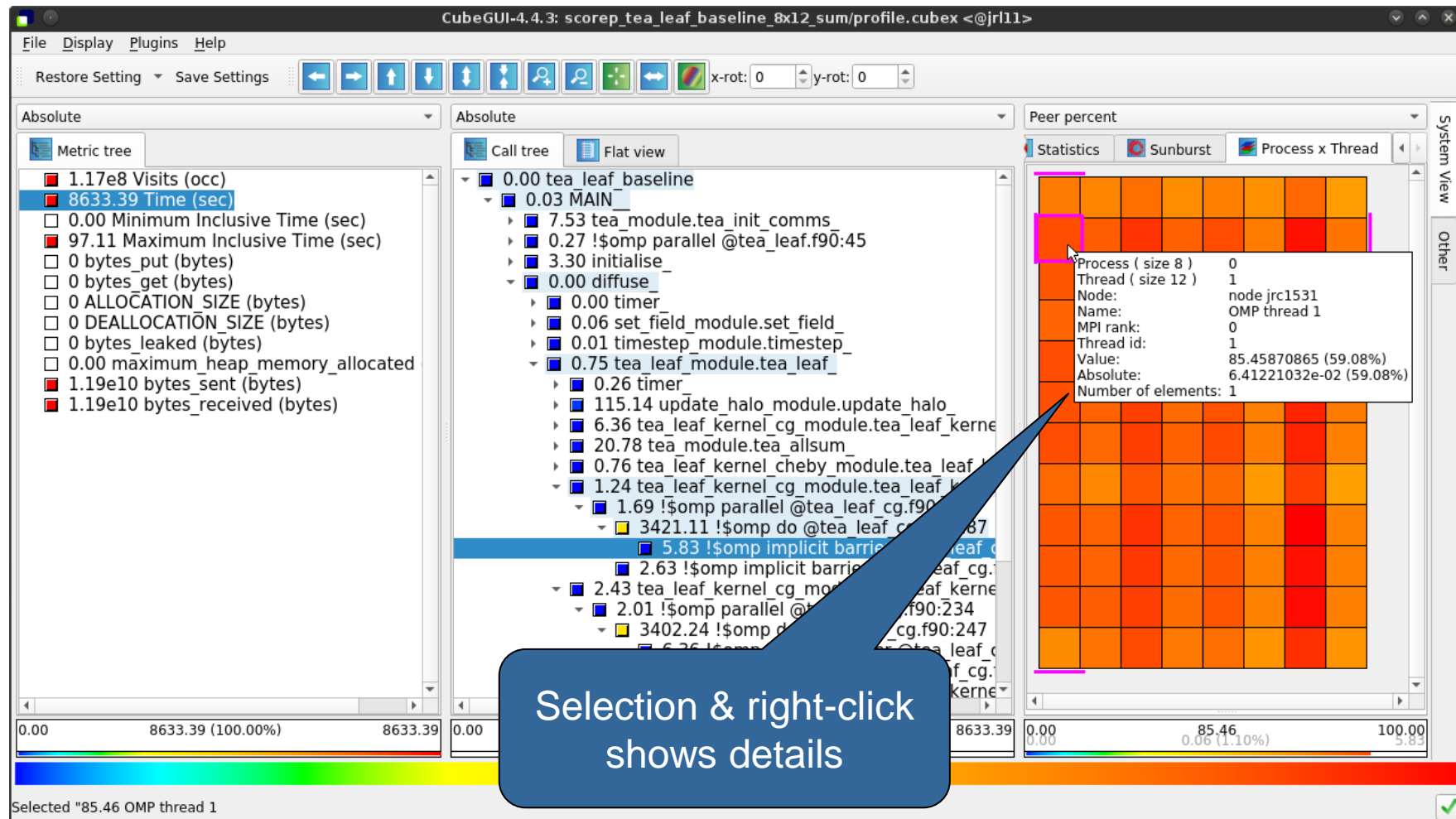
# Topology view



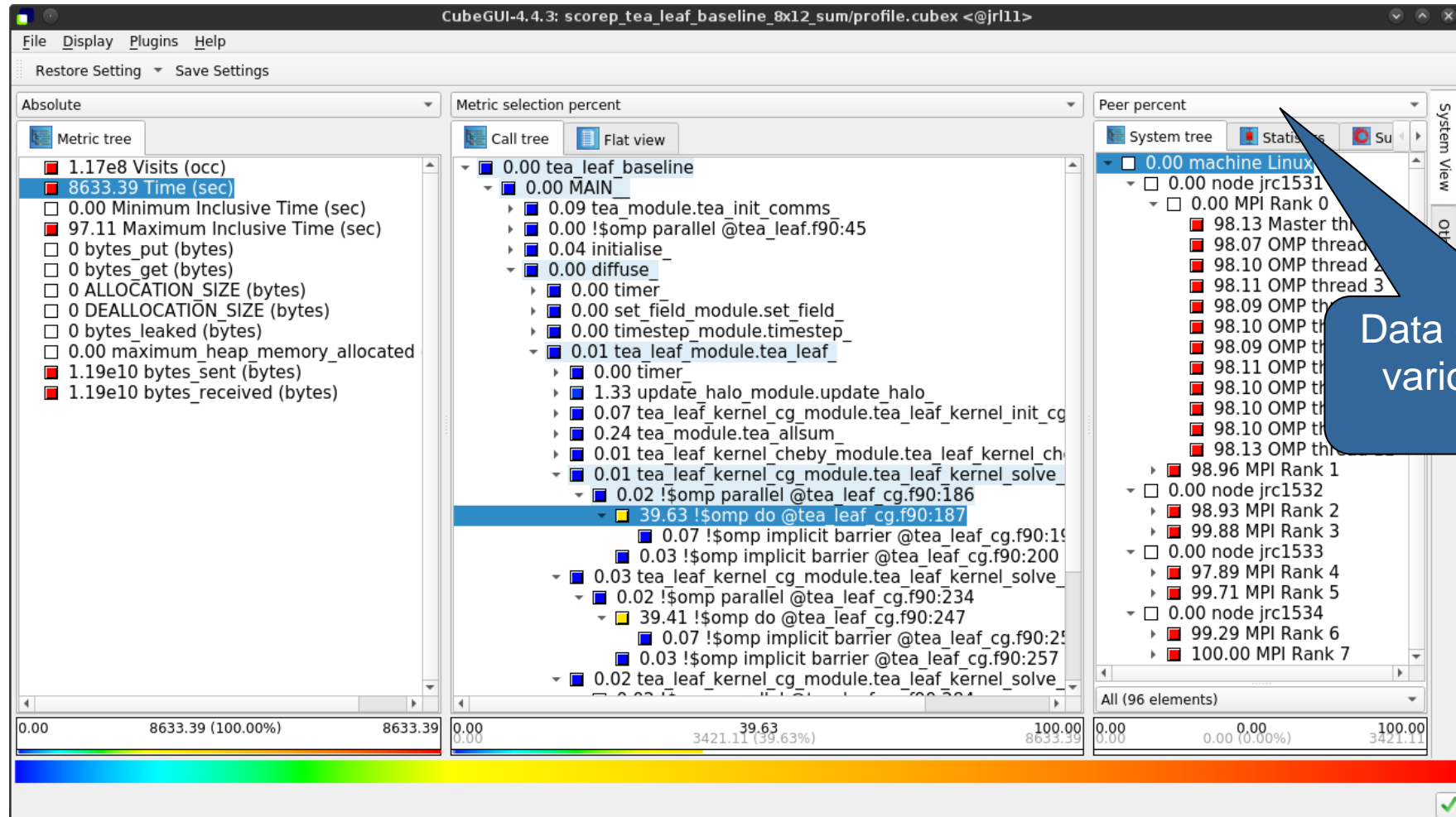
Shows topological distribution  
across the system  
(here: processes × threads)



## Topology view (cont.)



# Alternative display modes



# Important display modes

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- 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 node `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 with a speech bubble points to the context menu, containing the text: "Right-click opens context menu".

Right-click opens context menu



# 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

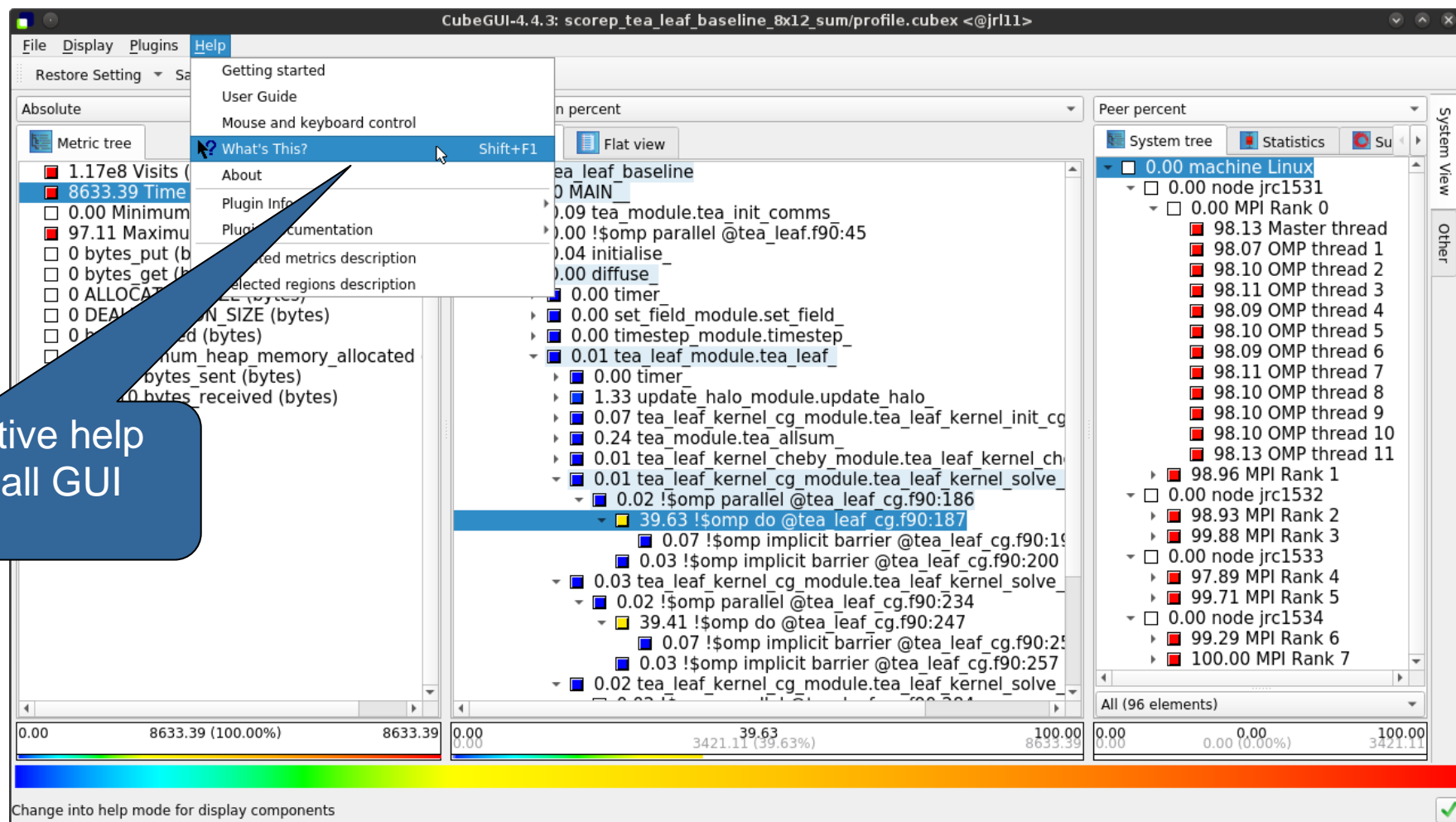
```
170 IMPLICIT NONE
171
172 INTEGER(KIND=4):: x_min,x_max,y_min,y_max
173 REAL(KIND=8), DIMENSION(x_min-2:x_max+2,y_min-2:y
174 REAL(KIND=8), DIMENSION(x_min-2:x_max+2,y_min-2:y
175 REAL(KIND=8), DIMENSION(x_min-2:x_max+2,y_min-2:y
176 REAL(KIND=8), DIMENSION(x_min-2:x_max+2,y_min-2:y
177
178 REAL(KIND=8) :: rx, ry
179
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
```

8633.39 0.00 3421.11 (39.63%) 8633.39

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

Select "Source" tab

# Context-sensitive help



Context-sensitive help  
available for all GUI  
items

## Scalasca report post-processing

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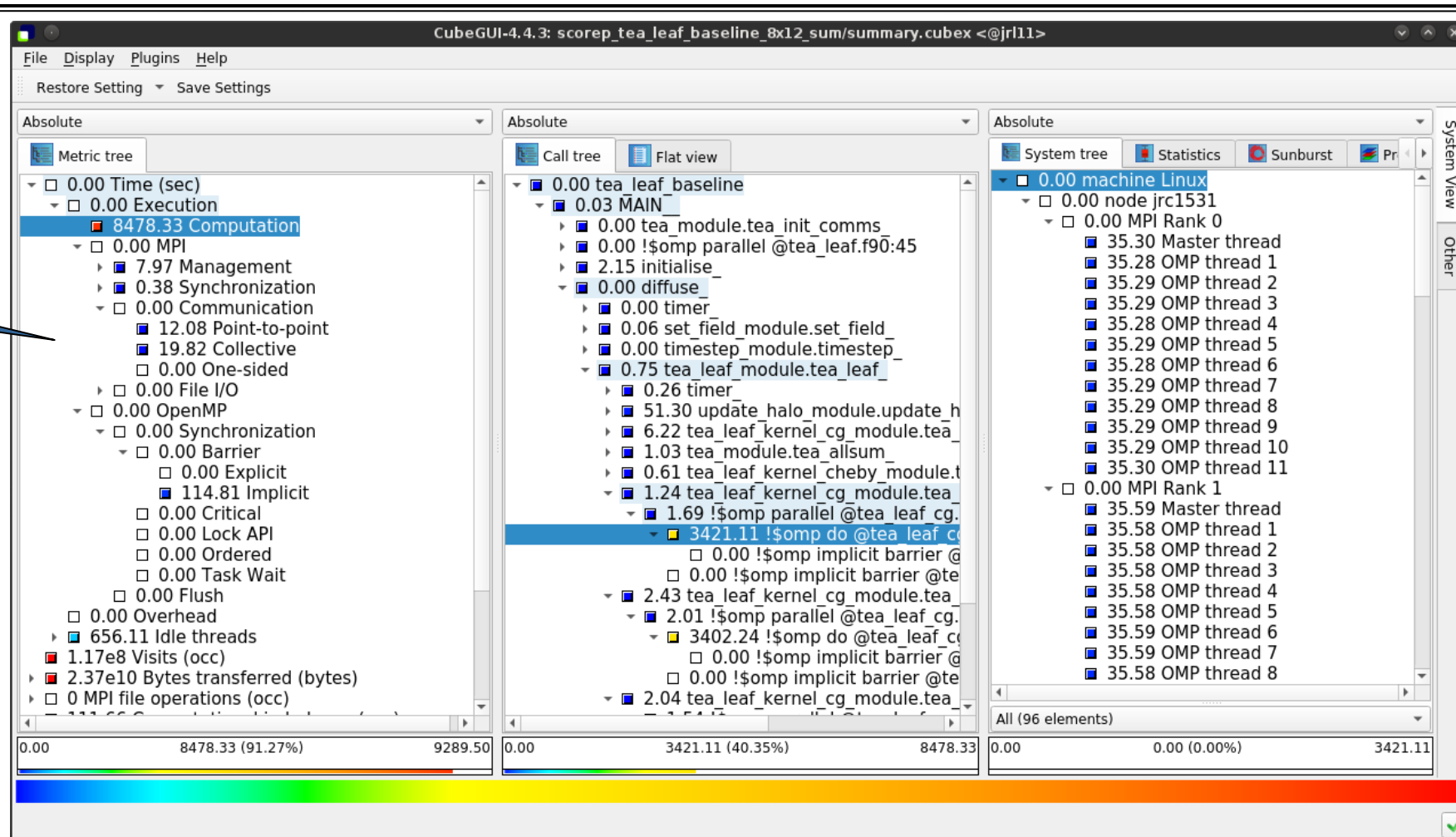
- Scalasca's report post-processing derives additional metrics and generates a structured metric hierarchy
- Automatically run (if needed) when using the **square** convenience command:

```
% 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]
```

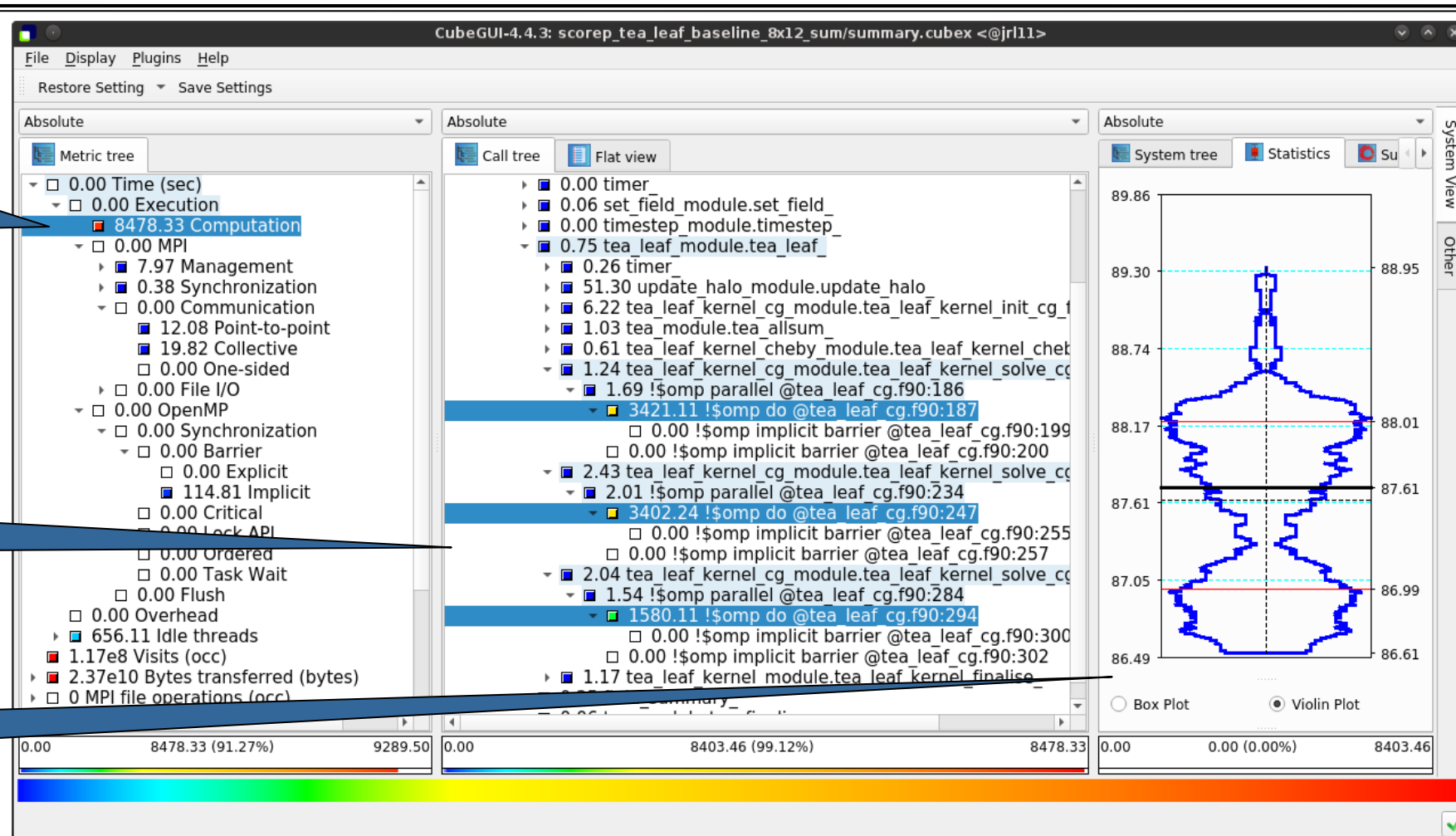
# Post-processed summary analysis report

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...

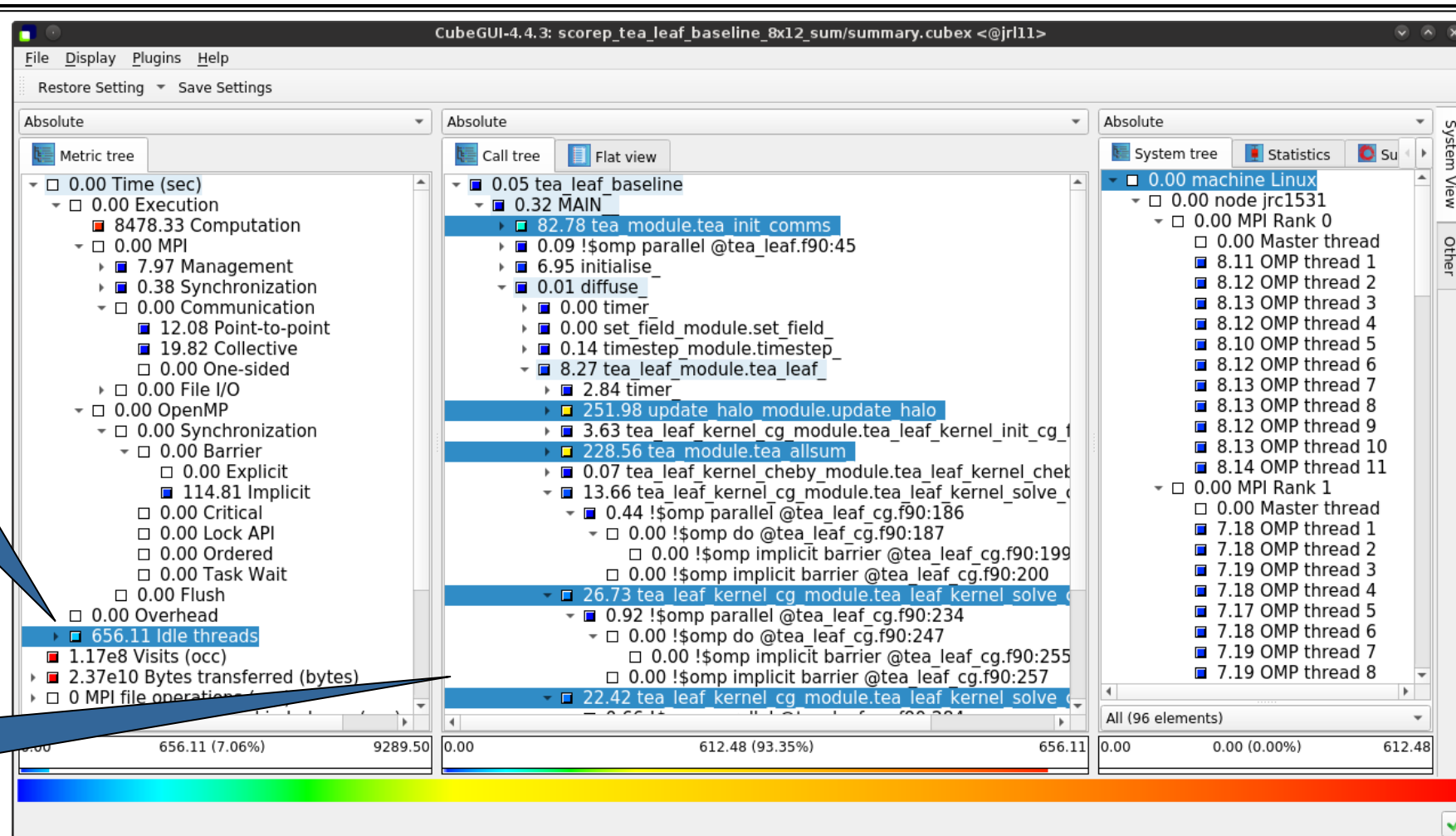
...almost entirely spent in 3 OpenMP do loops...

...with a slight imbalance across ranks & threads

## TeaLeaf summary report analysis (II)

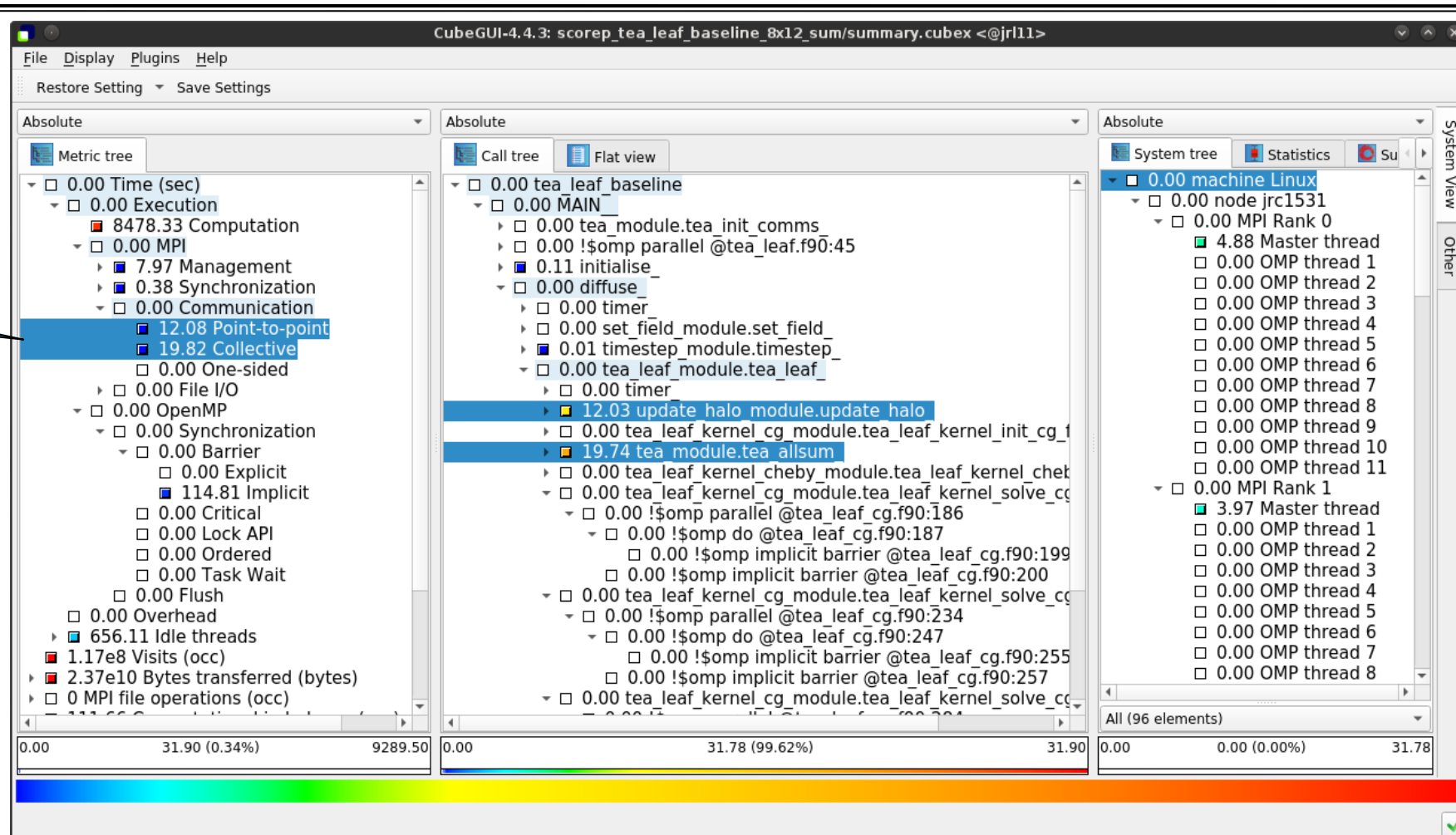
7% of the total CPU execution time is due to "idle threads"...

... 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

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- 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)

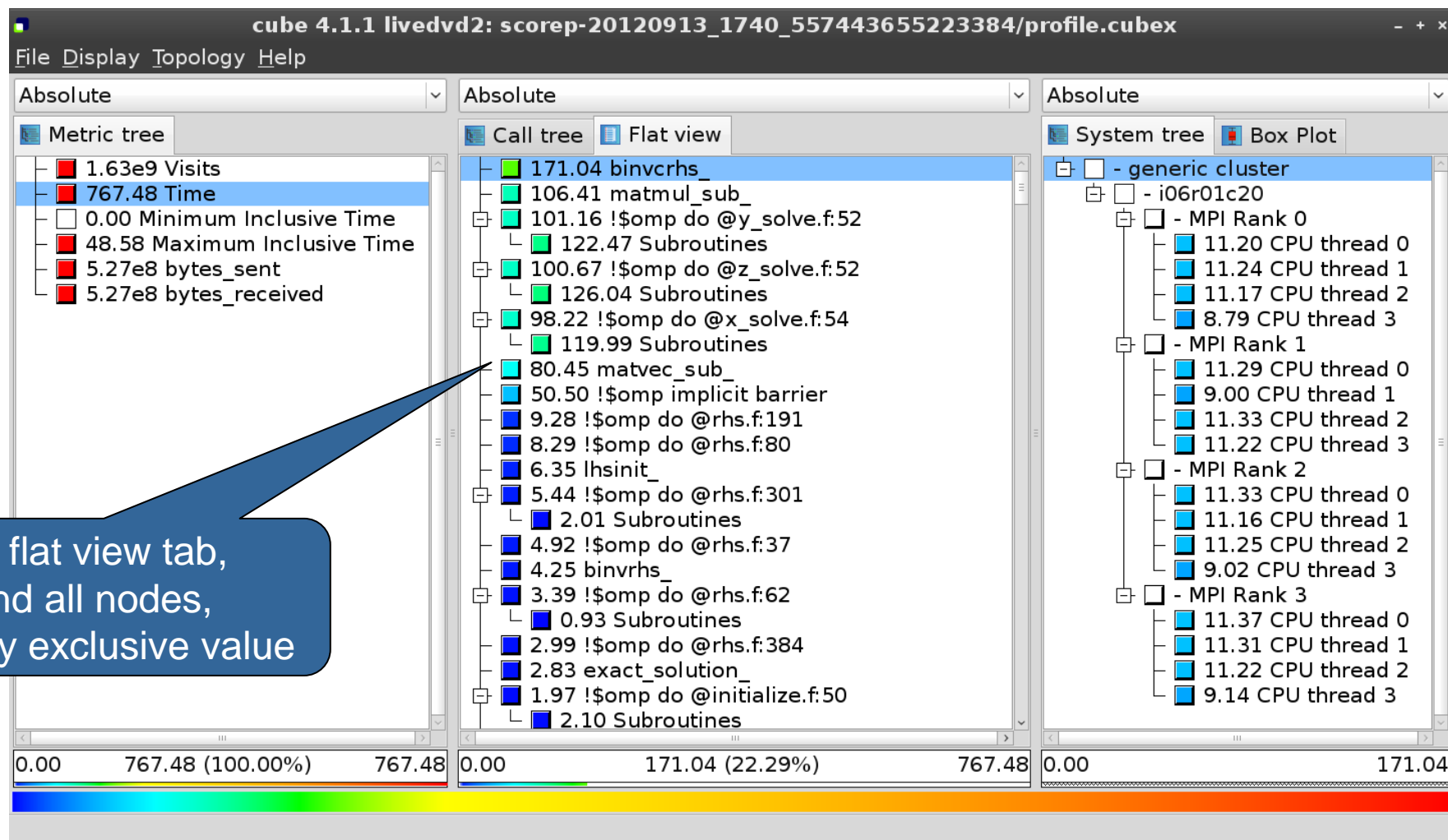




## Reference material



# Flat profile view



## Derived metrics

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- 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

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 calculation formula 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 (...)
- 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**

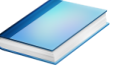
**Right Screenshot: Cube-4.3.1: scorep\_8x4\_sum/profile.cubex (on froggy1)**

This window shows the "System tree" view. The selected metric is "9.65e8 !\$omp do @exact\_rhs...".

- 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

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

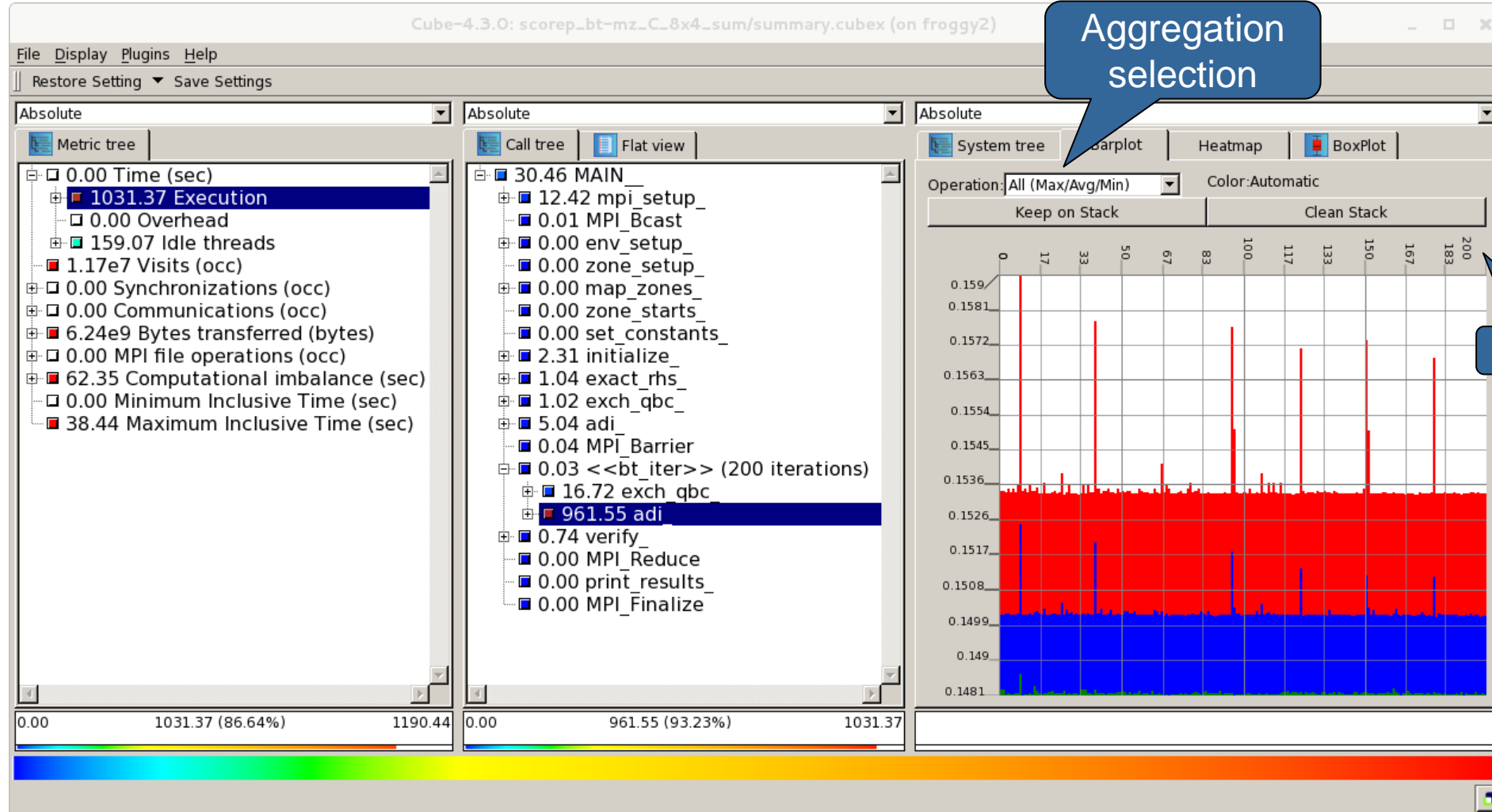


- Show time dependent behavior by “unrolling” iterations
- Preparations:
  - Mark loop body by using Score-P instrumentation API in your source code

```
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

