

# Analysis report examination with Cube

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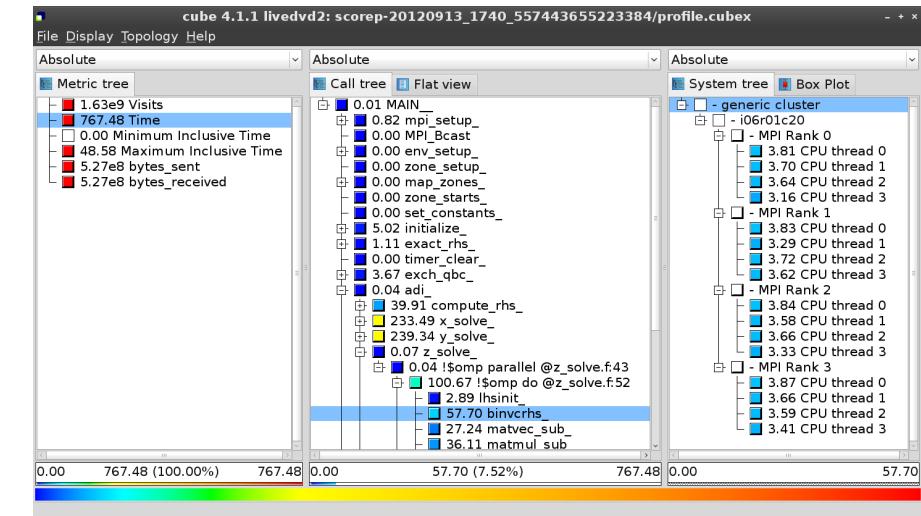
The Scalasca Team  
Jülich Supercomputing Centre



# 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 component
  - Can be installed independently of Score-P, e.g., on laptop or desktop
  - Latest release: Cube v4.8.2 (Oct 2023)



**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 (archer2)

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



- Run **remote** (*often convenient*)
  - start X server (e.g., Xming) locally, or use alternative such as mobaXterm
  - connect to Archer2 with X forwarding enabled
    - **-Y** may be faster but is insecure!
  - load scalasca module and start cube remotely

```
desk$ ssh -x login.archer2.ac.uk
Welcome to ARCHER2...
uan01$ module load scalasca
uan01$ cube ./scorep_sum/profile.cubex
```

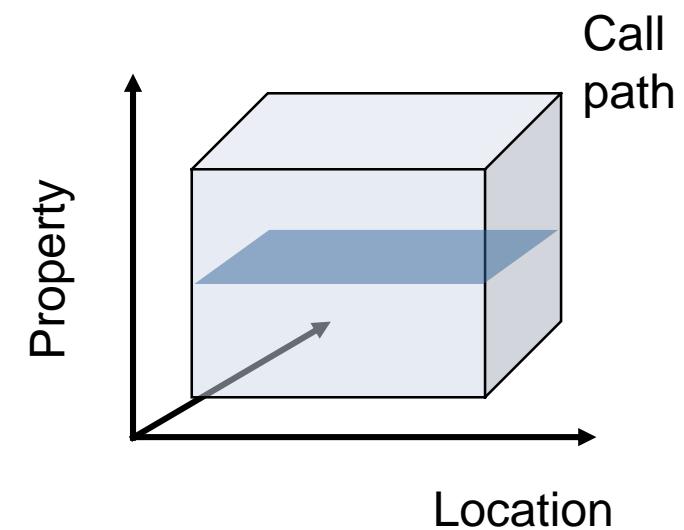
Sample measurements (CUBE files) on Archer2:  
/work/y23/shared/tutorial/samples

- Install & run **local** (*recommended*)
  - 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

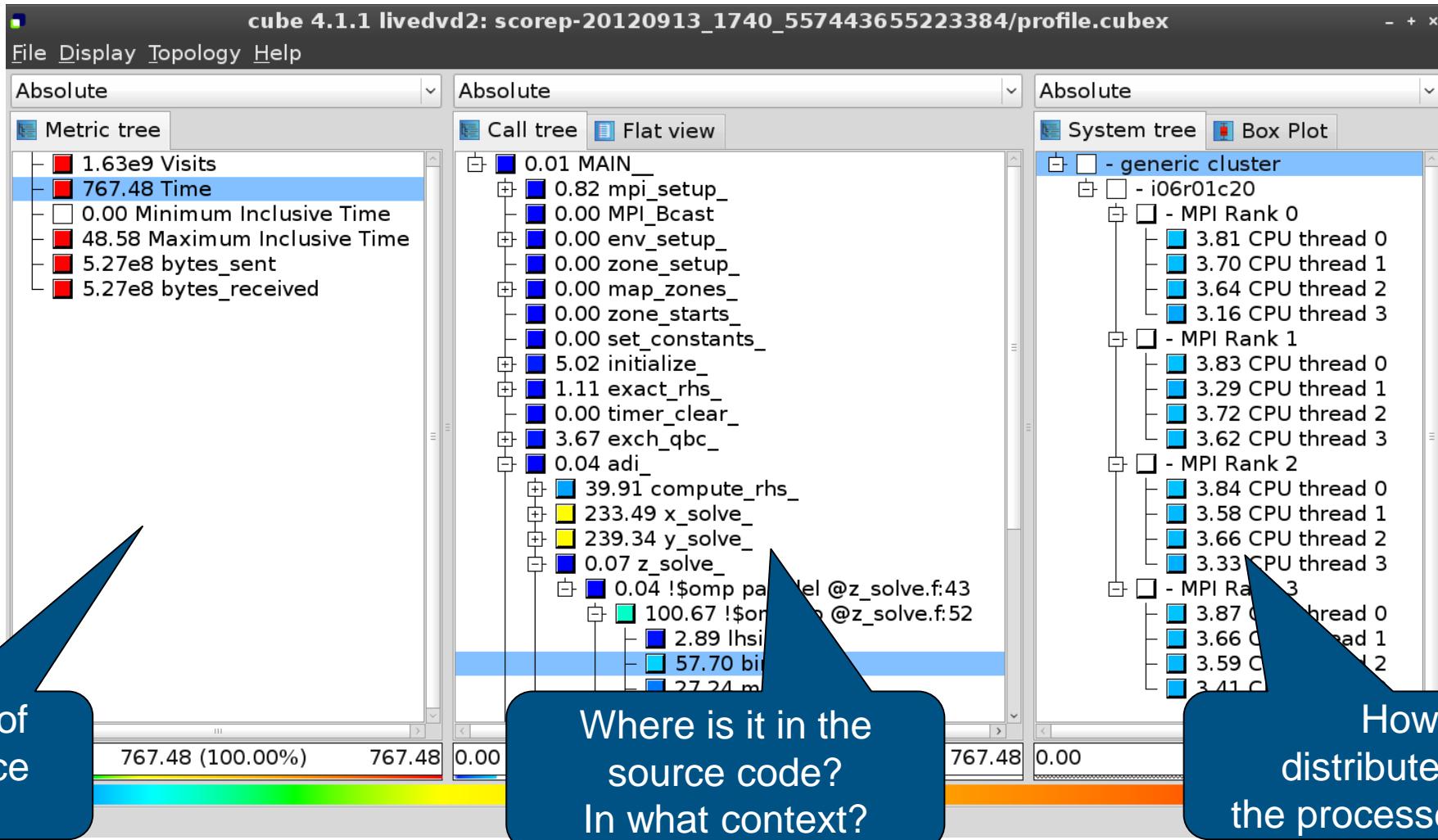
```
desk$ mkdir $HOME/mnt
desk$ sshfs [user@]remote.sys:[dir] $HOME/mnt
desk$ cd $HOME/mnt
desk$ cube ./scorep_sum/profile.cubex
```

# 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



# Analysis presentation



What kind of performance metric?

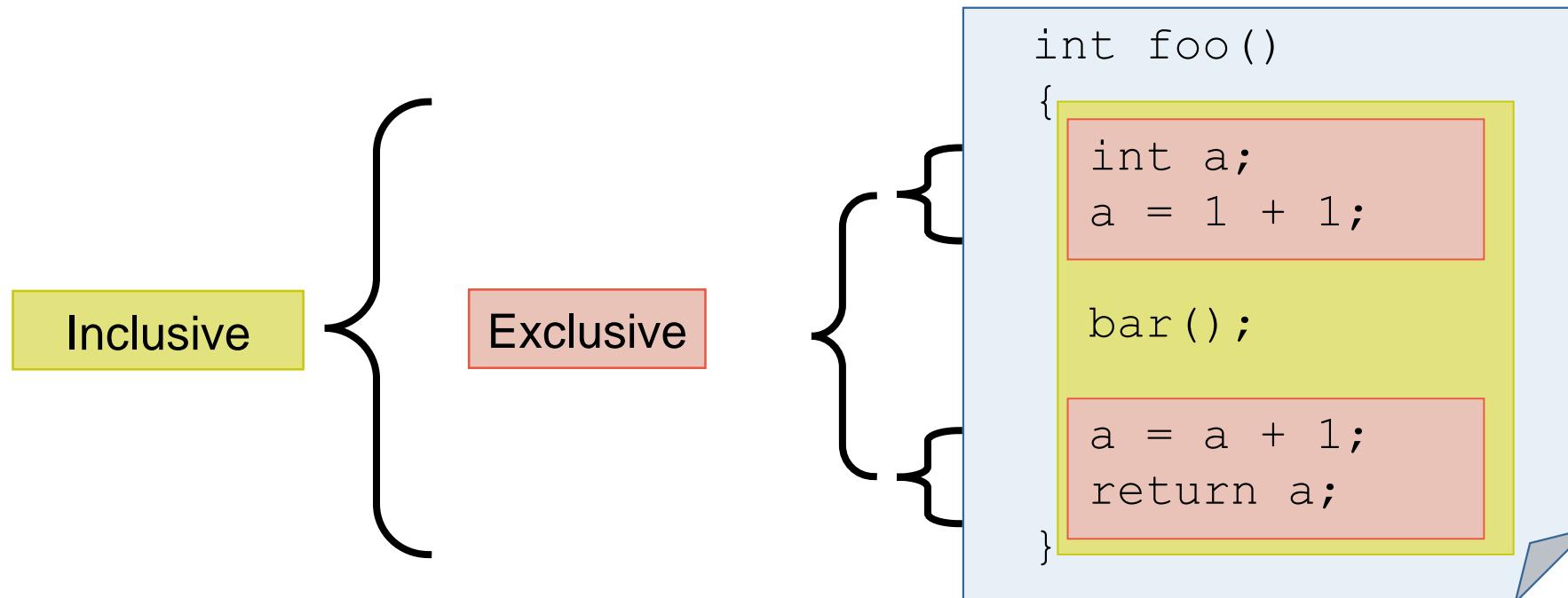
Where is it in the source code?  
In what context?

How is it distributed across the processes/threads?

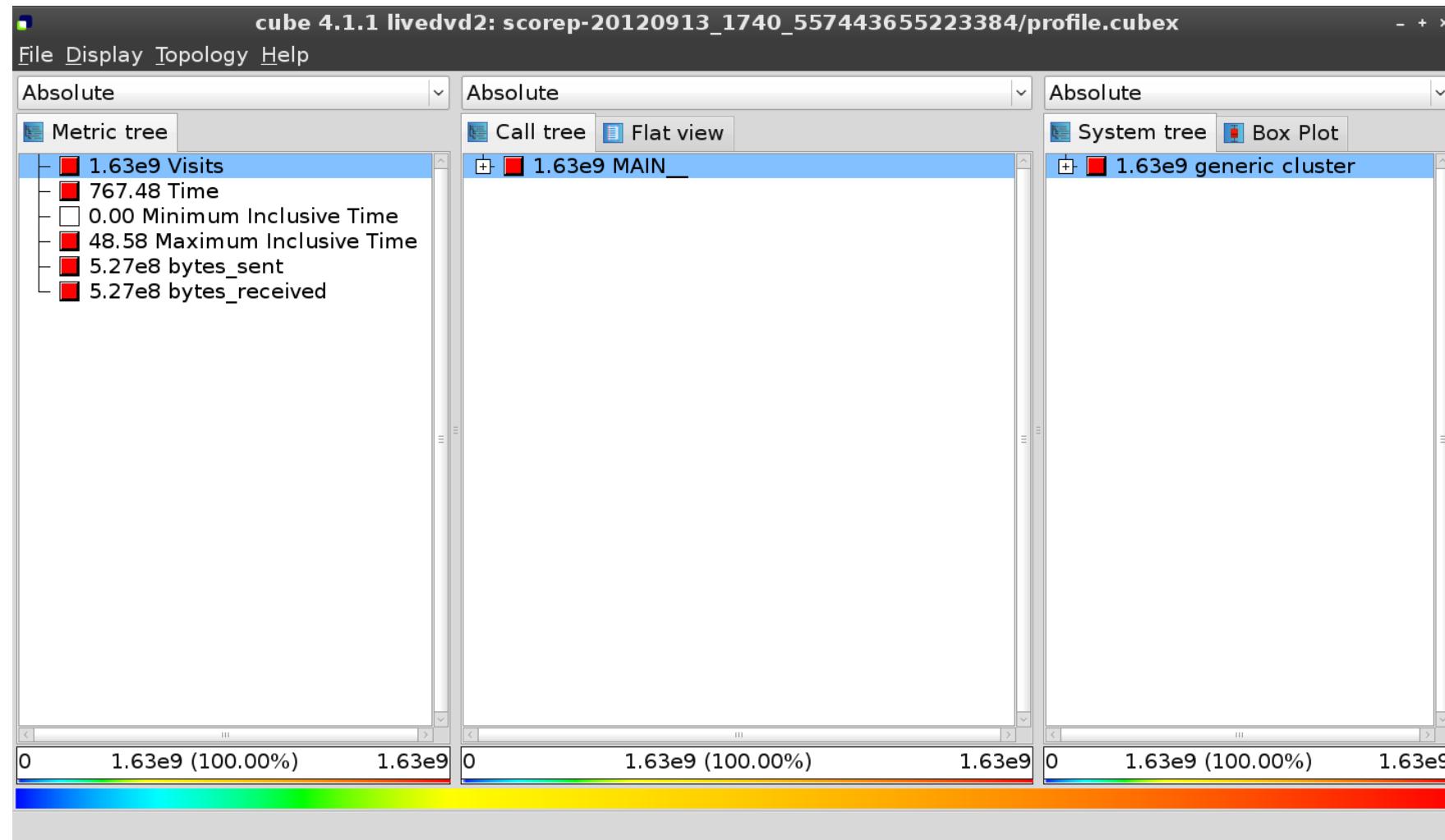
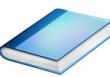
# Inclusive vs. exclusive values

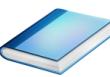


- Inclusive
  - Information of all sub-elements aggregated into single value
- Exclusive
  - Information cannot be subdivided further

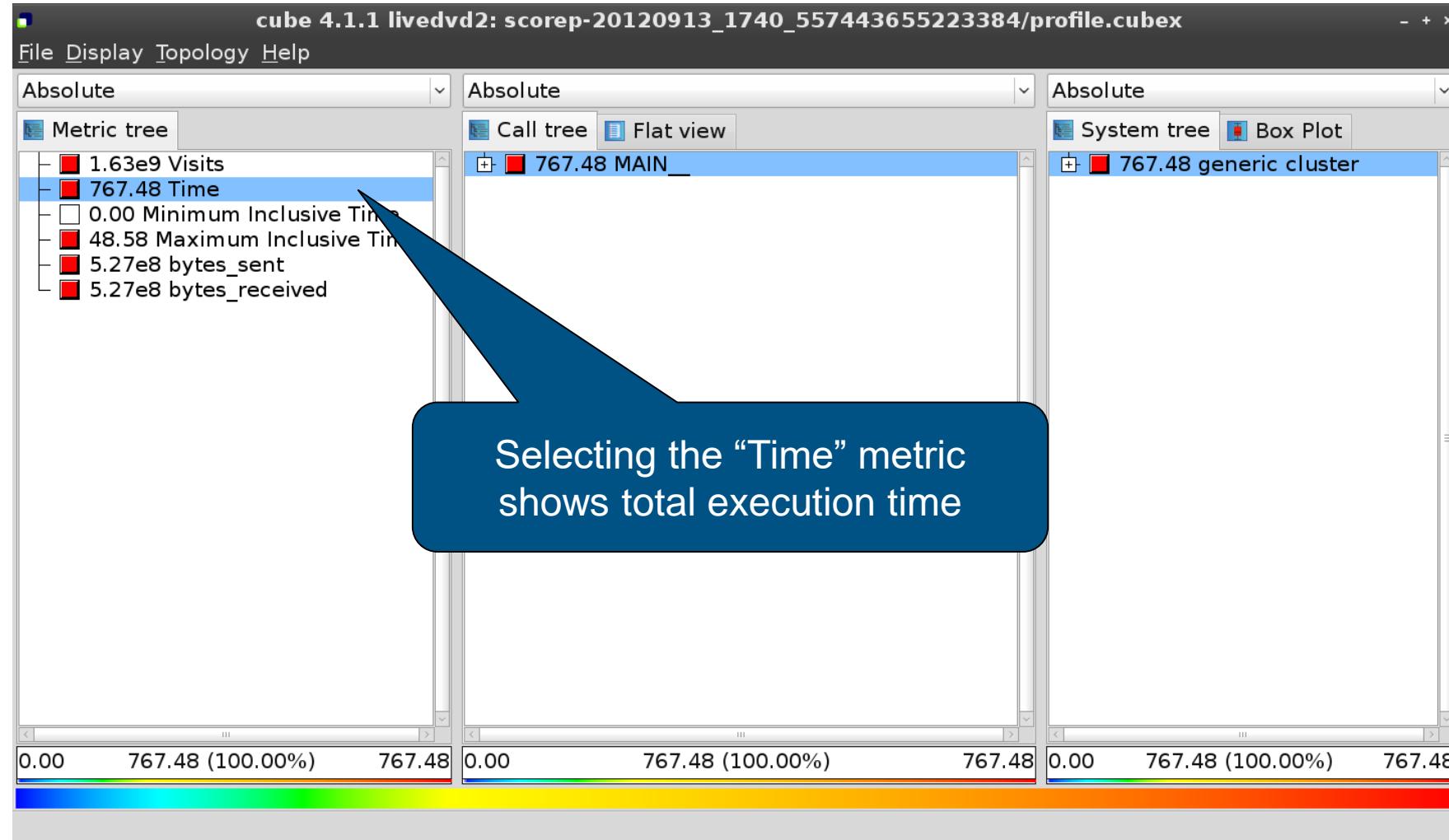


# Score-P analysis report exploration (opening view)



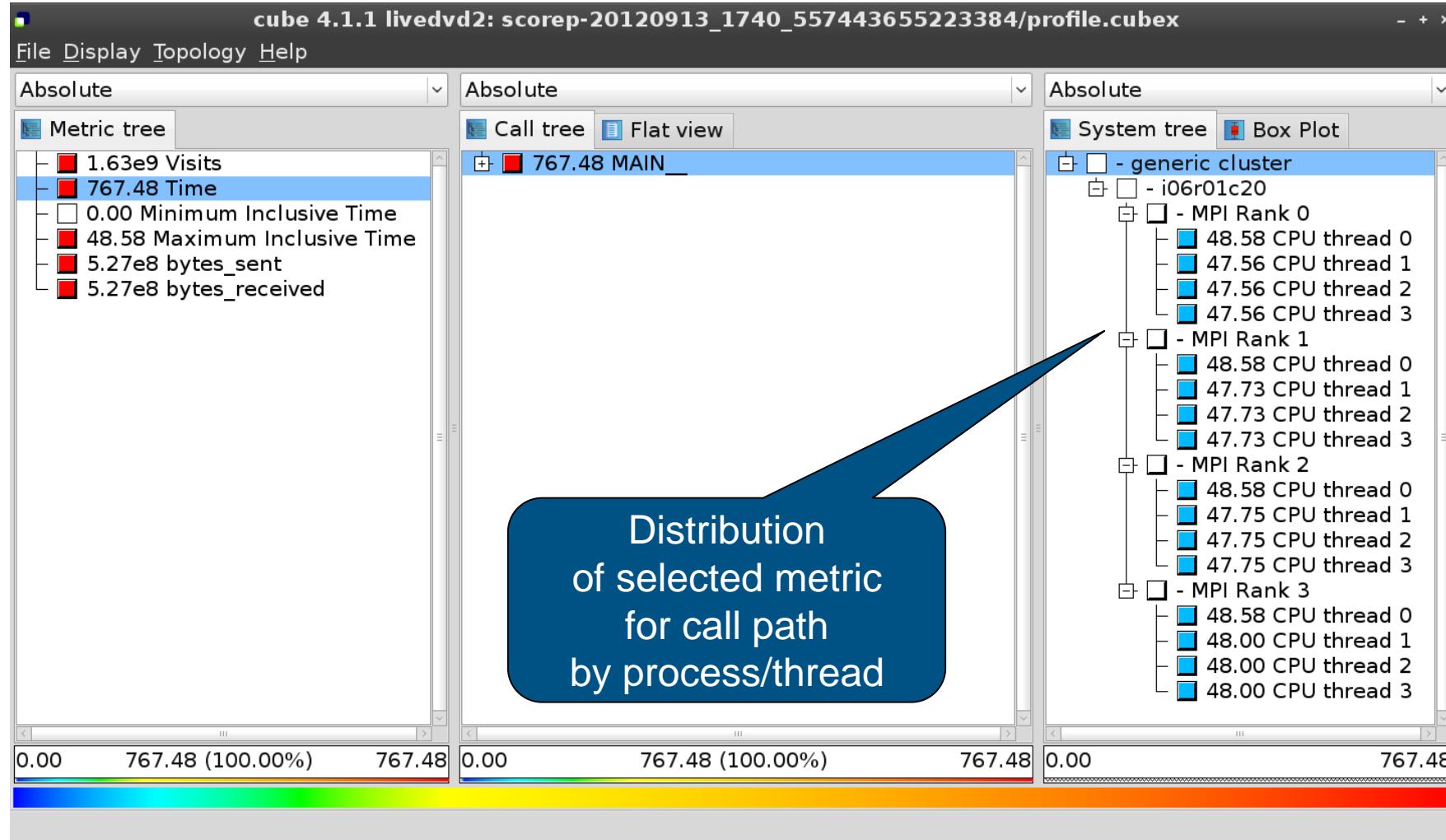


# Metric selection



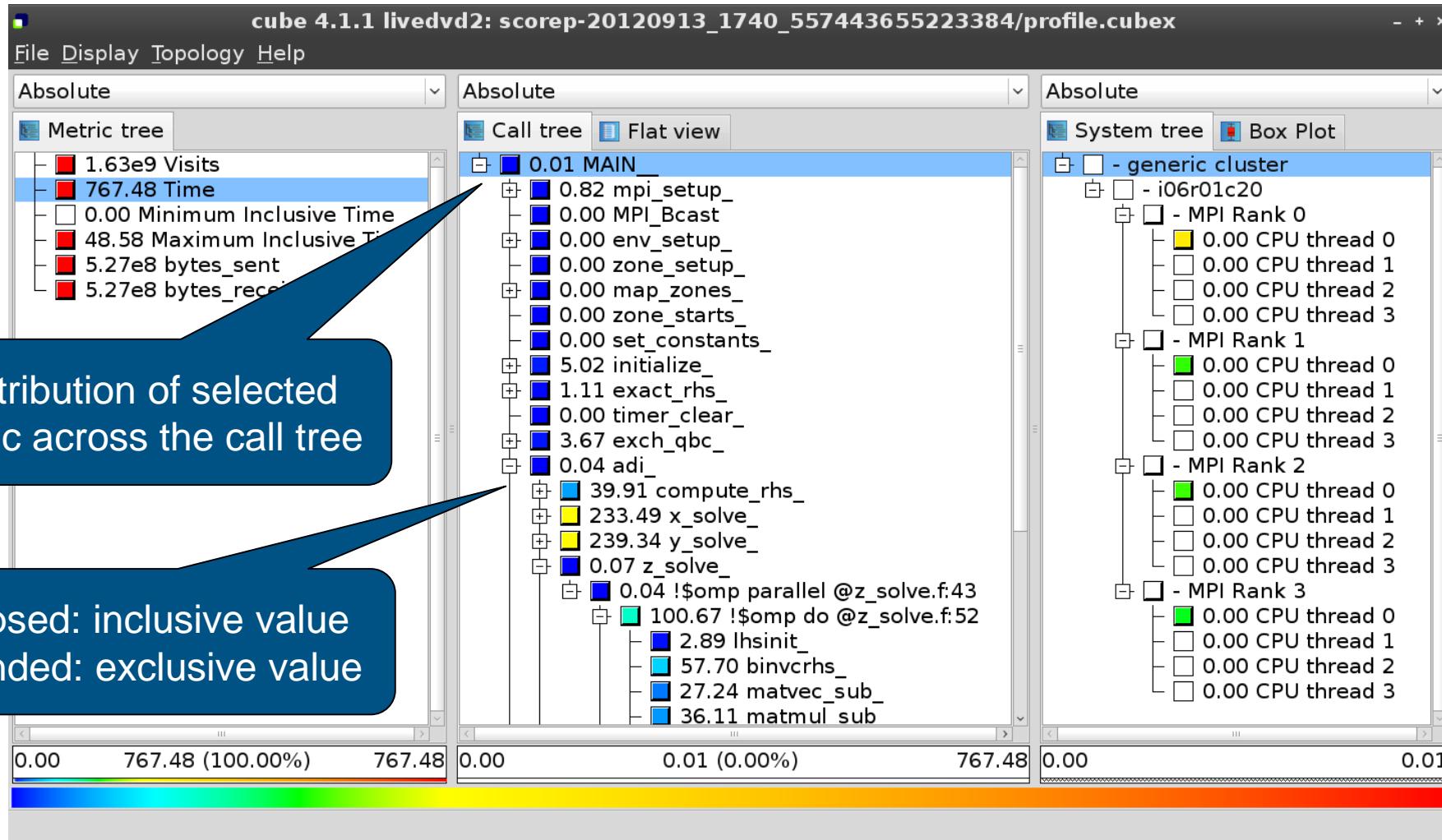


# Expanding the system tree



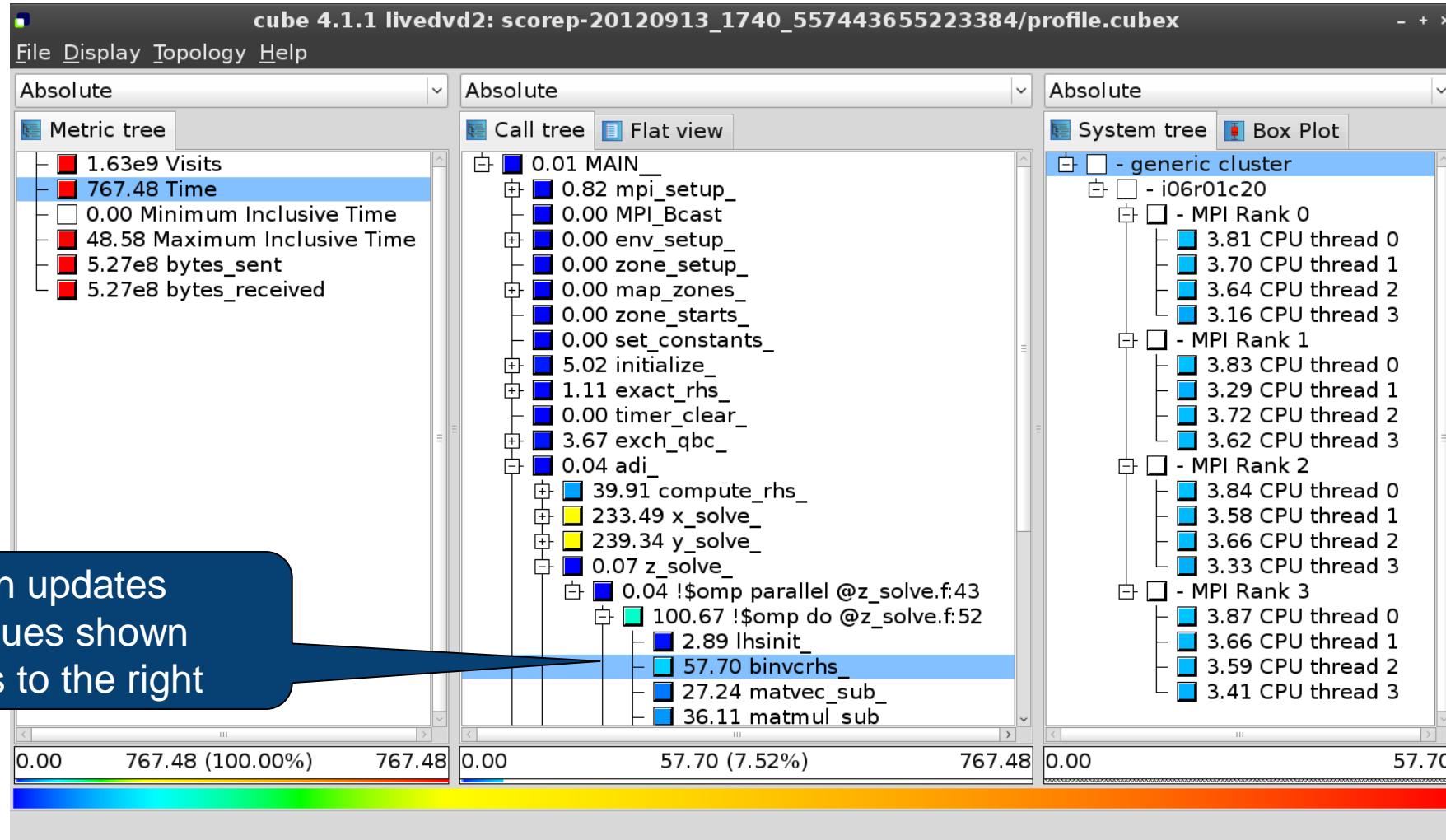


## Expanding the call tree



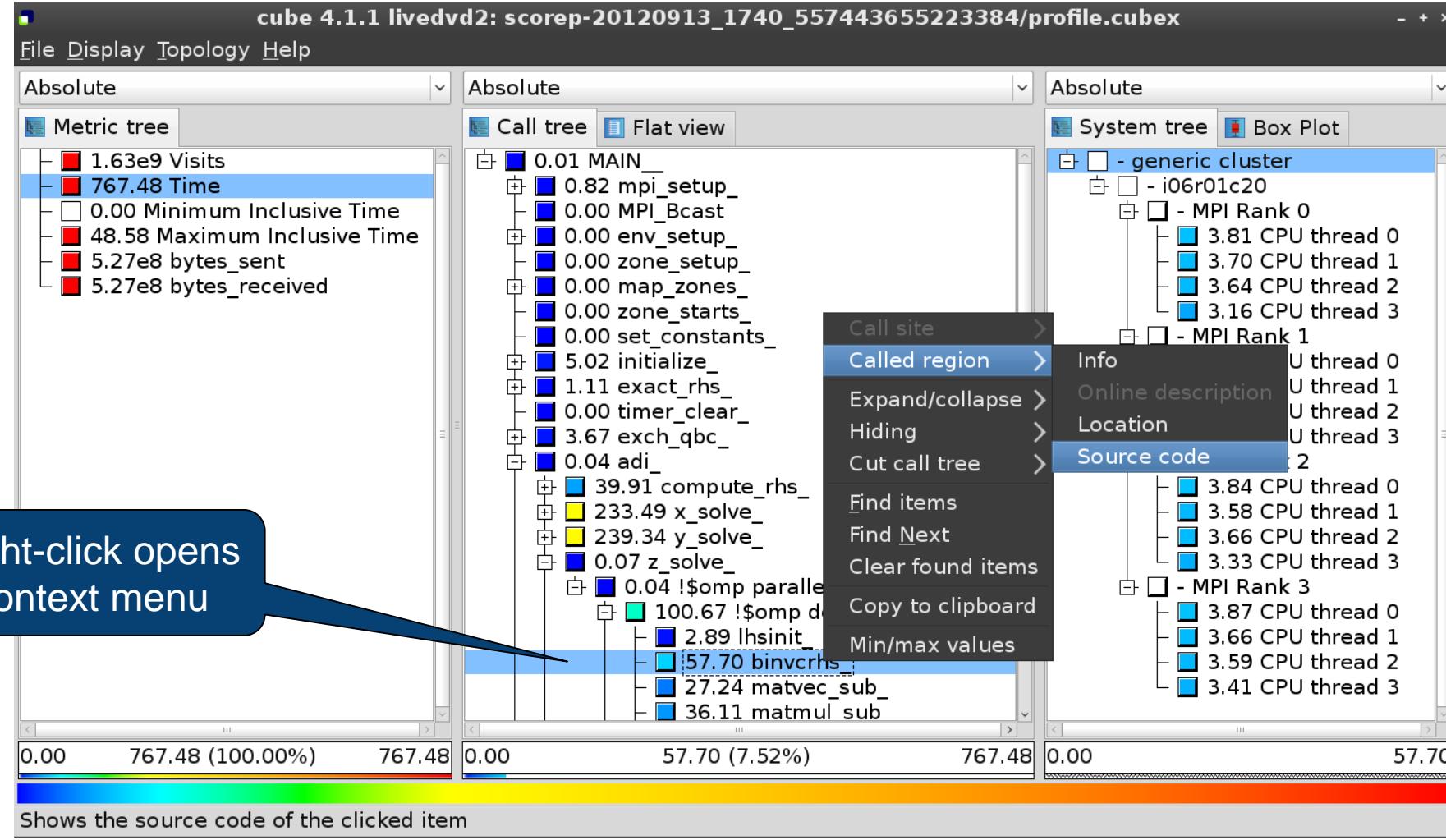


# Selecting a call path



Selection updates  
metric values shown  
in columns to the right

# Source-code view via context menu



# Source-code view



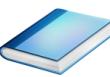
The screenshot shows a window titled "/home/geimer/Projects/Tests/NPB3.3-MZ-MPI/BT-MZ/solve\_subs.f". The code is as follows:

```
subroutine binvcrhs( lhs,c,r )  
c-----  
c-----  
c-----  
c-----  
implicit none  
double precision pivot, coeff, lhs  
dimension lhs(5,5)  
double precision c(5,5), r(5)  
c-----  
c-----  
pivot = 1.00d0/lhs(1,1)  
lhs(1,2) = lhs(1,2)*pivot  
lhs(1,3) = lhs(1,3)*pivot  
lhs(1,4) = lhs(1,4)*pivot  
lhs(1,5) = lhs(1,5)*pivot  
c(1,1) = c(1,1)*pivot  
c(1,2) = c(1,2)*pivot  
c(1,3) = c(1,3)*pivot  
c(1,4) = c(1,4)*pivot
```

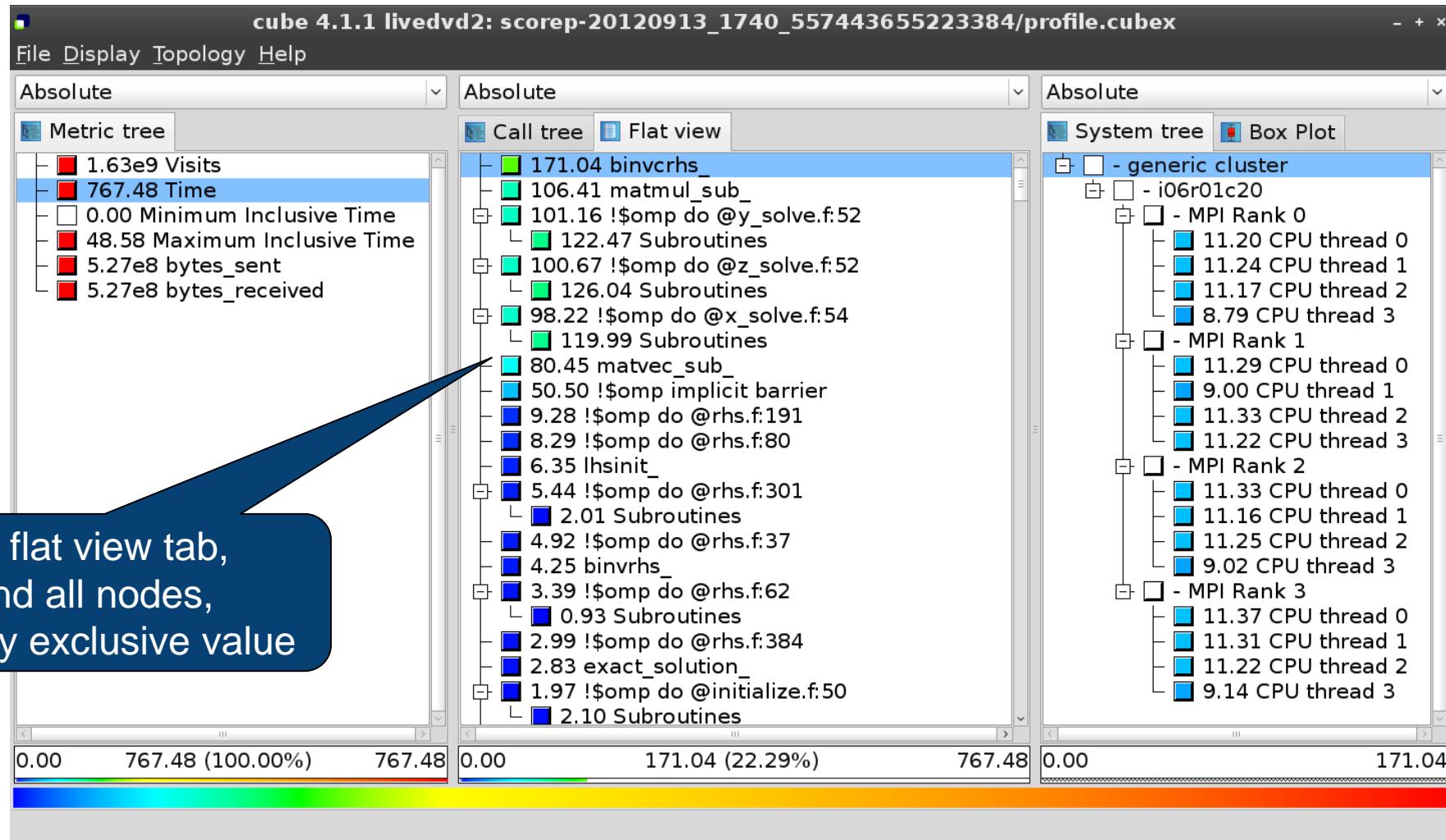
At the bottom of the window, there are buttons: "Read only" (radio button selected), "Save", "Save as", "Font...", and "Close".

**Note:**

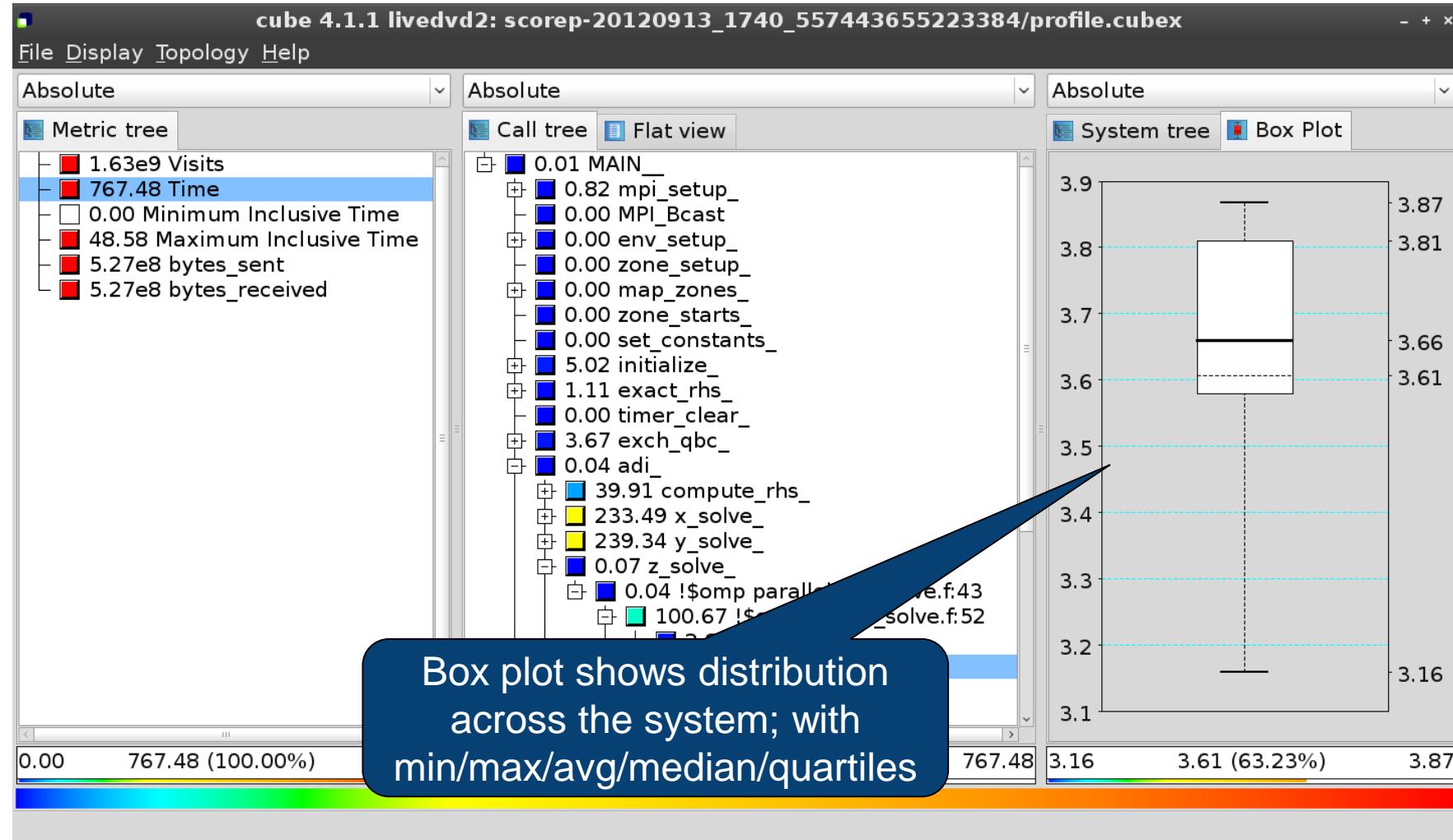
This feature depends on file and line number information provided by the instrumentation, i.e., it may not always be available



# Flat profile view

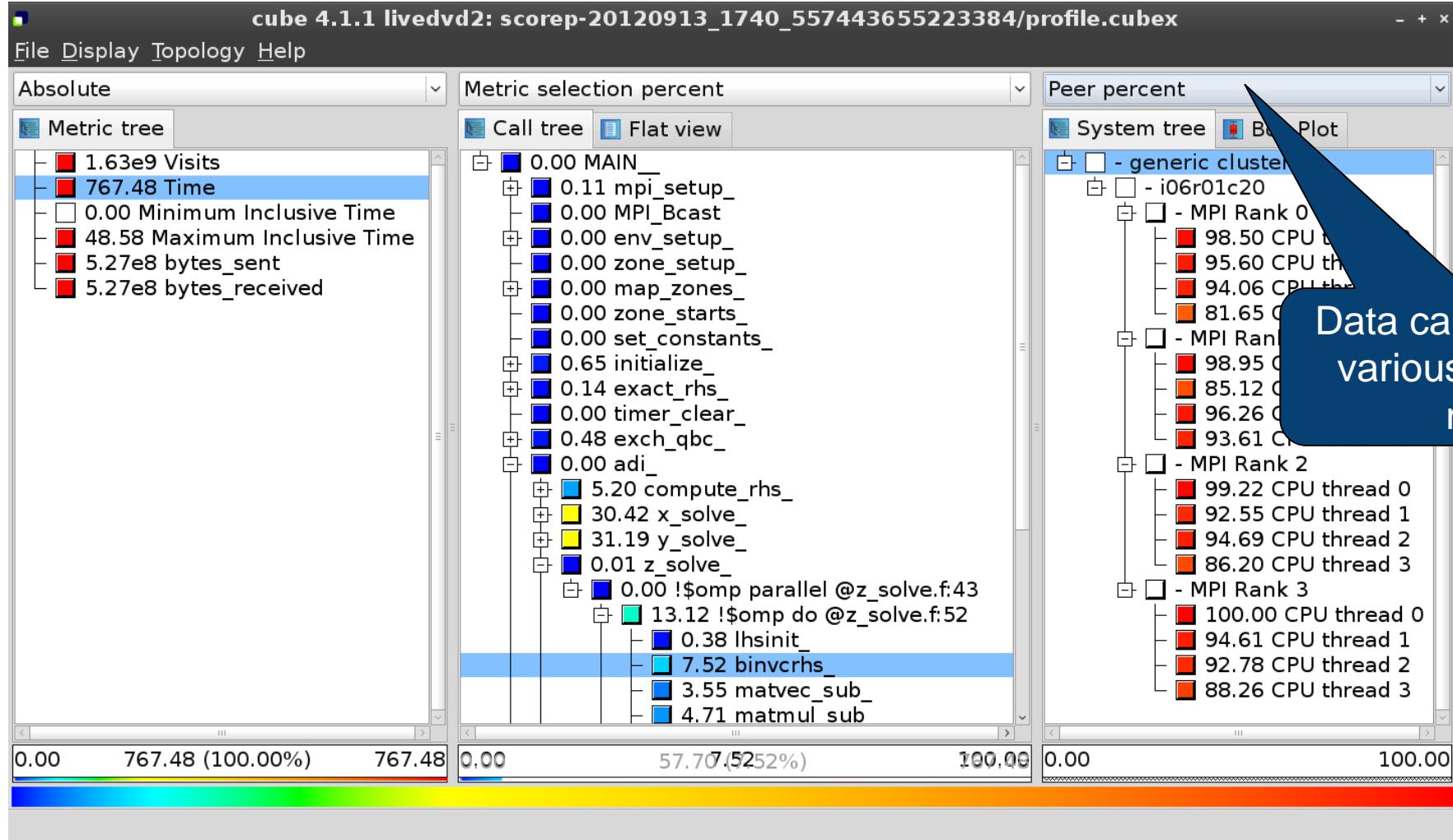


# Box plot view





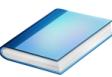
# Alternative display modes



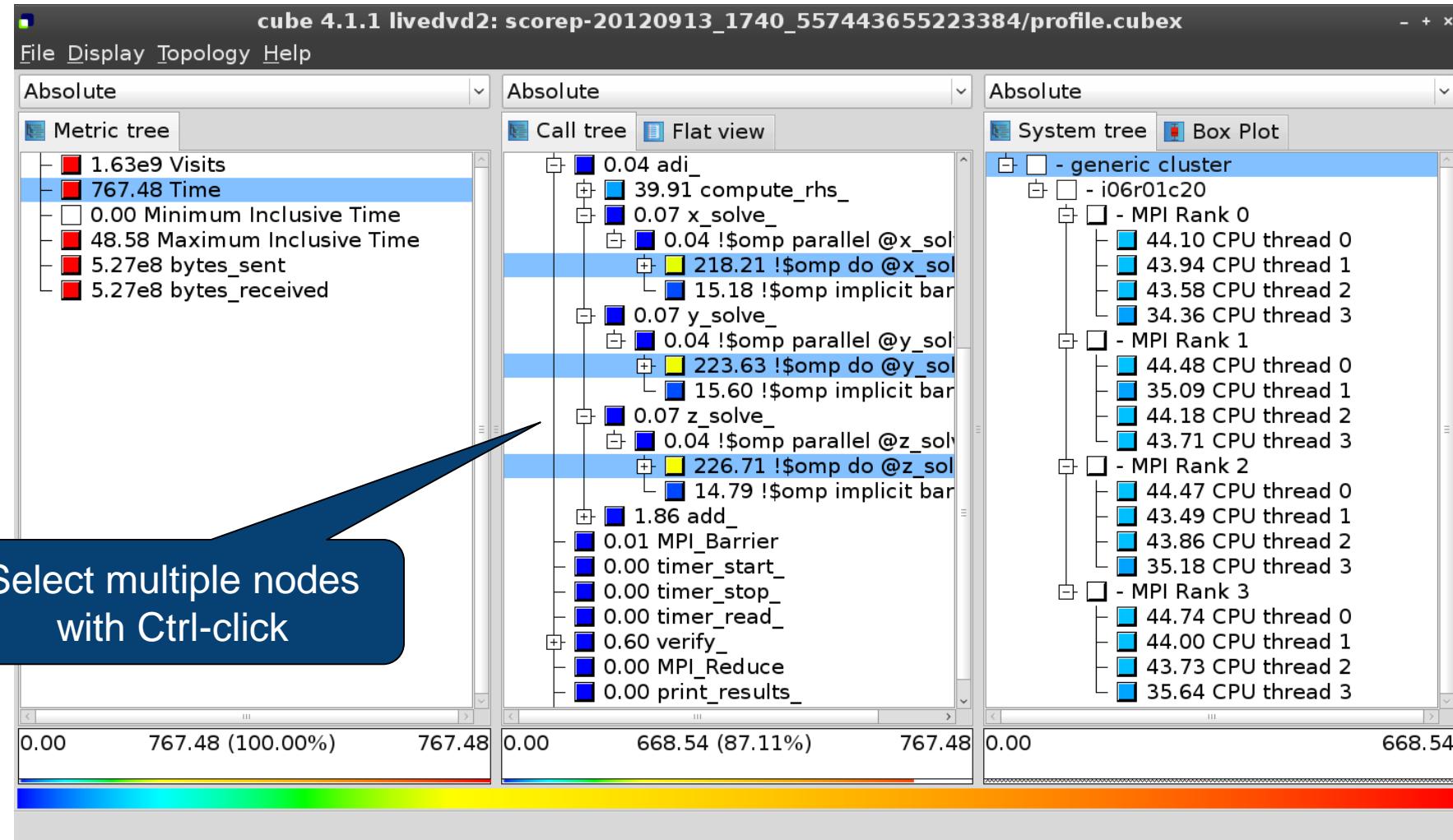
# Important display modes

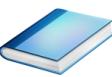


- Absolute
  - Absolute value shown in seconds/bytes/counts
- Selection percent
  - Value shown as percentage w.r.t. the selected node  
“on the left” (metric/call path)
- Peer percent (system tree only)
  - Value shown as percentage relative to the maximum peer value

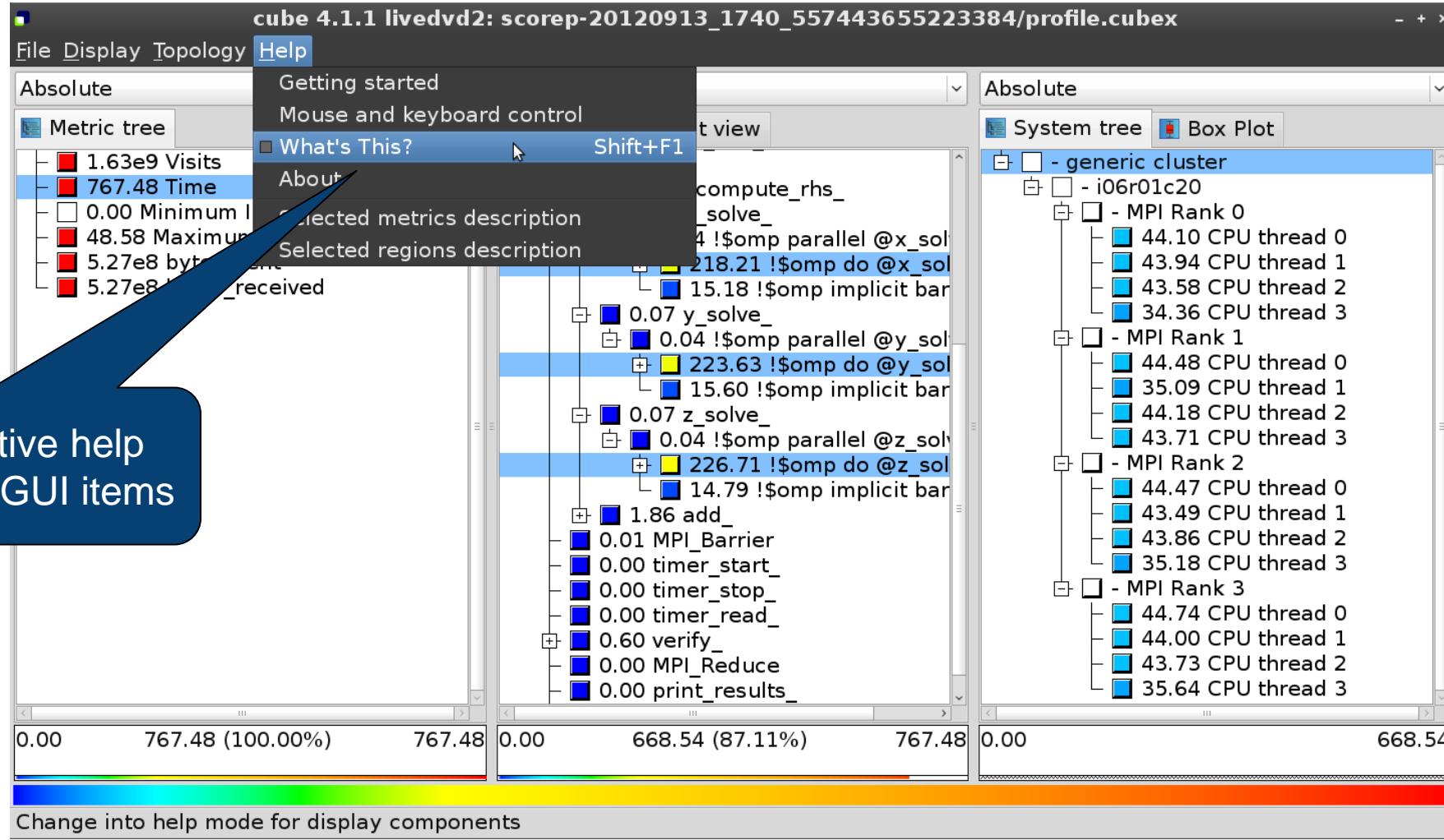


# Multiple selection





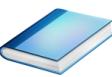
# Context-sensitive help



# 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

The screenshot shows the Cube 4.3.1 interface with three main panes:

- Metric tree:** Shows a collection of derived metrics, including "1.09e8 Visits (occ)", "1.01e6 Time (sec)", "0.00 Minimum Inclusive Time (sec)", "246.14 Maximum Inclusive Time (sec)", "7.18e12 bytes\_sent", and "7.18e12 bytes\_received".
- Call tree:** Shows the call graph for the "main" function, including nodes like "2512.10 ugshellInit", "1.01e6 ug::script::LoadUGScript", "2.11 ug::script::ParseBuffer", "0.04 ugshellFinalize", and "94.31 MPI\_Finalize".
- System tree:** Shows the system hierarchy for "machine Blue Gene/Q", including "rack 11", "midplane 1", "nodeboard 8", "nodecard 4", "0.65 MPI Rank 0", and "0.64 MPI Rank 1".

A modal dialog box is open in the center, titled "Create new metric as a child of metric". It contains the following fields:

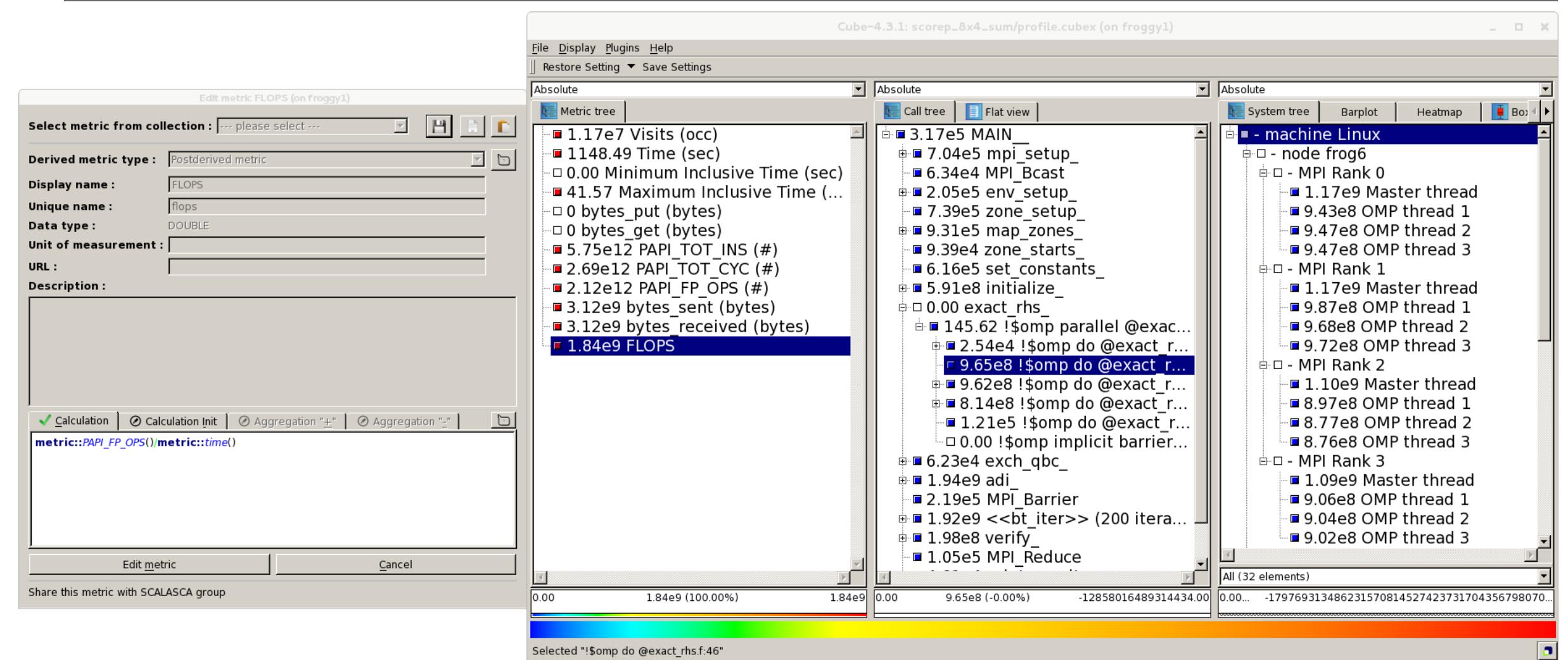
- Select metric from collection: Average execution time (kenobi)
- Derived metric type: Postderived metric
- Display name: Average visit time
- Unique name: avg\_visit\_time
- Data type: DOUBLE
- Unit of measurement: sec
- URL: (empty)
- Description: Calculates average time of region execution per visit.  
Autor is Michael Knobloch.

Below the dialog, a code editor shows the CubePL expression: `metric::time(i)|metric::visits(e)`. The status bar at the bottom indicates "Calculation" is selected.

Three callout boxes point to specific parts of the interface:

- Collection of derived metrics:** Points to the Metric tree pane.
- Parameters of the derived metric:** Points to the "Create new metric as a child of metric" dialog.
- CubePL expression:** Points to the code editor containing the expression `metric::time(i)|metric::visits(e)`.

# Example: FLOPS based on PAPI\_FP\_OPS and time



# 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 )
```

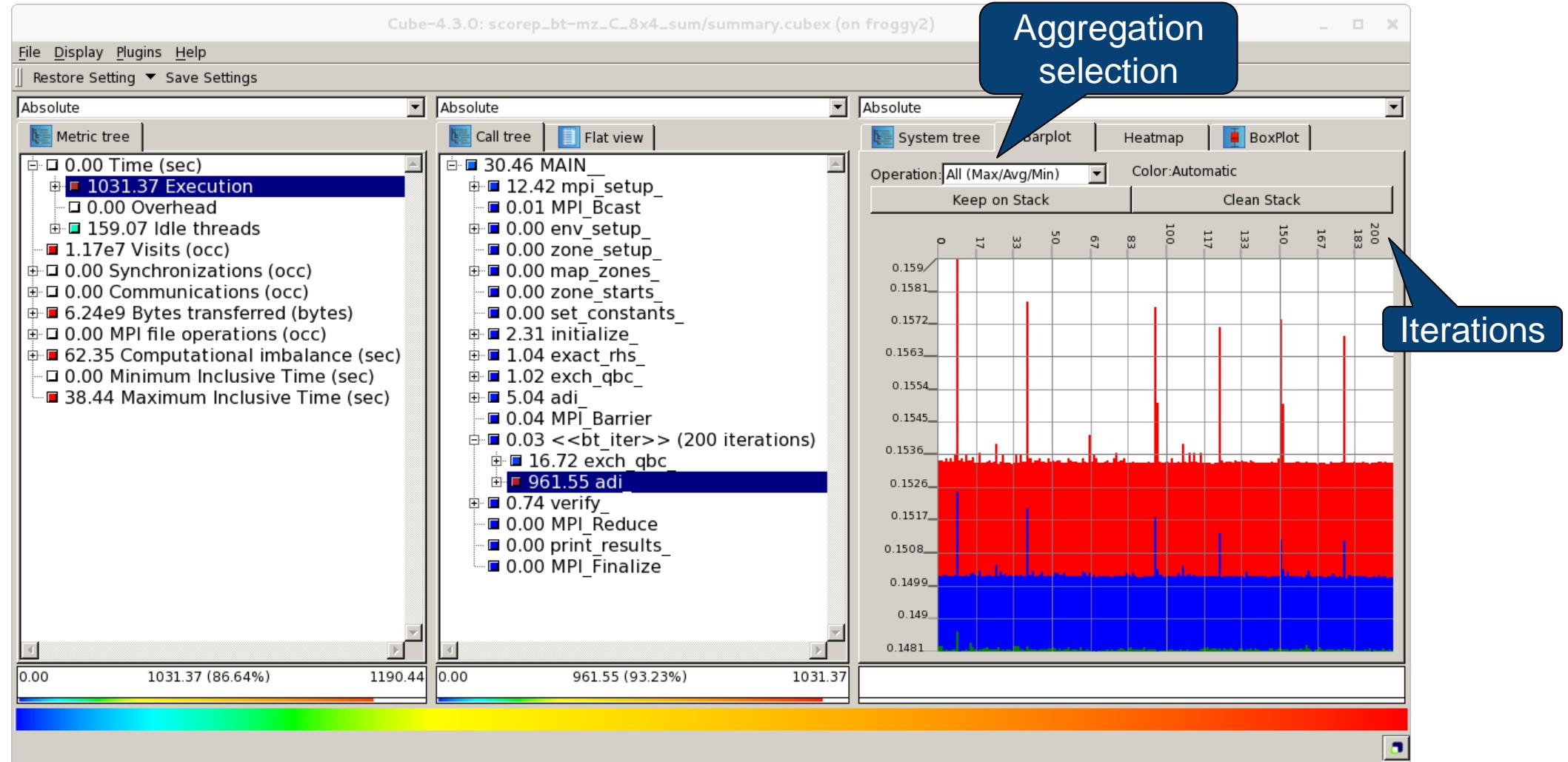
- Result in the Cube profile:
  - Iterations shown as separate call trees
    - Useful for checking results for specific iterations
  - Select your user-instrumented region and mark it as loop
  - Choose “Hide iterations”
  - View the Barplot statistics or the (thread x iterations) Heatmap

or

PARALLEL PERFORMANCE ANALYSIS USING SCALASCA (EDINBURGH, 29-30 APRIL 2024)

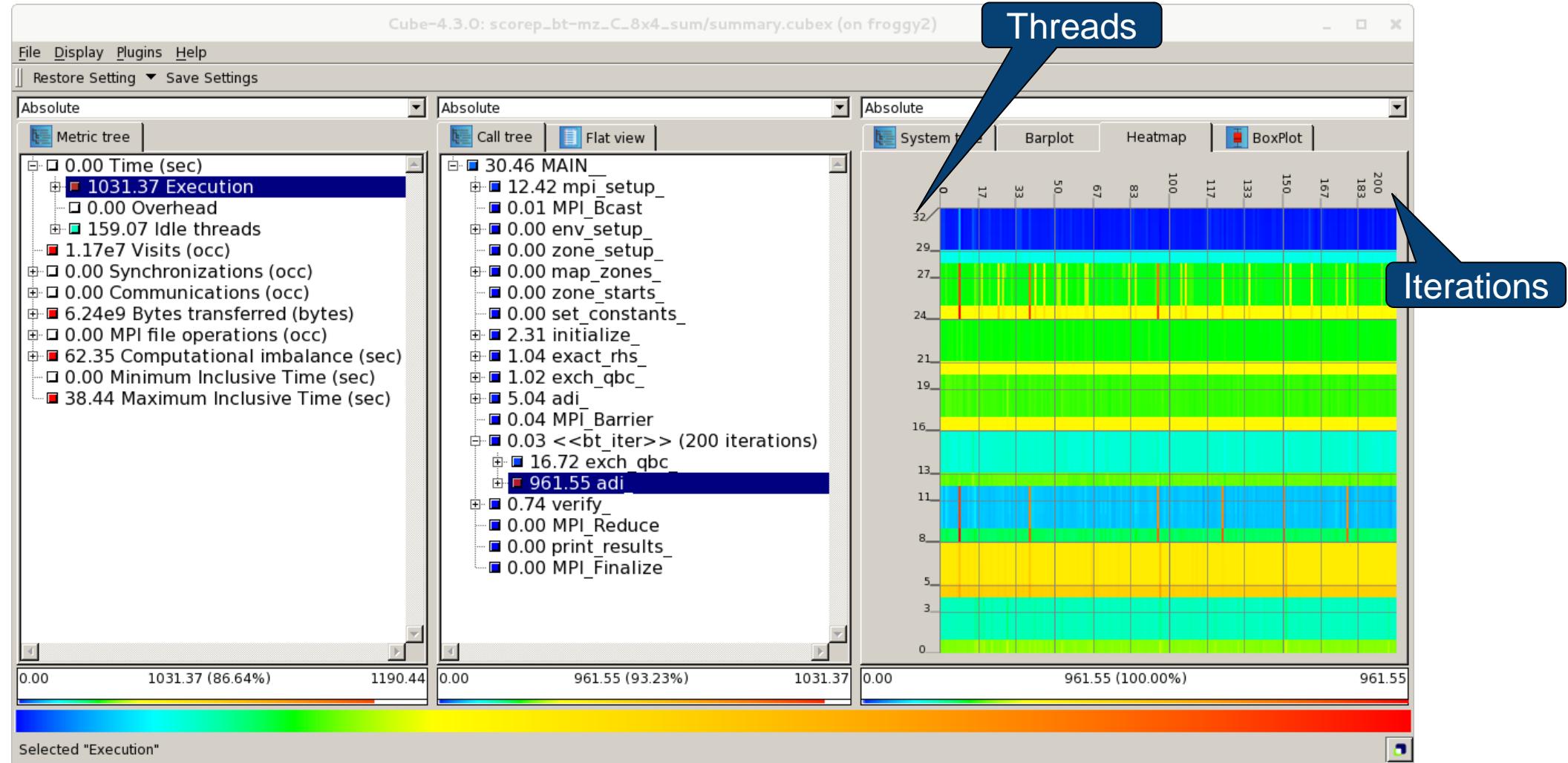


# Iteration profiling: Barplot





# Iteration profiling: Heatmap



# CUBE algebra utilities

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- Extracting solver sub-tree from analysis report

```
% cube_cut -r '<<ITERATION>>' scorep_bt-mz_C_16x8_sum/profile.cubex  
Writing cut.cubex... done.
```

- Calculating difference of two reports

```
% cube_diff scorep_bt-mz_C_16x8_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

## Square sneak preview

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- Scalasca provides **square** to facilitate analysis report exploration
  - square = scalasca –examine [OPTIONS] ( ./scorep\_expt\_sum | ./profile.cubex )
- Processes intermediate .cubex files produced by Score-P and Scout
  - profile.cubex -> summary.cubex
  - scout.cubex -> trace.cubex
- and (optionally) starts CUBE GUI with the post-processed file
  - containing additional derived metrics and metric hierarchies

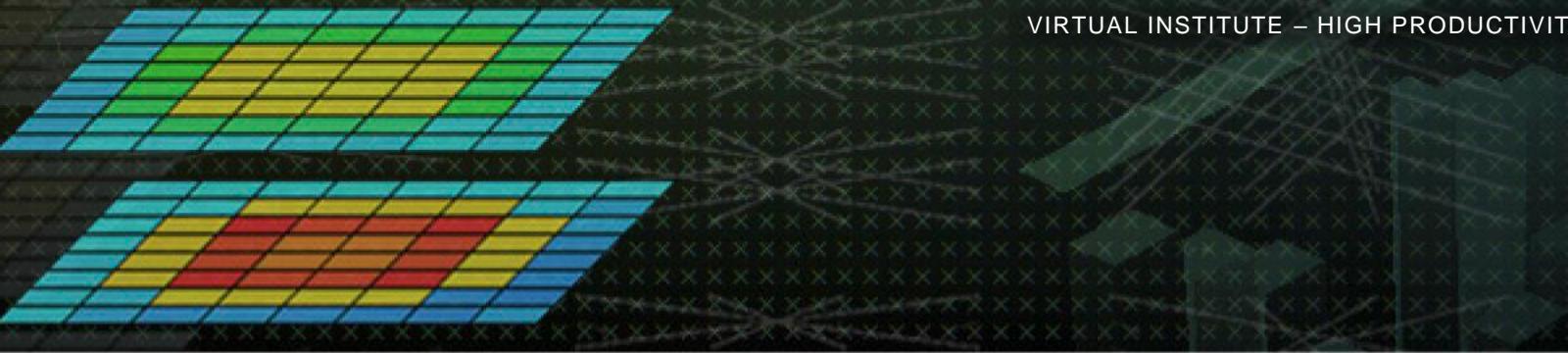


# Cube: Further information

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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:
  - <http://www.scalasca.org>
- User guide also part of installation:
  - <prefix>/share/doc/CubeGuide.pdf
- Contact:
  - mailto: [scalasca@fz-juelich.de](mailto:scalasca@fz-juelich.de)

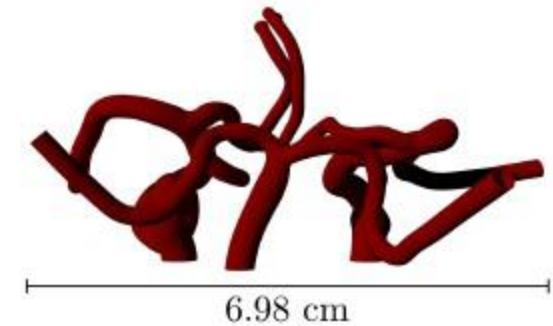




# Score-P/CUBE case study HemeLB

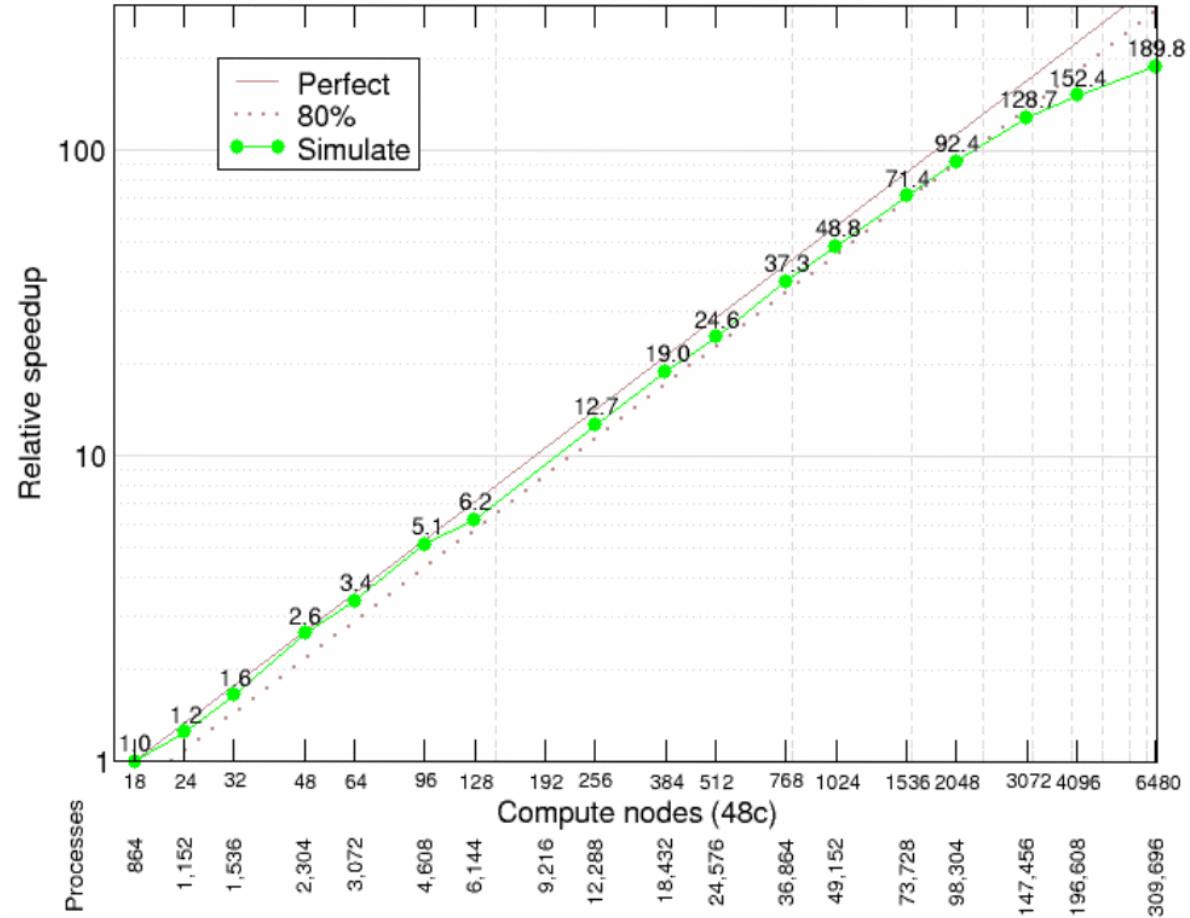
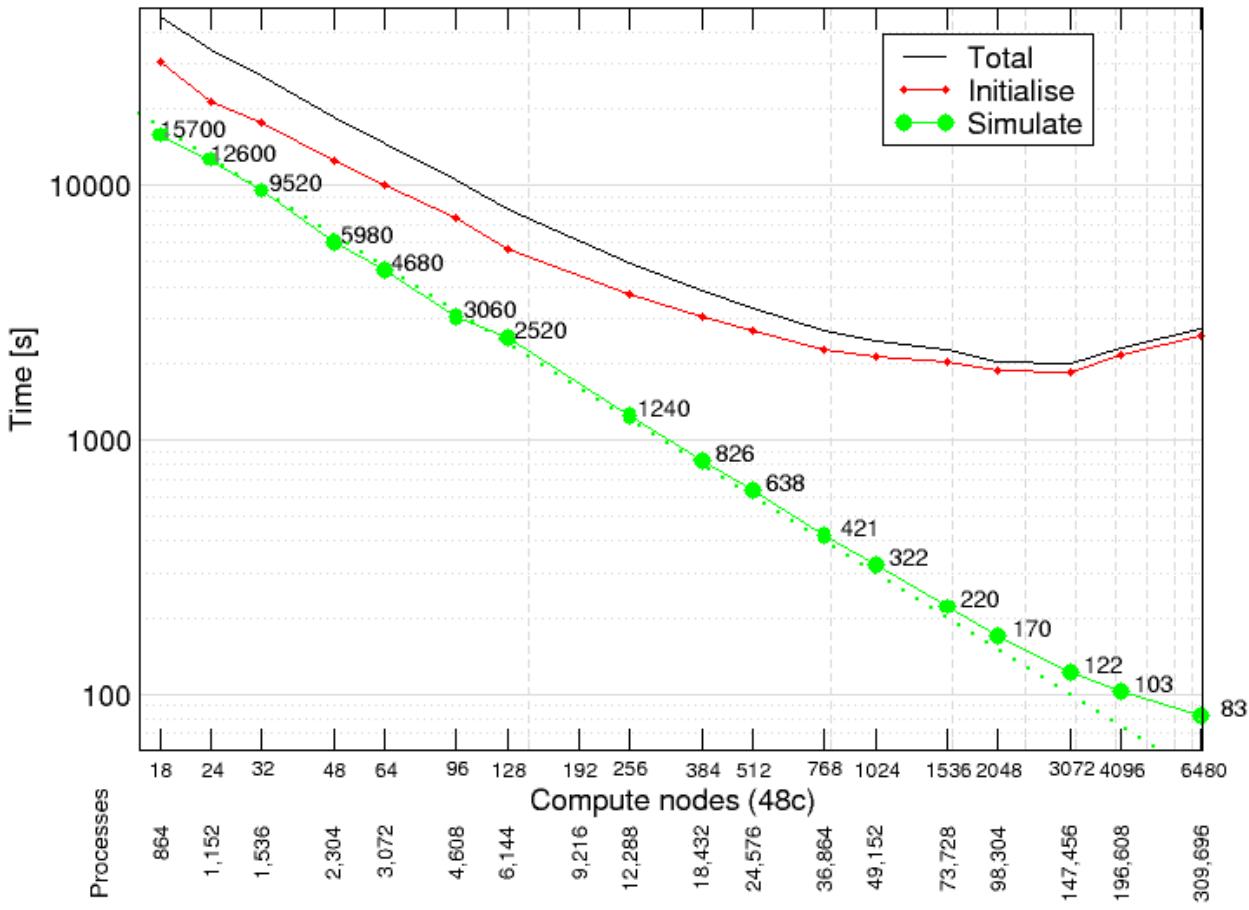
# HemeLB (SuperMUC-NG: no GPUs)

- 3D macroscopic blood flow in human arterial system developed by UC London (UK)
  - lattice-Boltzmann method tracking fluid particles on a lattice grid with complex boundary conditions
  - exascale flagship application of EU H2020 HPC Centre of Excellence for Computational Biomedicine
- HemeLB open-source code and test case: [www.hemelb.org](http://www.hemelb.org)
  - C++ parallelized with MPI [+ CUDA unused]
    - Intel Studio 2019u4 compiler and MPI library (v19.0.4.243)
    - configured with 2 'reader' processes (intermediate MPI file writing disabled)
    - MPI-3 shared-memory model employed within compute nodes to reduce memory requirements when distributing lattice blocks from reader processes
  - Focus of analysis 5,000 time-step (500 $\mu$ s) simulation of cerebrovascular "circle of Willis" geometry
    - 6.4 $\mu$ m lattice resolution (21.15 GiB): 10,154,448,502 lattice sites
- Executed on *SuperMUC-NG* Lenovo ThinkSystem SD650 (LRZ):
  - 2x 24-core Intel Xeon Platinum 8174 ('Skylake') @ 3.1GHz
  - 48 MPI processes/node, 6452 (of 6480) compute nodes: 309,696 MPI processes
  - 190x speed-up from 864 cores: 80% scaling efficiency to over 100,000 cores



⇒ ***Identification & quantification of impact of load balance and its variation***

# HemeLB@SNG strong scaling of FOA *RunSimulation*



[Execution of 9,216 processes on 192 compute nodes not possible due to insufficient compute nodes with adequate memory in 'fat' partition (768 GiB vs. regular 96 GiB node memory)]

# HemeLB@SNG strong scaling efficiency of FOA *RunSimulation*

Compute nodes	24	32	48	64	96	128	192	256	384	512	768	1024	1536	2048	3072	4096	6452
Processes	1152	1536	2304	3072	4608	6144	9216	12288	18432	24576	36864	49152	73728	98304	147456	196608	309696
<b>Global scaling efficiency</b>	0.79	0.79	0.84	0.80	0.82	0.75		0.73	0.72	0.73	0.74	0.68	0.68	0.65	0.62	0.57	0.45
- Parallel efficiency	0.79	0.80	0.87	0.83	0.86	0.80		0.75	0.74	0.74	0.77	0.71	0.72	0.70	0.72	0.70	0.73
- - Load balance efficiency	0.79	0.80	0.88	0.84	0.86	0.80		0.75	0.74	0.75	0.78	0.72	0.74	0.72	0.74	0.73	0.80
- - Communication efficiency	1.00	1.00	1.00	1.00	1.00	1.00		1.00	1.00	0.99	0.99	0.99	0.98	0.98	0.97	0.96	0.92
- - Computation scaling	1.00	0.99	0.96	0.96	0.95	0.93		0.98	0.98	0.98	0.96	0.96	0.94	0.93	0.87	0.81	0.61
- - Instructions scaling	1.00	1.00	1.00	1.00	1.00	1.00		1.00	1.00	1.00	0.99	0.97	0.94	0.89	0.79	0.67	0.45
- - IPC scaling	1.00	0.99	0.96	0.96	0.95	0.93		0.98	0.98	0.99	0.98	0.99	1.00	1.04	1.11	1.21	1.36
IPC	1.411	1.395	1.353	1.355	1.342	1.316		1.377	1.387	1.396	1.383	1.390	1.417	1.473	1.566	1.704	1.919
												Key: <0.65 <0.75 <0.85 <0.95 <1.00 >1.00					

Global scaling efficiency fairly good around 80%, before degrading at larger scales

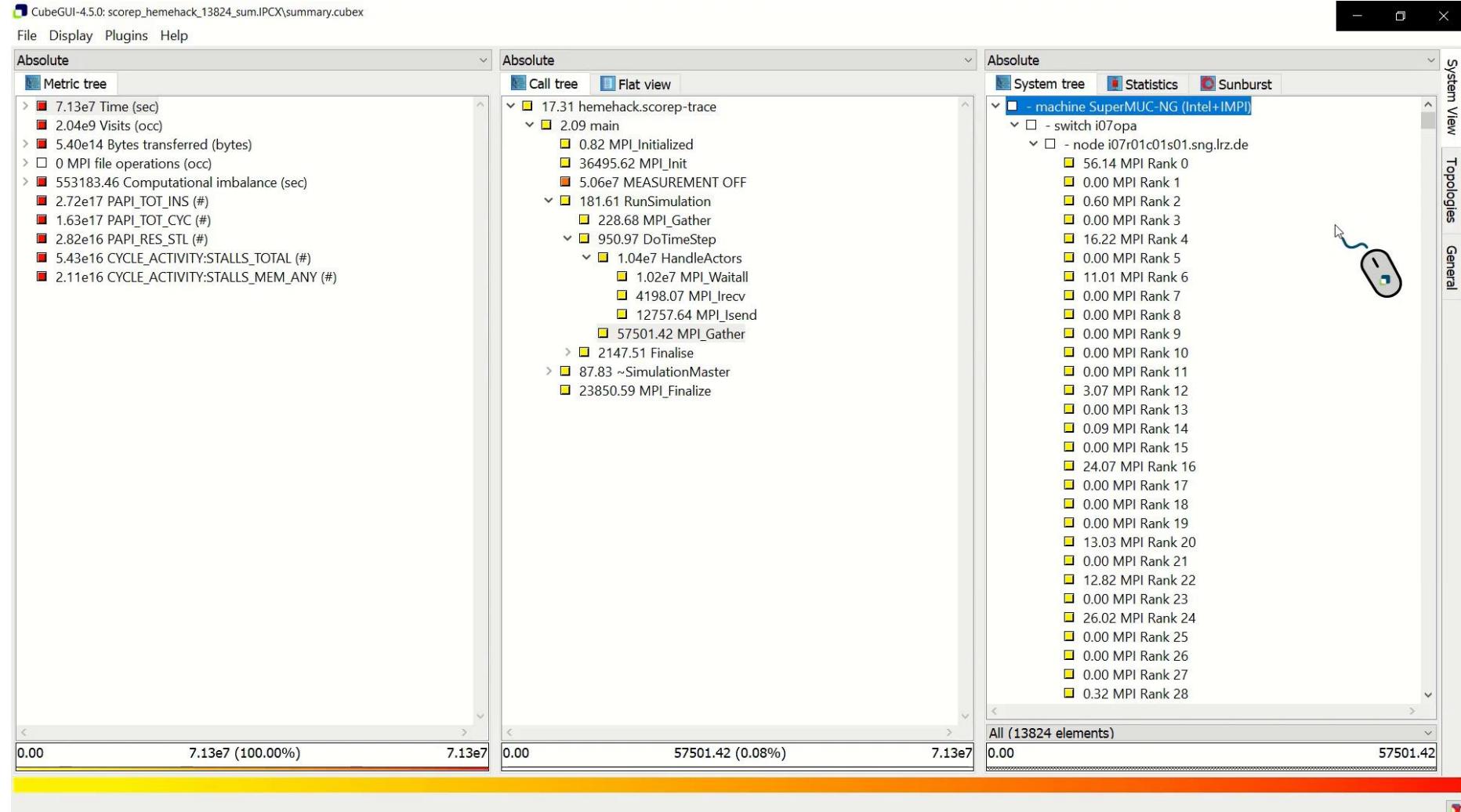
- Parallel efficiency deteriorating following Load balance efficiency
    - Communication efficiency excellent throughout
  - Computation scaling (relative to 1152 processes) very good except at largest scale
    - Degradation of Instructions scaling partially compensated by improving IPC scaling
- [POP CoE scaling efficiency model: [www.pop-coe.eu](http://www.pop-coe.eu)]



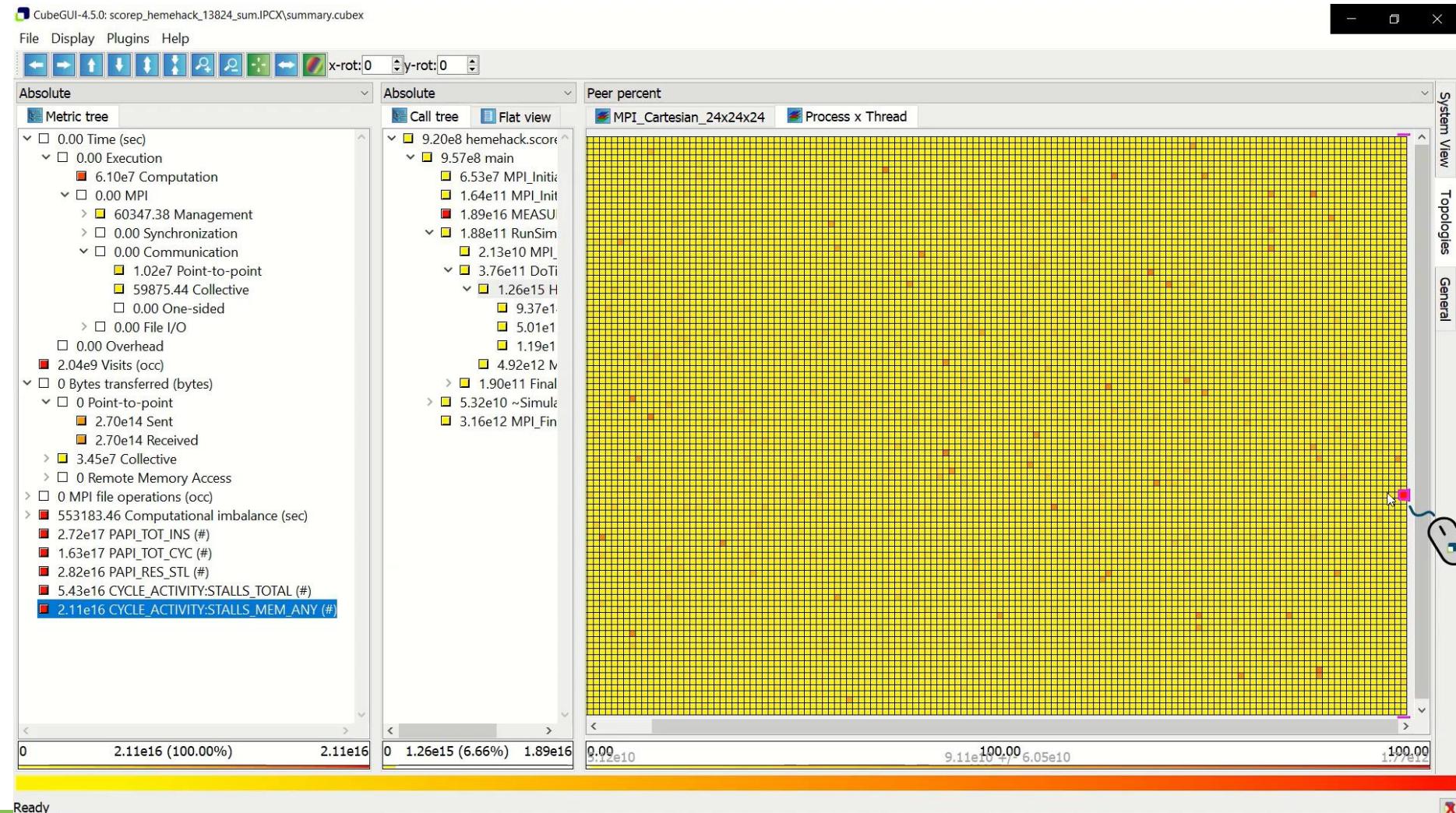
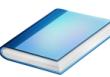
# Initial tree presentation: Time of MPI\_Gather per MPI process



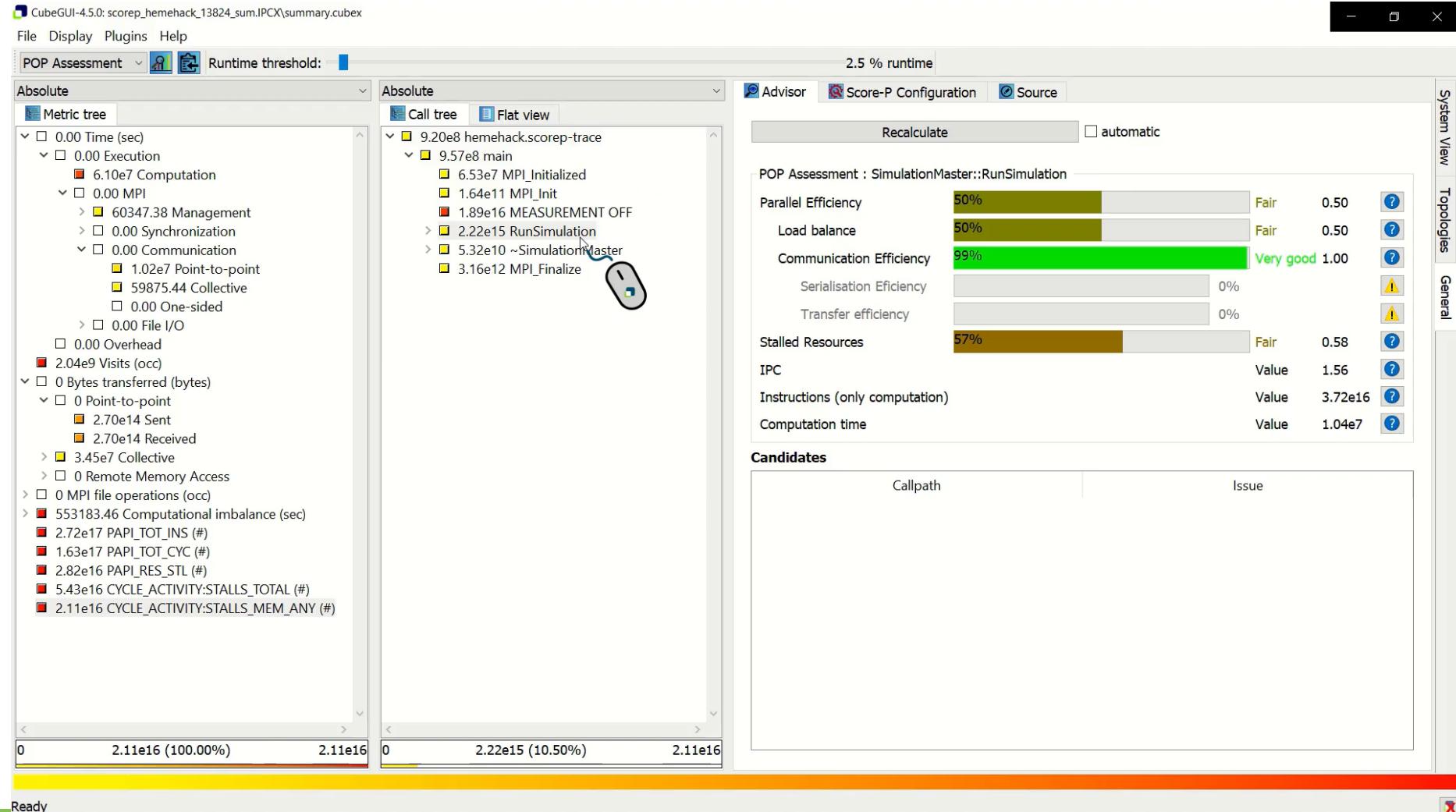
DOI 10.5281/zenodo.4080701



# Topological presentation: STALLS\_MEM\_ANY for HandleActors



# Advisor: POP efficiency assessment for RunSimulation



# HemeLB (JUWELS-Volta)

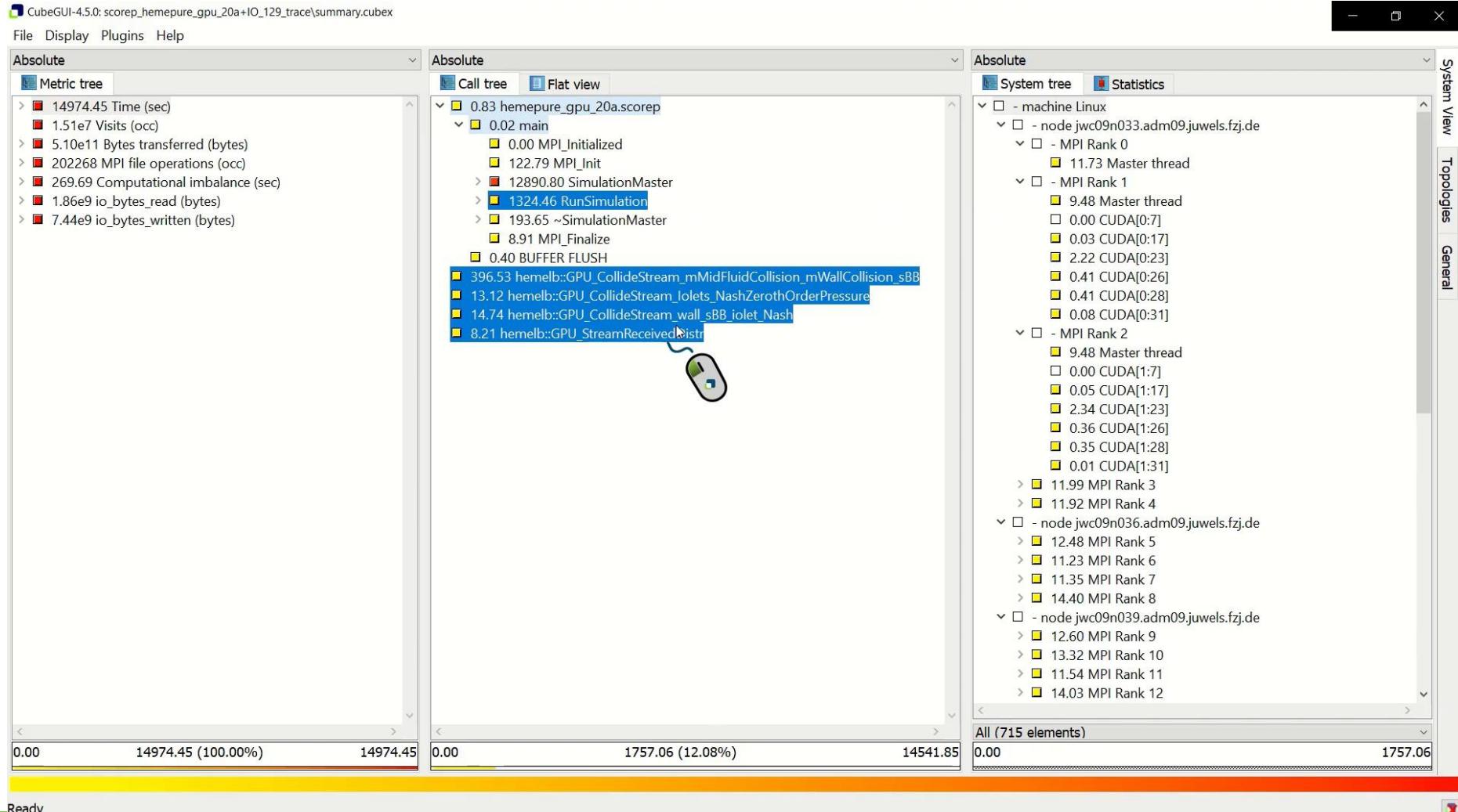
- 3D macroscopic blood flow in human arterial system developed by UC London (UK)
    - lattice-Boltzmann method tracking fluid particles on a lattice grid with complex boundary conditions
    - exascale flagship application of EU H2020 HPC Centre of Excellence for Computational Biomedicine
  - HemeLB open-source code and test case: [www.hemelb.org](http://www.hemelb.org)
    - C++ parallelized with MPI + CUDA (in development)
      - GCC/8.3.0 compiler, CUDA/10.1.105 and ParaStationMPI/5.4 library
      - configured with 2 'reader' processes and intermediate MPI file writing
      - rank 0 'monitor' process doesn't participate in simulation
  - Focus of analysis 2,000 time-step (each 100 $\mu$ s) simulation of CBM2019\_Arteries\_patched geometry
    - 1.78 GiB: 66,401,494 lattice sites, 1+38 iolets
  - Executed on *JUWELS-Volta* (@JSC):
    - 2x 20-core Intel Xeon Platinum 8168 ('Skylake') CPUs + 4 Nvidia V100 'Volta' GPUs
    - 4\* MPI processes/node (one per GPU), 32 (of 56) compute nodes: 129 MPI processes
- ⇒ ***Identification & quantification of impact of load balance and its variation***



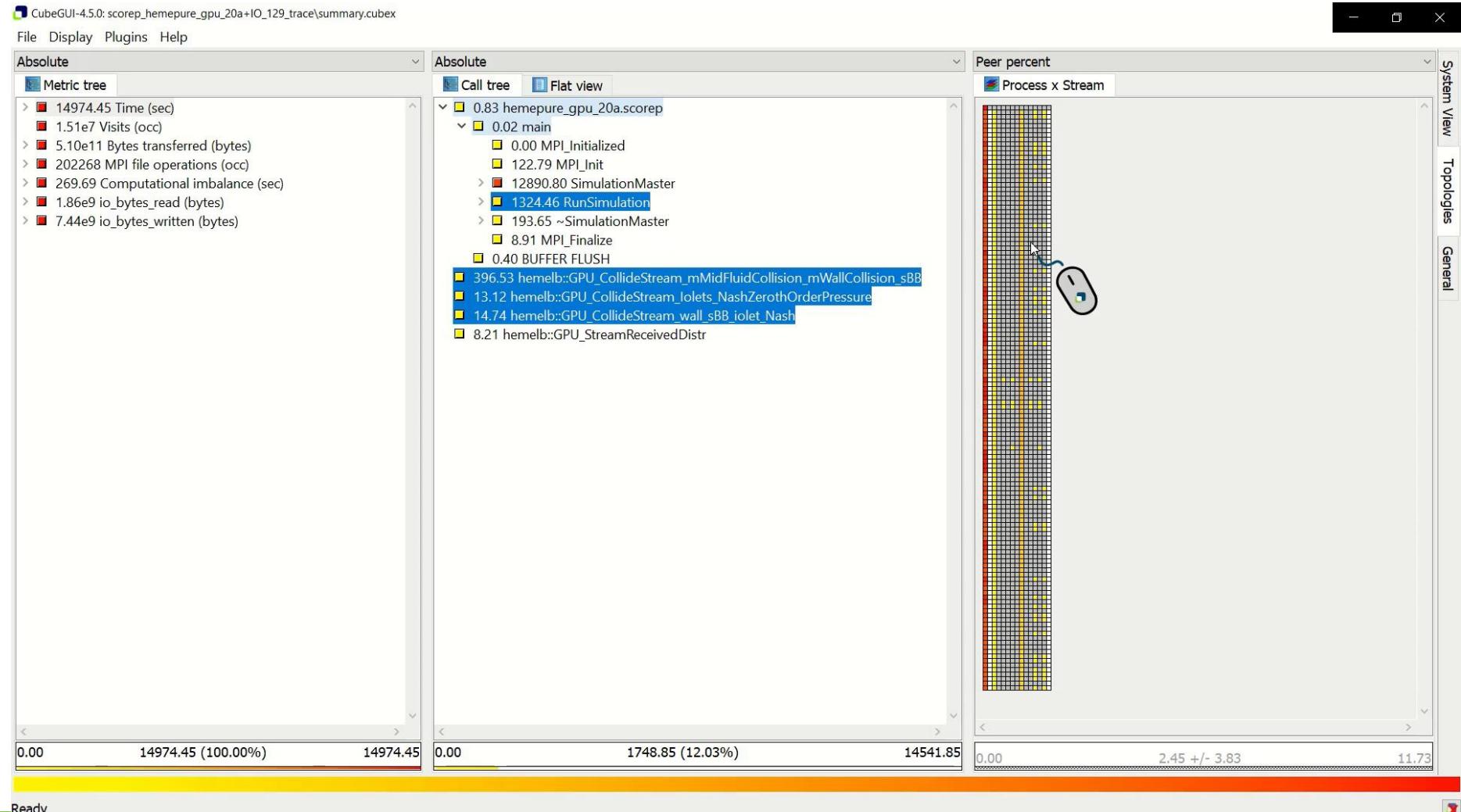
# Tree: Time for asynch. CUDA kernels on separate CUDA streams



DOI 10.5281/zenodo.4081080

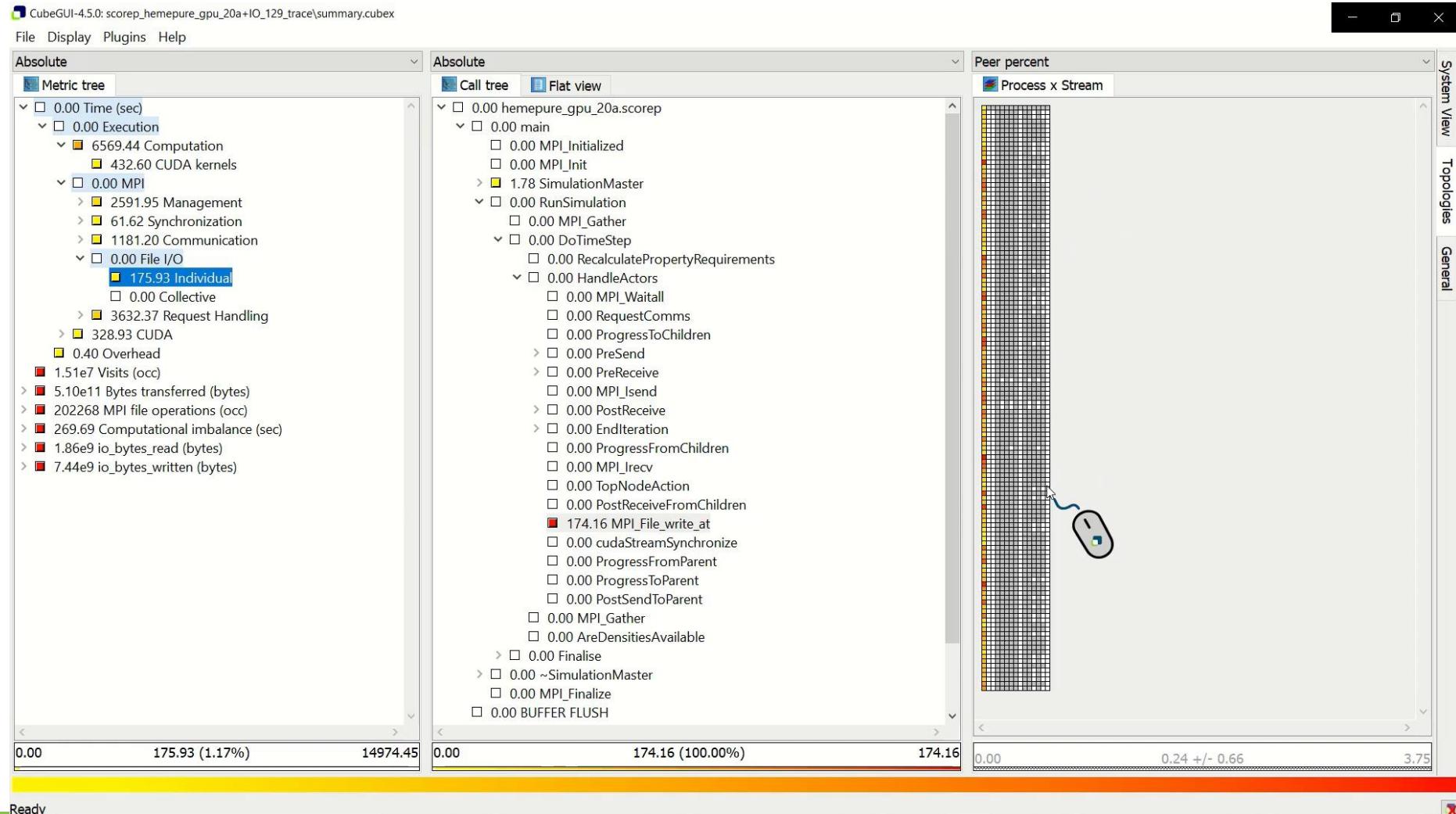


# Topo: Time for asynch. CUDA kernels on separate CUDA streams

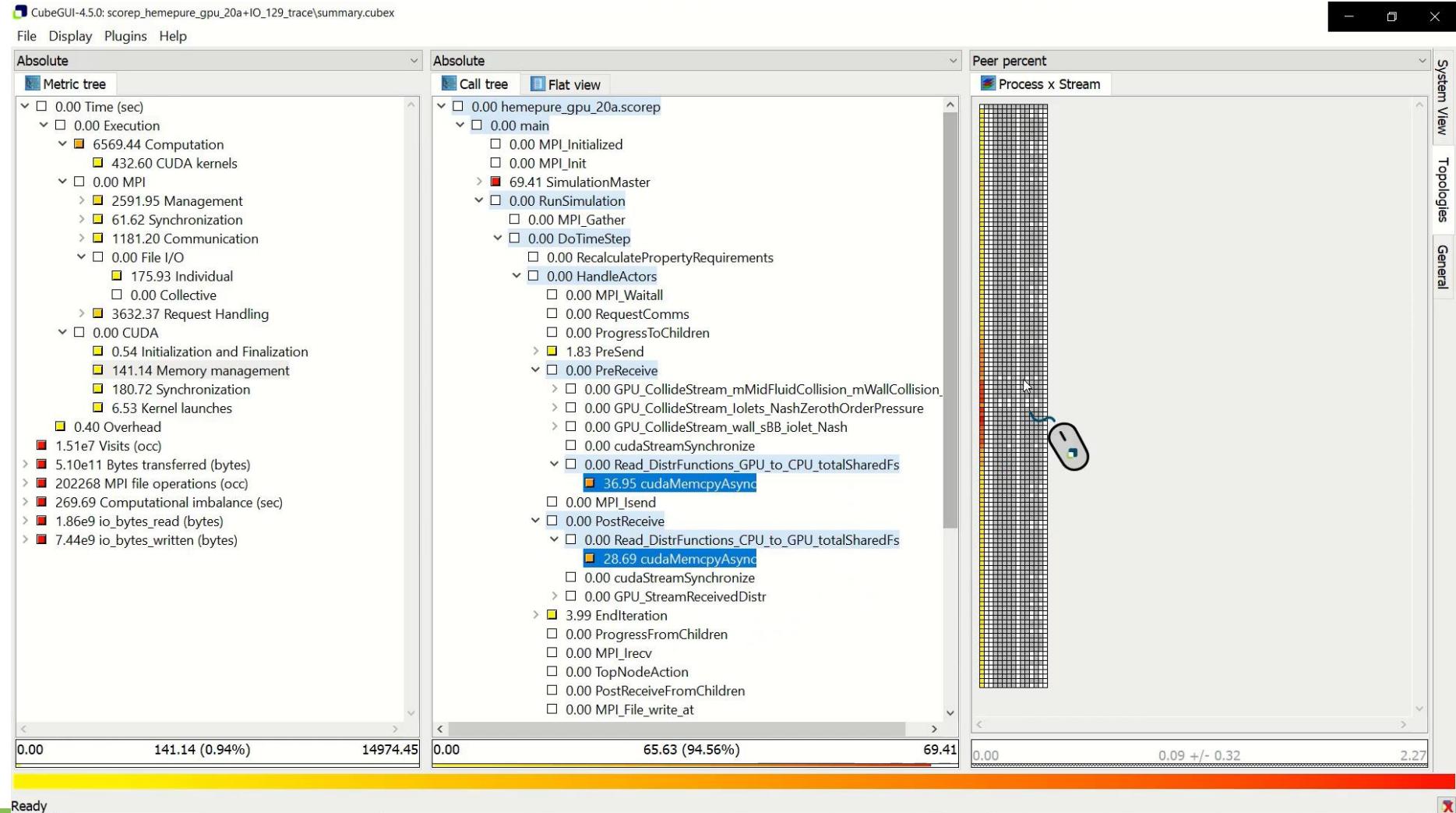




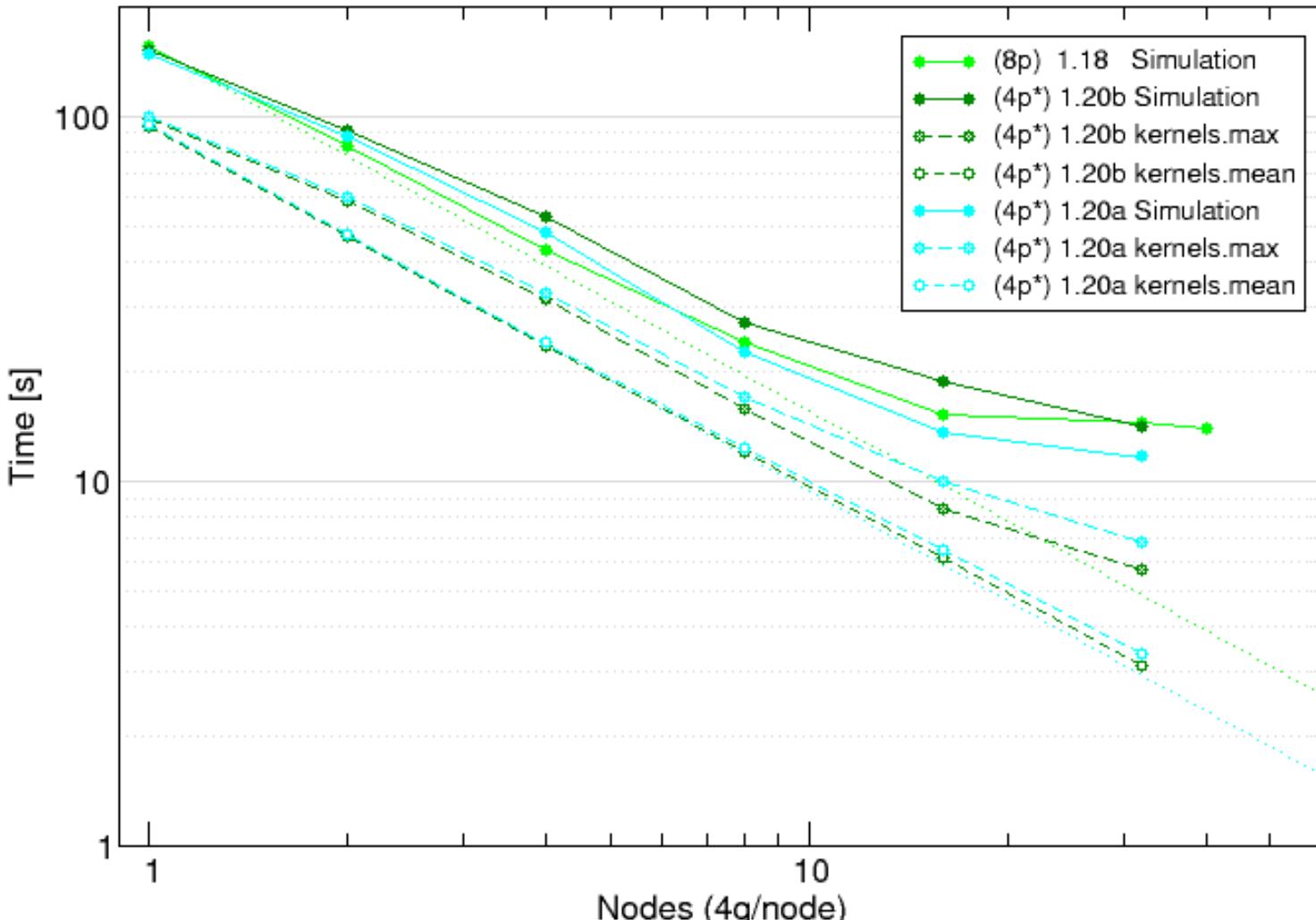
**Topo: Time for MPI file writing on CPU varies per MPI process**



# Topo: Time for CUDA asynchronous memory copies is imbalanced



# HemeLB@JUWELS-Volta strong scaling of FOA *RunSimulation*



- Reference execution with 8ppn
  - multiple processes offloading GPU kernels generally unproductive
- Comparison of versions (4ppn)
  - v1.20a generally better
- Synchronous MPI file writing is the primary bottleneck
- CUDA kernels on GPUs
  - less than half of Simulation time (therefore GPUs mostly idle)
  - total kernel time scales very well (0.93 scaling efficiency)
  - load balance deteriorates (0.95 for single node, 0.50 for 32 nodes)

## HemeLB@JUWELS/Volta strong scaling efficiency of *RunSimulation*

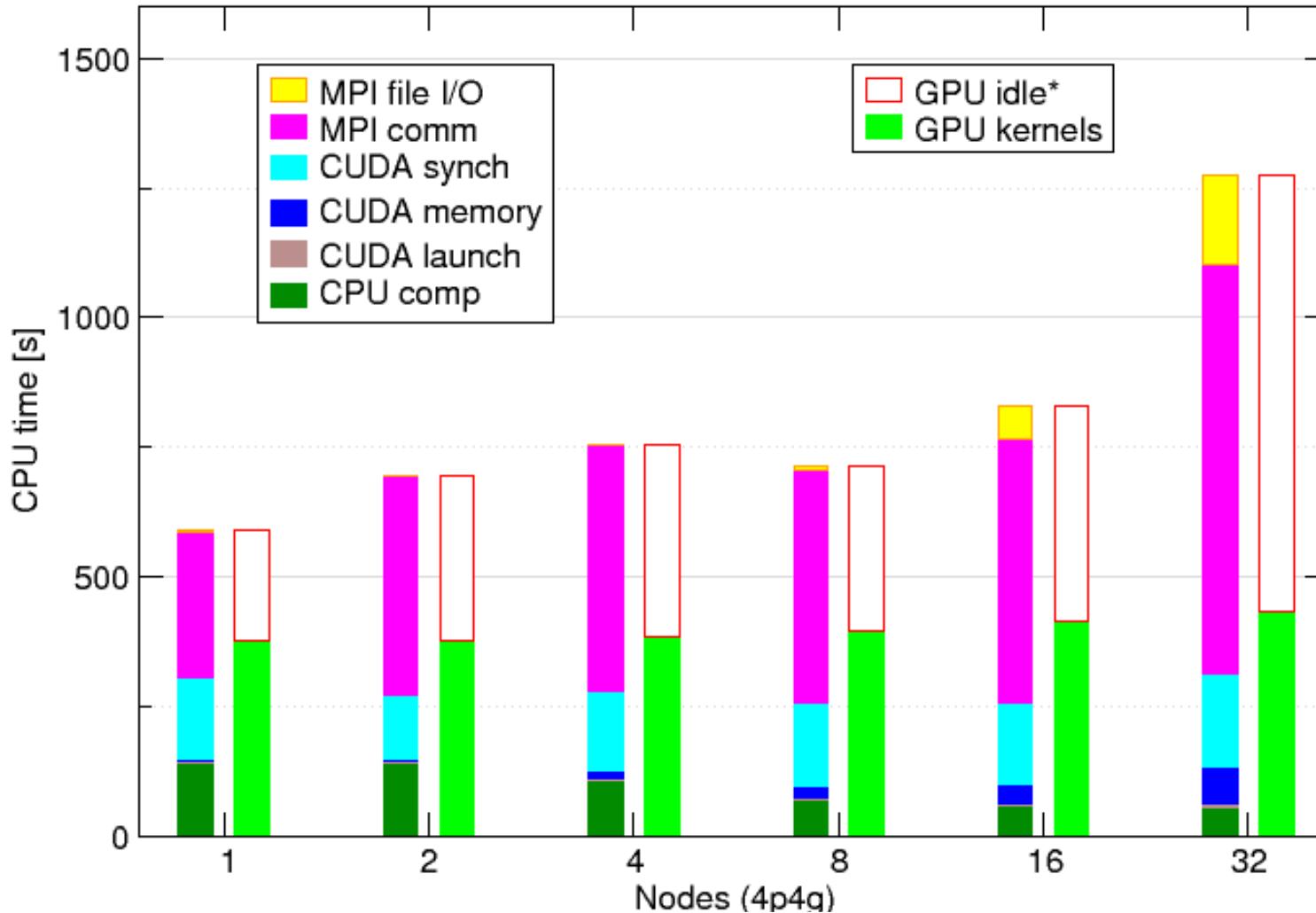
	1n 5p	2n 9p	4n 17p	8n 33p	16n 65p	32n 129p	Key:
Simulation time [s]	147.87	88.38	48.13	22.66	13.68	11.67	1.1 1.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0.0
Global scaling efficiency	0.64	0.53	0.49	0.52	0.43	0.25	
– Parallel efficiency	0.64	0.53	0.50	0.54	0.47	0.29	
– – Load balance efficiency (GPU)	0.95	0.78	0.73	0.73	0.65	0.50	
– – Communication efficiency (GPU)	0.67	0.68	0.68	0.75	0.73	0.58	
– Computation scaling (GPU)	1.00	1.00	0.99	0.96	0.92	0.87	

Only considering GPUs (ignoring all CPU cores, 90% of which are completely unused)

- Single (quad-GPU) node already suffers significant communication inefficiency
    - includes MPI file writing, but doesn't degrade much as additional nodes are included
  - Load balance of GPUs deteriorates progressively
  - GPU computation scaling remains reasonably good
- [POP CoE scaling efficiency model: [www.pop-coe.eu](http://www.pop-coe.eu)]



# HemeLB@JUWELS-Volta strong scaling of FOA *RunSimulation*



- CPU+GPU time breakdown
- CUDA kernels on GPUs
  - less than half of Simulation time (therefore GPUs mostly idle)
  - total kernel time scales very well (0.87 scaling efficiency)
- MPI processes on CPUs
  - computation time decreases
  - CUDA synchronization time fairly constant, but time for memory management increases somewhat
  - MPI communication time dominates, with much more time for file writing with 16+ nodes