International HPC Summer School 2022: Performance analysis and optimization

Analysis report examination with Cube

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Cube

- Parallel program analysis report exploration tools
  - Libraries for XML+binary report reading & writing
  - Algebra utilities for report processing
  - GUI for interactive analysis exploration
    - Requires Qt4 ≥4.6 or Qt 5

- Originally developed as part of the Scalasca toolset

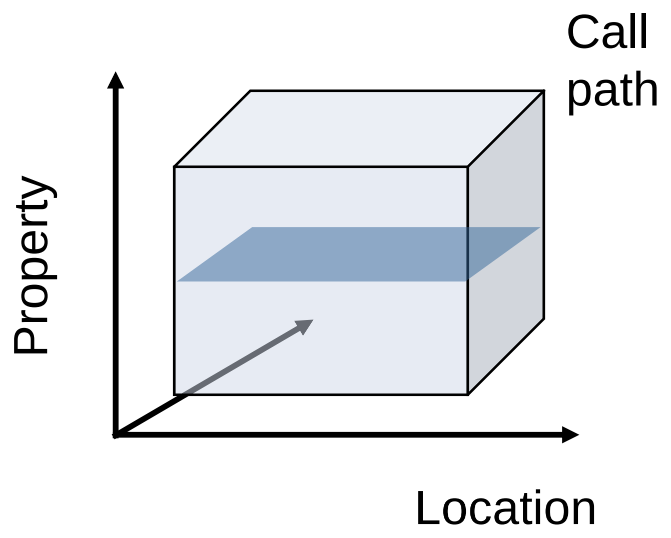
- Now available as a separate component
  - Can be installed independently of Score-P, e.g., on laptop or desktop
  - Latest release 4.7 (April 2022)

Analysis presentation and exploration

- Representation of values (severity matrix) on three hierarchical axes
  - Performance property (metric)
  - Call path (program location)
  - System location (process/thread)

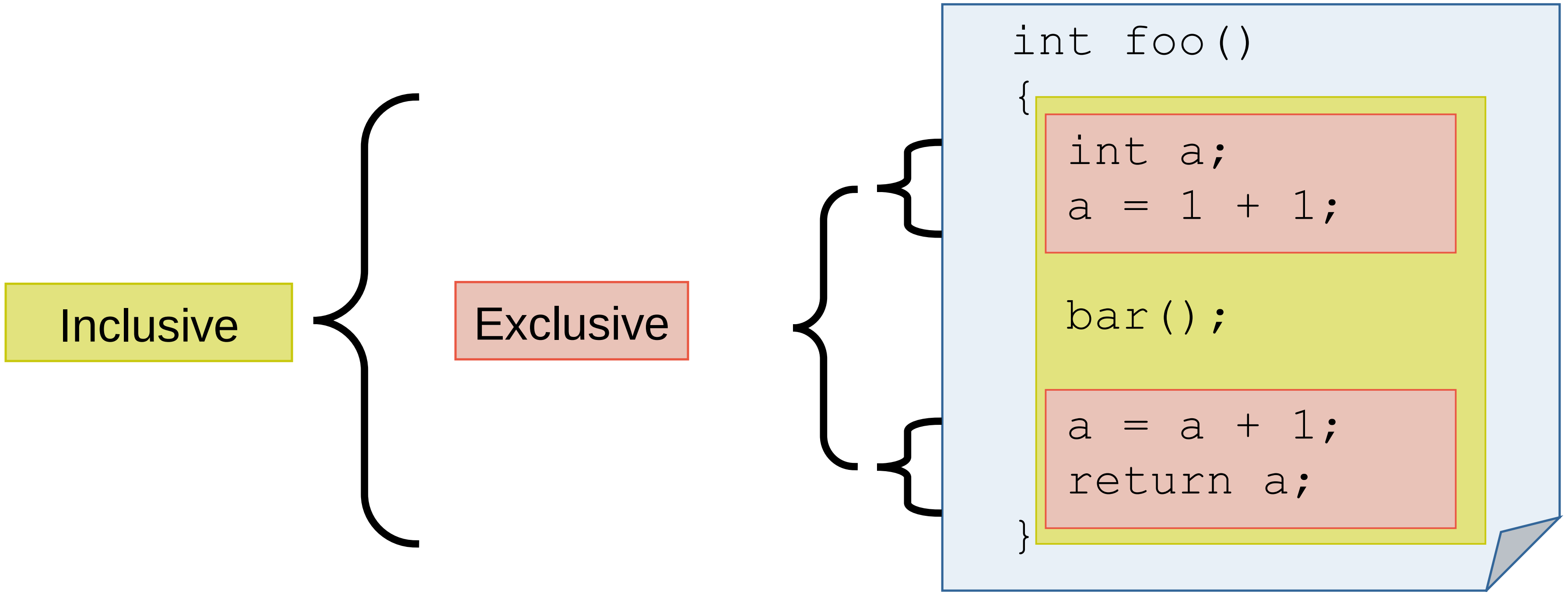
- Three coupled tree browsers

- Cube displays severities
  - As value: for precise comparison
  - As color: for easy identification of hotspots
  - Inclusive value when closed & exclusive value when expanded
  - Customizable via display modes



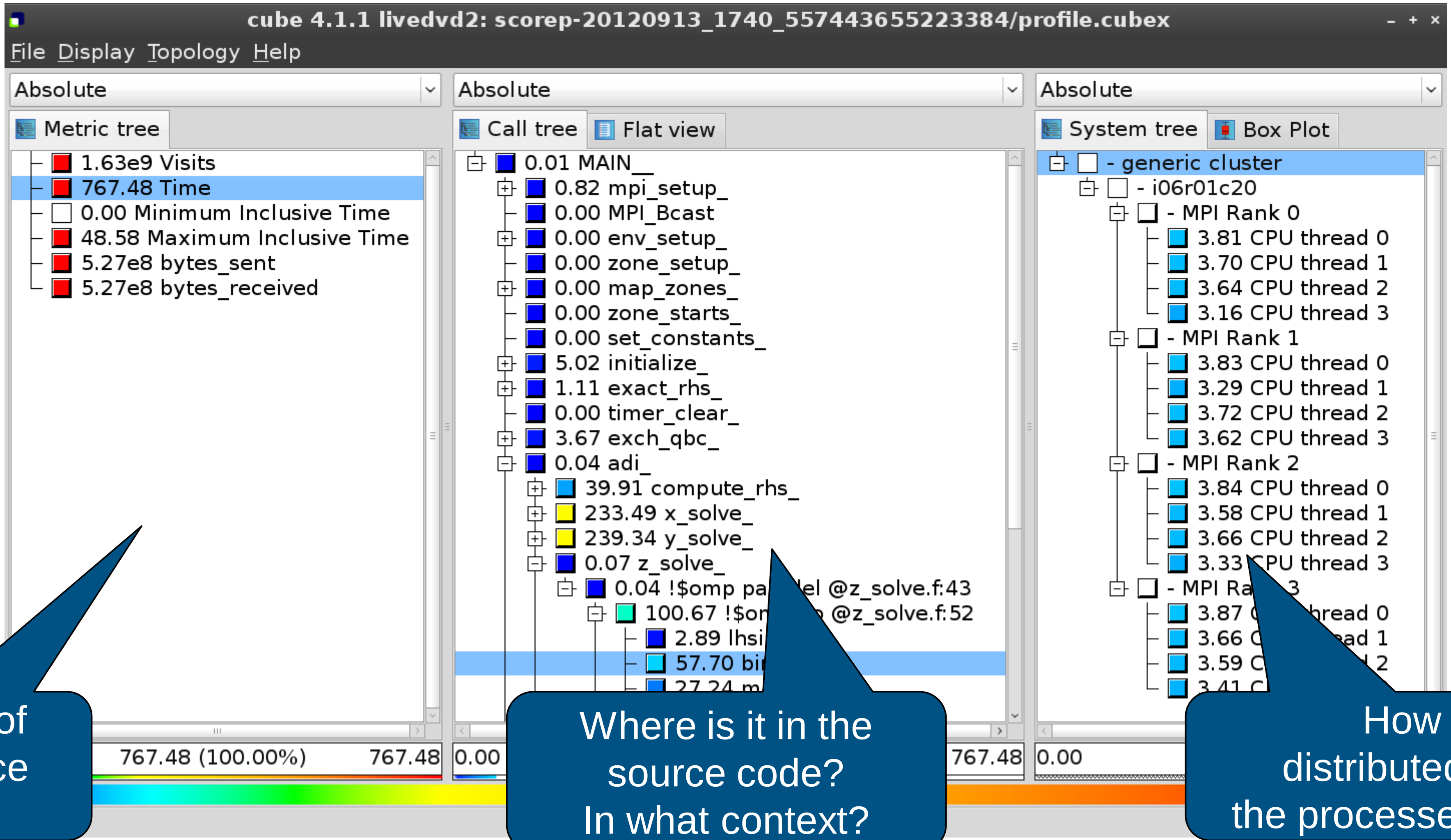
Inclusive vs. exclusive values

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



```
int foo()
{
  int a;
  a = 1 + 1;

  bar();

  a = a + 1;
  return a;
}
```

Analysis presentation



cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex

File Display Topology Help

Absolute | Absolute | Absolute

Metric tree:

```
1.63e9 Visits
767.48 Time
0.00 Minimum Inclusive Time
48.58 Maximum Inclusive Time
5.27e8 bytes_sent
5.27e8 bytes_received
```

Call tree / Flat view:

```
0.01 MAIN__
  0.82 mpi_setup_
  0.00 MPI_Bcast
  0.00 env_setup_
  0.00 zone_setup_
  0.00 map_zones_
  0.00 zone_starts_
  0.00 set_constants_
  5.02 initialize_
  1.11 exact_rhs_
  0.00 timer_clear_
  3.67 exch_qbc_
  0.04 adi_
    39.91 compute_rhs_
    233.49 x_solve_
    239.34 y_solve_
    0.07 z_solve_
      0.04 !$omp pa    lel @z_solve.f:43
        100.67 !$om      @z_solve.f:52
          2.89 lhsi
          57.70 bi
          27.24 m
```

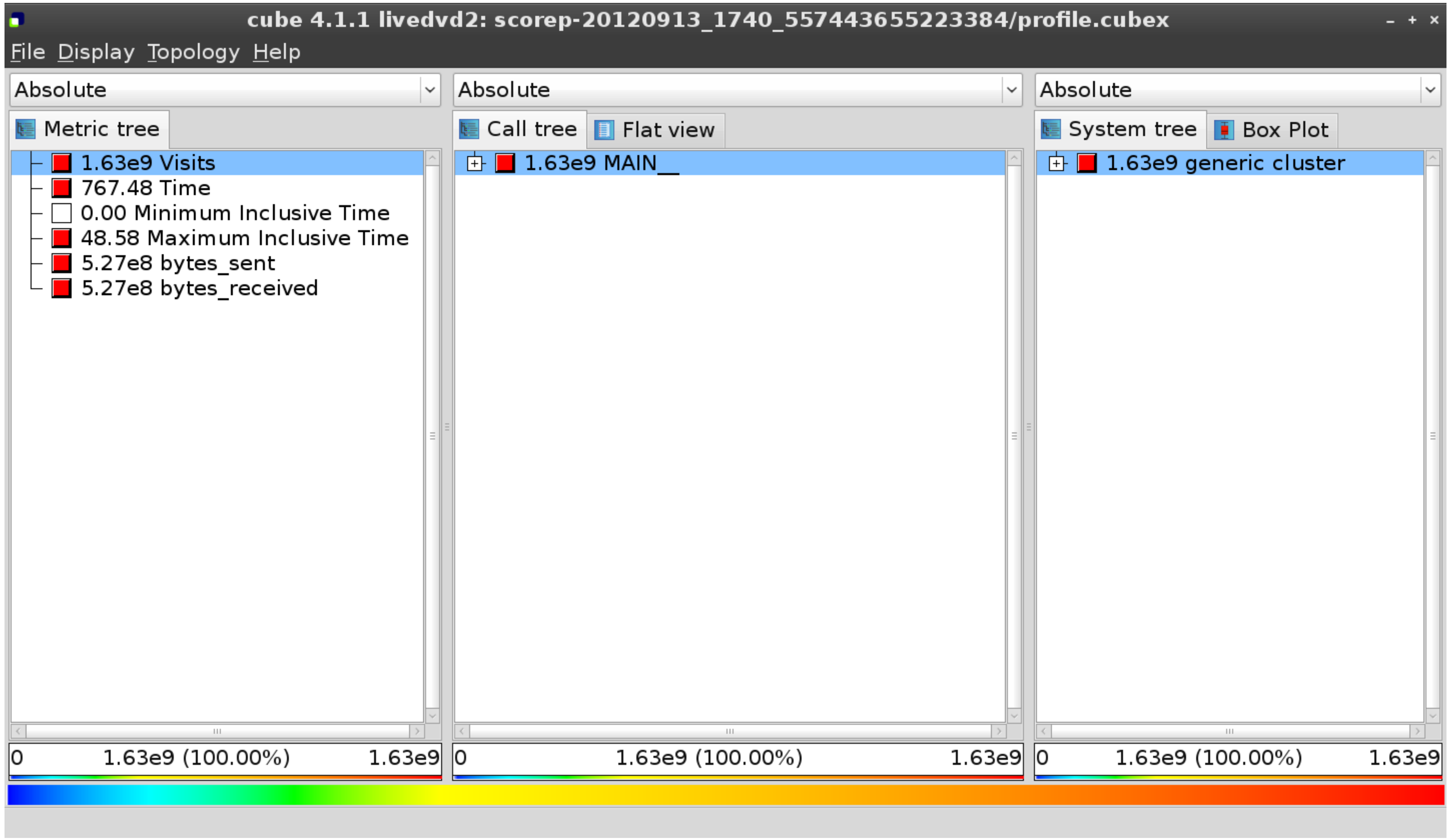
System tree / Box Plot:

```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      3.81 CPU thread 0
      3.70 CPU thread 1
      3.64 CPU thread 2
      3.16 CPU thread 3
    - MPI Rank 1
      3.83 CPU thread 0
      3.29 CPU thread 1
      3.72 CPU thread 2
      3.62 CPU thread 3
    - MPI Rank 2
      3.84 CPU thread 0
      3.58 CPU thread 1
      3.66 CPU thread 2
      3.33 CPU thread 3
    - MPI Ra    3
      3.87 C      hread 0
      3.66 C      ead 1
      3.59 C      2
      3.41 C
```

767.48 (100.00%) 767.48 | 0.00 767.48 | 0.00

What kind of performance metric?
Where is it in the source code? In what context?
How is it distributed across the processes/threads?

Score-P analysis report exploration (opening view)


cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex

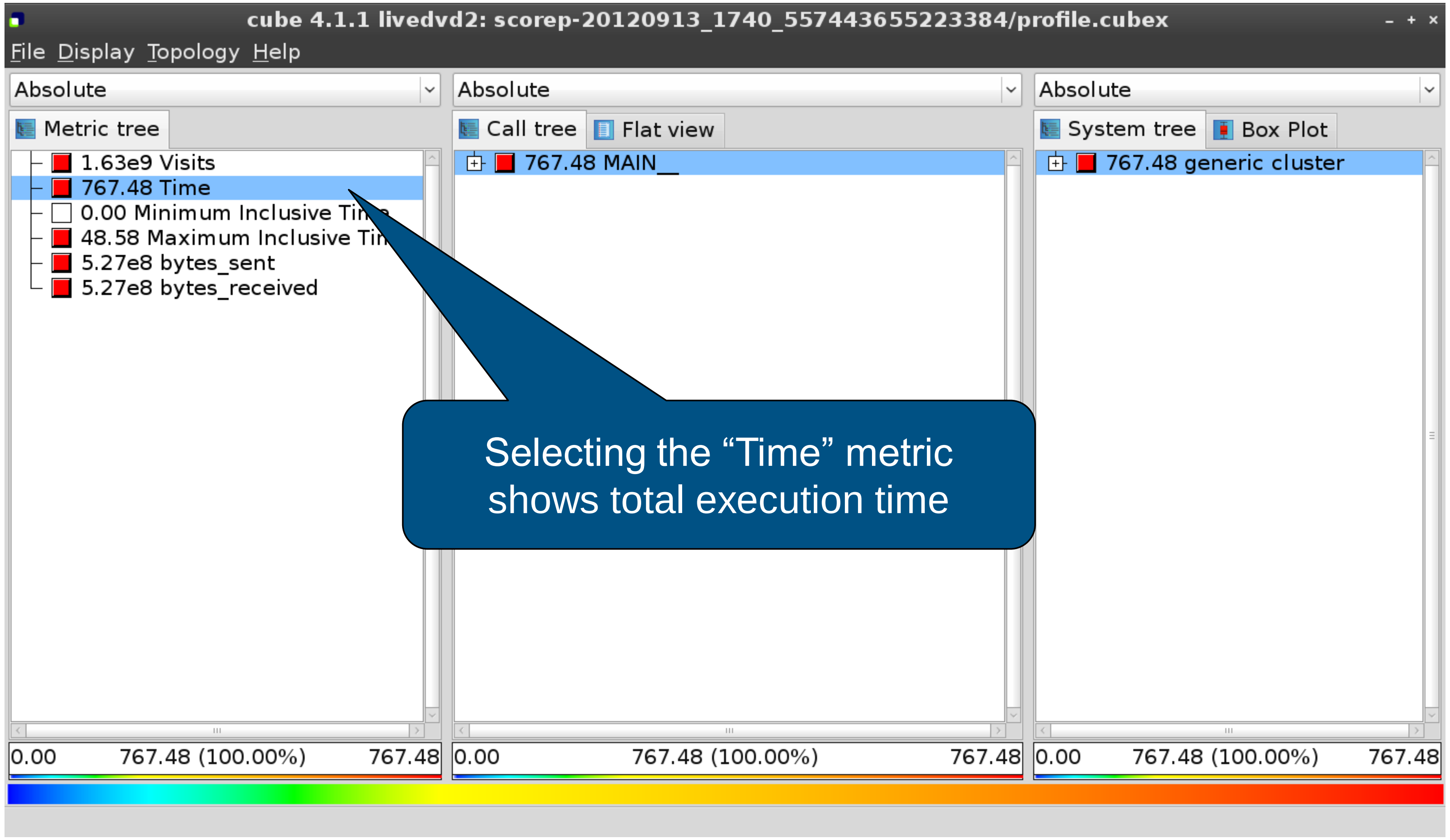
```
1.63e9 Visits
767.48 Time
0.00 Minimum Inclusive Time
48.58 Maximum Inclusive Time
5.27e8 bytes_sent
5.27e8 bytes_received
```

```
1.63e9 MAIN__
```

```
1.63e9 generic cluster
```

```
0    1.63e9 (100.00%)    1.63e9
```

Metric selection


cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex
File Display Topology Help
Absolute
Absolute
Absolute
Metric tree
Call tree
Flat view
System tree
Box Plot

- 🟥 1.63e9 Visits
- 🟥 767.48 Time
- ☐ 0.00 Minimum Inclusive Time
- 🟥 48.58 Maximum Inclusive Time
- 🟥 5.27e8 bytes_sent
- 🟥 5.27e8 bytes_received

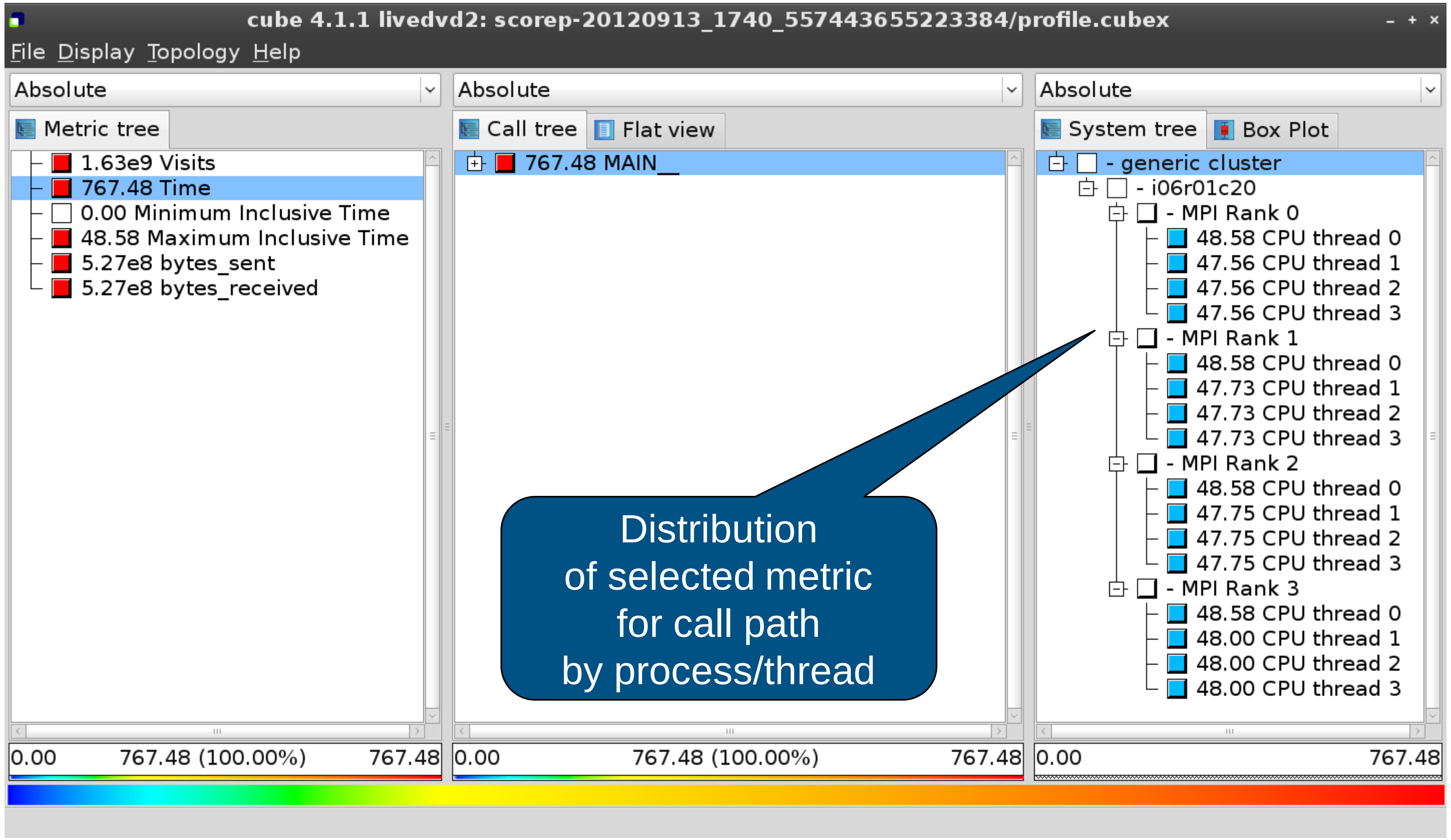
🟥 767.48 MAIN__

🟥 767.48 generic cluster

0.00 767.48 (100.00%) 767.48

Selecting the "Time" metric shows total execution time

Expanding the system tree


cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex

File Display Topology Help

Absolute | Absolute | Absolute

Metric tree | Call tree | Flat view | System tree | Box Plot

Metric tree:
```
├ 🟥 1.63e9 Visits
├ 🟥 767.48 Time
├ ☐ 0.00 Minimum Inclusive Time
├ 🟥 48.58 Maximum Inclusive Time
├ 🟥 5.27e8 bytes_sent
└ 🟥 5.27e8 bytes_received
```

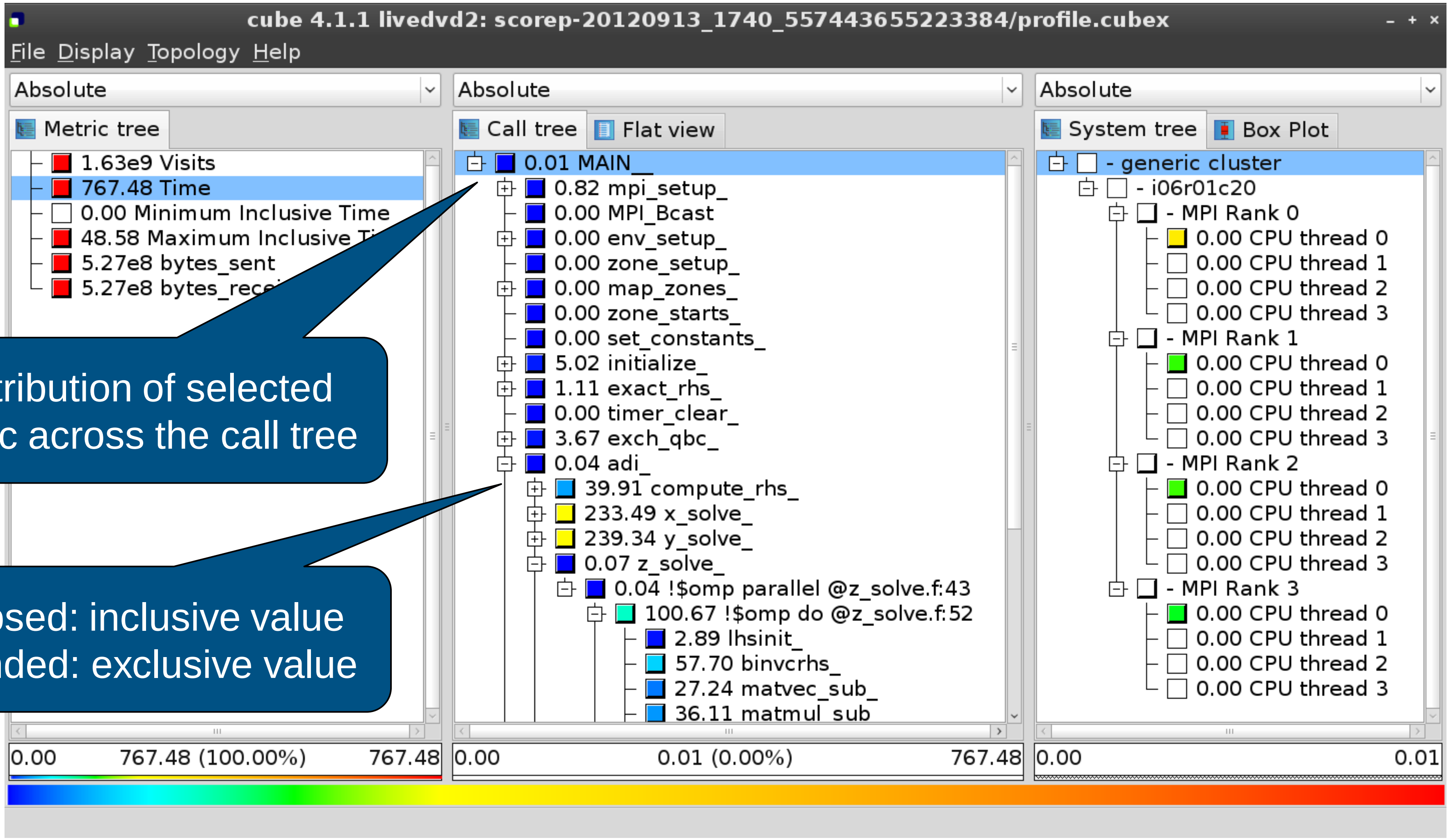
Call tree:
```
⊞ 🟥 767.48 MAIN__
```

System tree:
```
⊟ ☐ - generic cluster
  ⊟ ☐ - i06r01c20
    ⊟ ☐ - MPI Rank 0
        🟦 48.58 CPU thread 0
        🟦 47.56 CPU thread 1
        🟦 47.56 CPU thread 2
        🟦 47.56 CPU thread 3
    ⊟ ☐ - MPI Rank 1
        🟦 48.58 CPU thread 0
        🟦 47.73 CPU thread 1
        🟦 47.73 CPU thread 2
        🟦 47.73 CPU thread 3
    ⊟ ☐ - MPI Rank 2
        🟦 48.58 CPU thread 0
        🟦 47.75 CPU thread 1
        🟦 47.75 CPU thread 2
        🟦 47.75 CPU thread 3
    ⊟ ☐ - MPI Rank 3
        🟦 48.58 CPU thread 0
        🟦 48.00 CPU thread 1
        🟦 48.00 CPU thread 2
        🟦 48.00 CPU thread 3
```

0.00 767.48 (100.00%) 767.48 | 0.00 767.48 (100.00%) 767.48 | 0.00 767.48

Distribution of selected metric for call path by process/thread

Expanding the call tree


cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex
File Display Topology Help
Absolute
Metric tree
Call tree
Flat view
System tree
Box Plot

```
1.63e9 Visits
767.48 Time
0.00 Minimum Inclusive Time
48.58 Maximum Inclusive Ti
5.27e8 bytes_sent
5.27e8 bytes_rece
```

```
0.01 MAIN__
  0.82 mpi_setup_
  0.00 MPI_Bcast
  0.00 env_setup_
  0.00 zone_setup_
  0.00 map_zones_
  0.00 zone_starts_
  0.00 set_constants_
  5.02 initialize_
  1.11 exact_rhs_
  0.00 timer_clear_
  3.67 exch_qbc_
  0.04 adi_
    39.91 compute_rhs_
    233.49 x_solve_
    239.34 y_solve_
    0.07 z_solve_
      0.04 !$omp parallel @z_solve.f:43
        100.67 !$omp do @z_solve.f:52
          2.89 lhsinit_
          57.70 binvcrhs_
          27.24 matvec_sub_
          36.11 matmul_sub
```

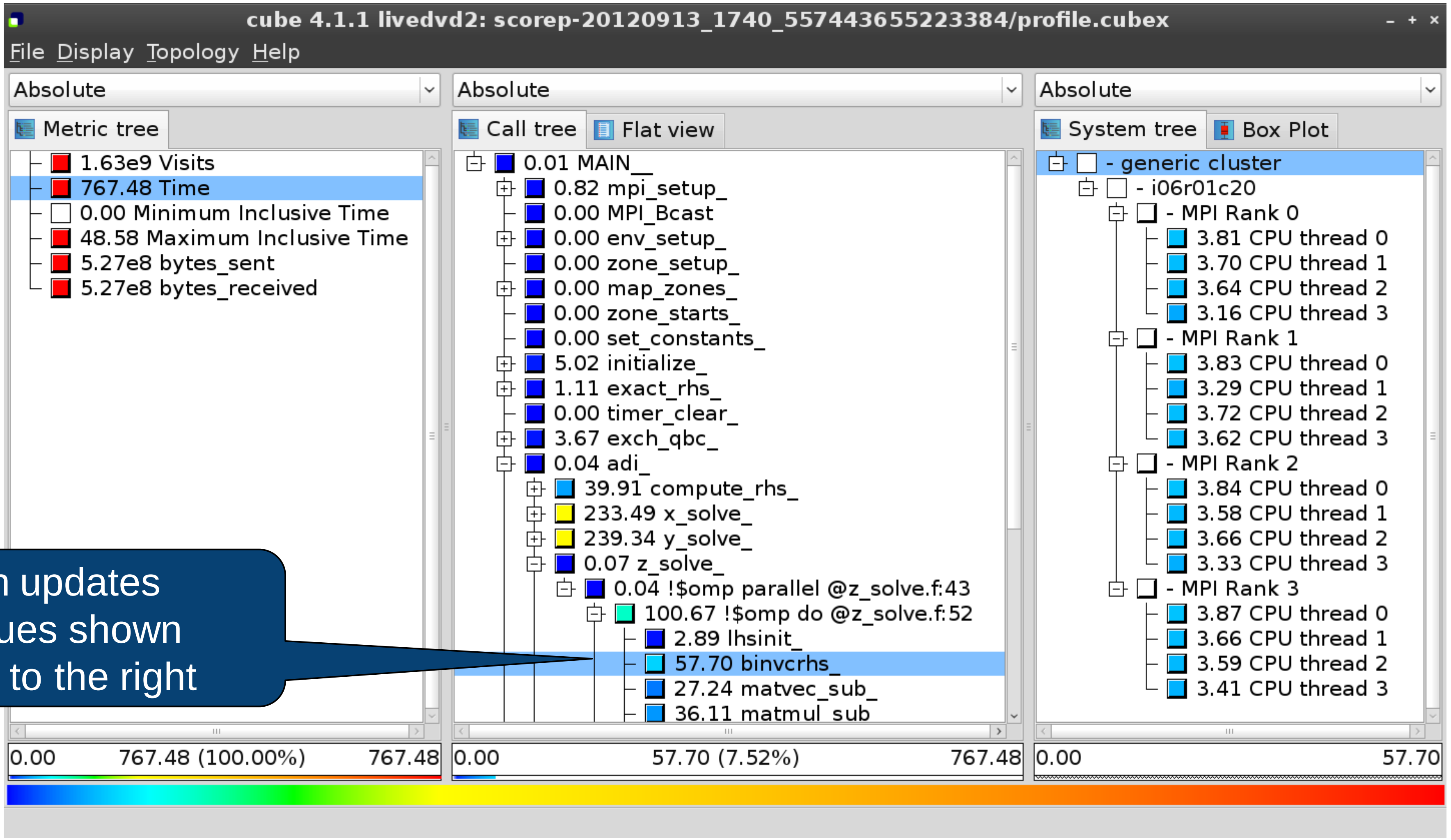
```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      0.00 CPU thread 0
      0.00 CPU thread 1
      0.00 CPU thread 2
      0.00 CPU thread 3
    - MPI Rank 1
      0.00 CPU thread 0
      0.00 CPU thread 1
      0.00 CPU thread 2
      0.00 CPU thread 3
    - MPI Rank 2
      0.00 CPU thread 0
      0.00 CPU thread 1
      0.00 CPU thread 2
      0.00 CPU thread 3
    - MPI Rank 3
      0.00 CPU thread 0
      0.00 CPU thread 1
      0.00 CPU thread 2
      0.00 CPU thread 3
```

```
0.00   767.48 (100.00%)   767.48
0.00   0.01 (0.00%)   767.48
0.00   0.01
```

Distribution of selected metric across the call tree

Collapsed: inclusive value
Expanded: exclusive value

Selecting a call path



cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex

File Display Topology Help

Absolute | Absolute | Absolute

Metric tree
- 1.63e9 Visits
- 767.48 Time
- 0.00 Minimum Inclusive Time
- 48.58 Maximum Inclusive Time
- 5.27e8 bytes_sent
- 5.27e8 bytes_received

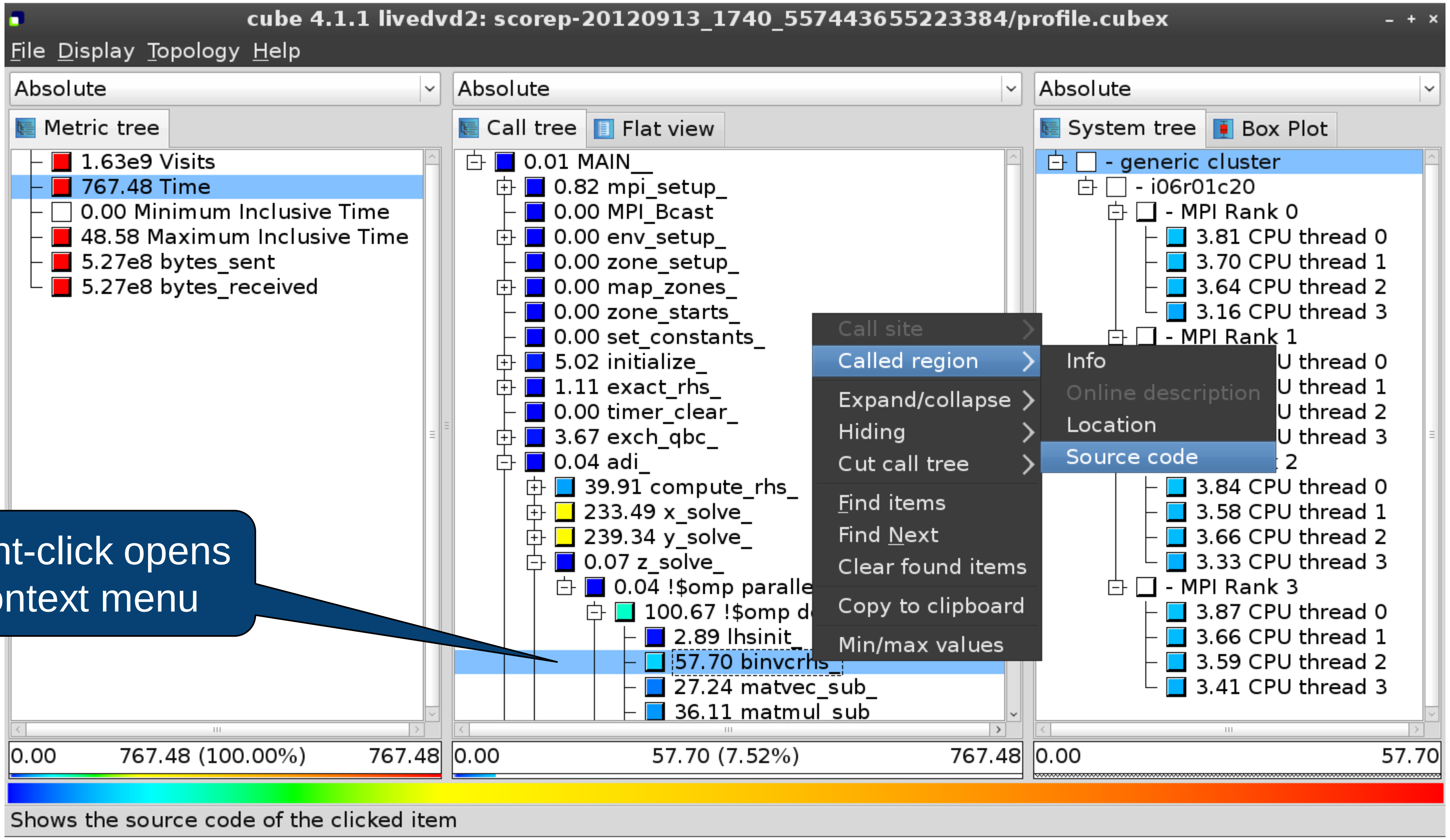
Call tree | Flat view
```
0.01 MAIN__
  0.82 mpi_setup_
  0.00 MPI_Bcast
  0.00 env_setup_
  0.00 zone_setup_
  0.00 map_zones_
  0.00 zone_starts_
  0.00 set_constants_
  5.02 initialize_
  1.11 exact_rhs_
  0.00 timer_clear_
  3.67 exch_qbc_
  0.04 adi_
    39.91 compute_rhs_
    233.49 x_solve_
    239.34 y_solve_
    0.07 z_solve_
      0.04 !$omp parallel @z_solve.f:43
        100.67 !$omp do @z_solve.f:52
          2.89 lhsinit_
          57.70 binvcrhs_
          27.24 matvec_sub_
          36.11 matmul_sub_
```

System tree | Box Plot
```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      3.81 CPU thread 0
      3.70 CPU thread 1
      3.64 CPU thread 2
      3.16 CPU thread 3
    - MPI Rank 1
      3.83 CPU thread 0
      3.29 CPU thread 1
      3.72 CPU thread 2
      3.62 CPU thread 3
    - MPI Rank 2
      3.84 CPU thread 0
      3.58 CPU thread 1
      3.66 CPU thread 2
      3.33 CPU thread 3
    - MPI Rank 3
      3.87 CPU thread 0
      3.66 CPU thread 1
      3.59 CPU thread 2
      3.41 CPU thread 3
```

0.00 767.48 (100.00%) 767.48 | 0.00 57.70 (7.52%) 767.48 | 0.00 57.70

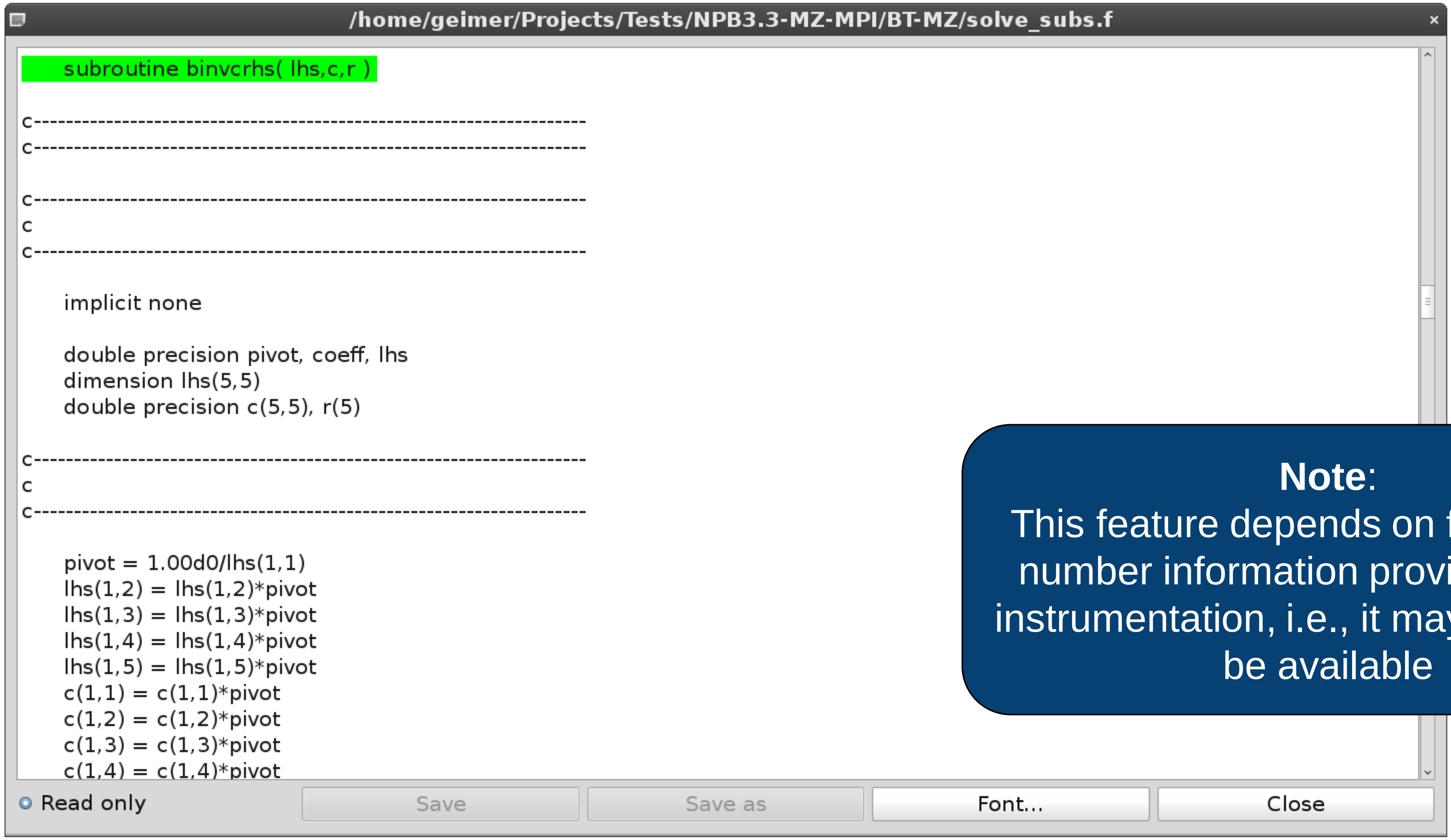
Selection updates metric values shown in columns to the right

Source-code view via context menu



Right-click opens context menu

Source-code view

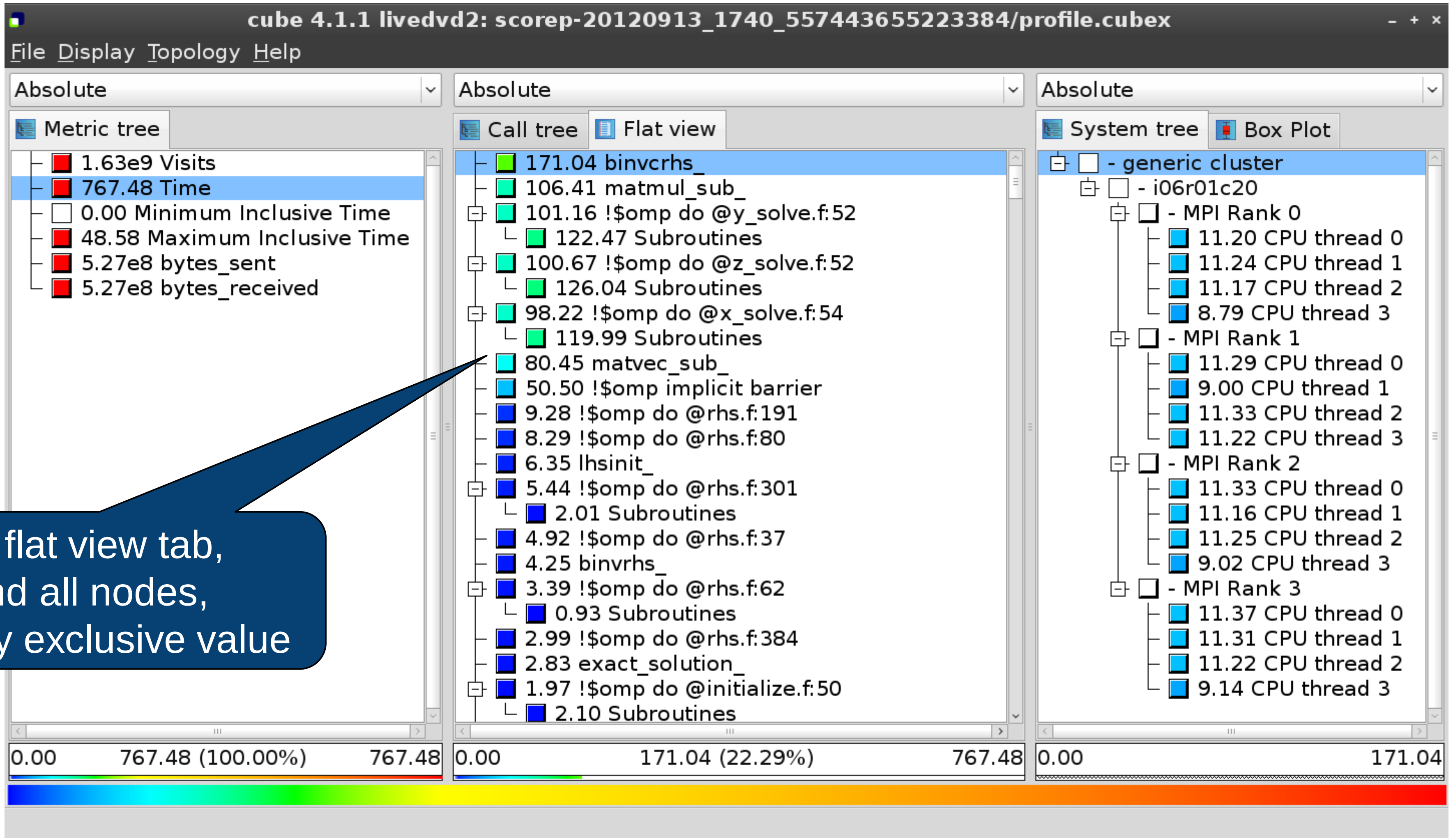

/home/geimer/Projects/Tests/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f

```
      subroutine binvcrhs( lhs,c,r )

c---------------------------------------------------------------------
c---------------------------------------------------------------------

c---------------------------------------------------------------------
c
c---------------------------------------------------------------------

      implicit none

      double precision pivot, coeff, lhs
      dimension lhs(5,5)
      double precision c(5,5), r(5)

c---------------------------------------------------------------------
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
```

Read only
Save
Save as
Font...
Close

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

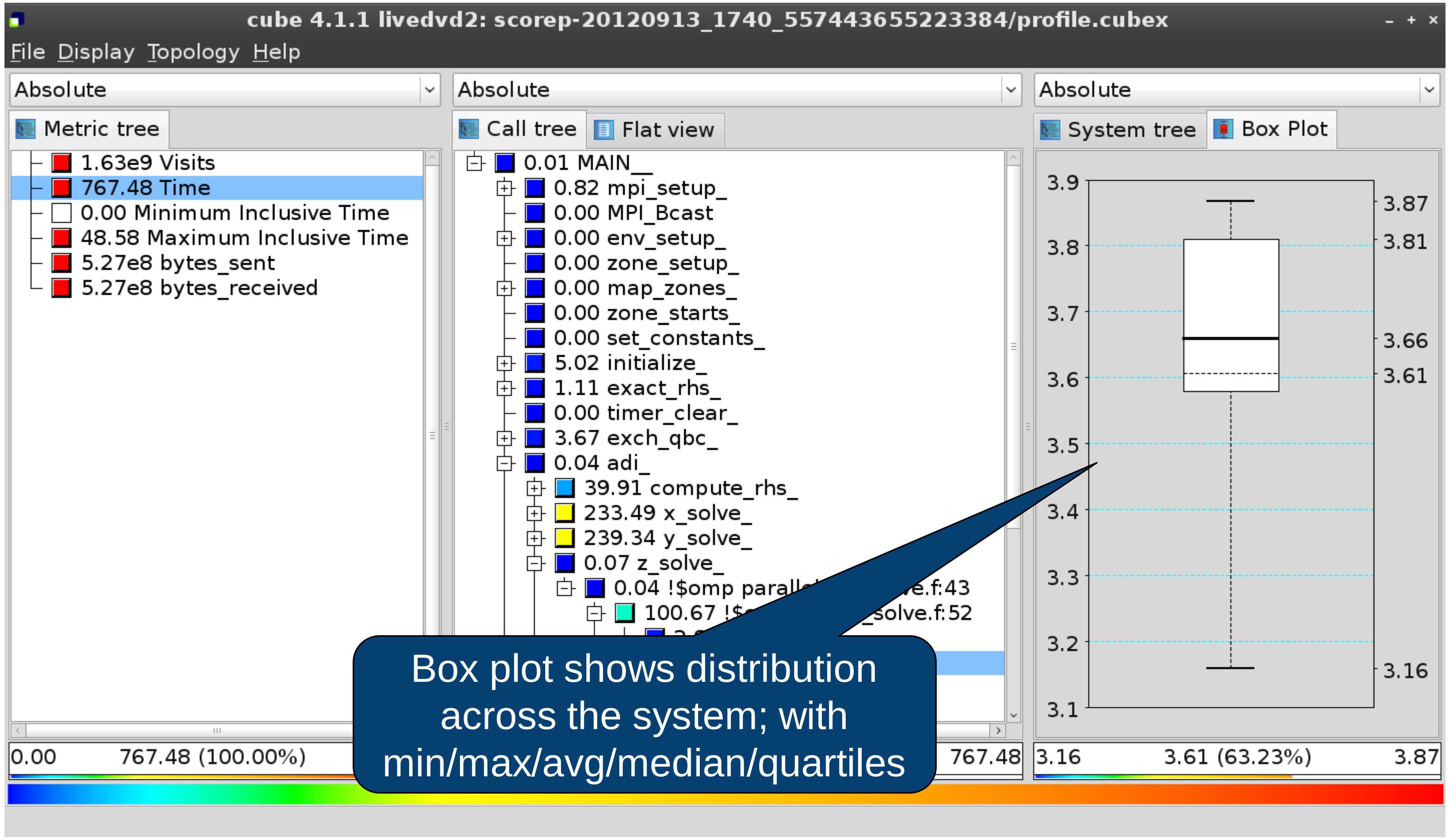
Flat profile view


cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex
File Display Topology Help
Absolute
Absolute
Absolute
Metric tree
Call tree
Flat view
System tree
Box Plot

```
Metric tree                      Flat view                               System tree
1.63e9 Visits                    171.04 binvcrhs_                        - generic cluster
767.48 Time                      106.41 matmul_sub_                        - i06r01c20
0.00 Minimum Inclusive Time      101.16 !$omp do @y_solve.f:52               - MPI Rank 0
48.58 Maximum Inclusive Time       122.47 Subroutines                          11.20 CPU thread 0
5.27e8 bytes_sent                100.67 !$omp do @z_solve.f:52                 11.24 CPU thread 1
5.27e8 bytes_received              126.04 Subroutines                          11.17 CPU thread 2
                                 98.22 !$omp do @x_solve.f:54                  8.79 CPU thread 3
                                   119.99 Subroutines                        - MPI Rank 1
                                 80.45 matvec_sub_                             11.29 CPU thread 0
                                 50.50 !$omp implicit barrier                  9.00 CPU thread 1
                                 9.28 !$omp do @rhs.f:191                      11.33 CPU thread 2
                                 8.29 !$omp do @rhs.f:80                       11.22 CPU thread 3
                                 6.35 lhsinit_                               - MPI Rank 2
                                 5.44 !$omp do @rhs.f:301                      11.33 CPU thread 0
                                   2.01 Subroutines                            11.16 CPU thread 1
                                 4.92 !$omp do @rhs.f:37                       11.25 CPU thread 2
                                 4.25 binvrhs_                                 9.02 CPU thread 3
                                 3.39 !$omp do @rhs.f:62                     - MPI Rank 3
                                   0.93 Subroutines                            11.37 CPU thread 0
                                 2.99 !$omp do @rhs.f:384                      11.31 CPU thread 1
                                 2.83 exact_solution_                          11.22 CPU thread 2
                                 1.97 !$omp do @initialize.f:50                9.14 CPU thread 3
                                   2.10 Subroutines

0.00   767.48 (100.00%)   767.48 | 0.00   171.04 (22.29%)   767.48 | 0.00   171.04
```

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

Box plot view


cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex

File Display Topology Help

Absolute | Absolute | Absolute

Metric tree
- 1.63e9 Visits
- 767.48 Time
- 0.00 Minimum Inclusive Time
- 48.58 Maximum Inclusive Time
- 5.27e8 bytes_sent
- 5.27e8 bytes_received

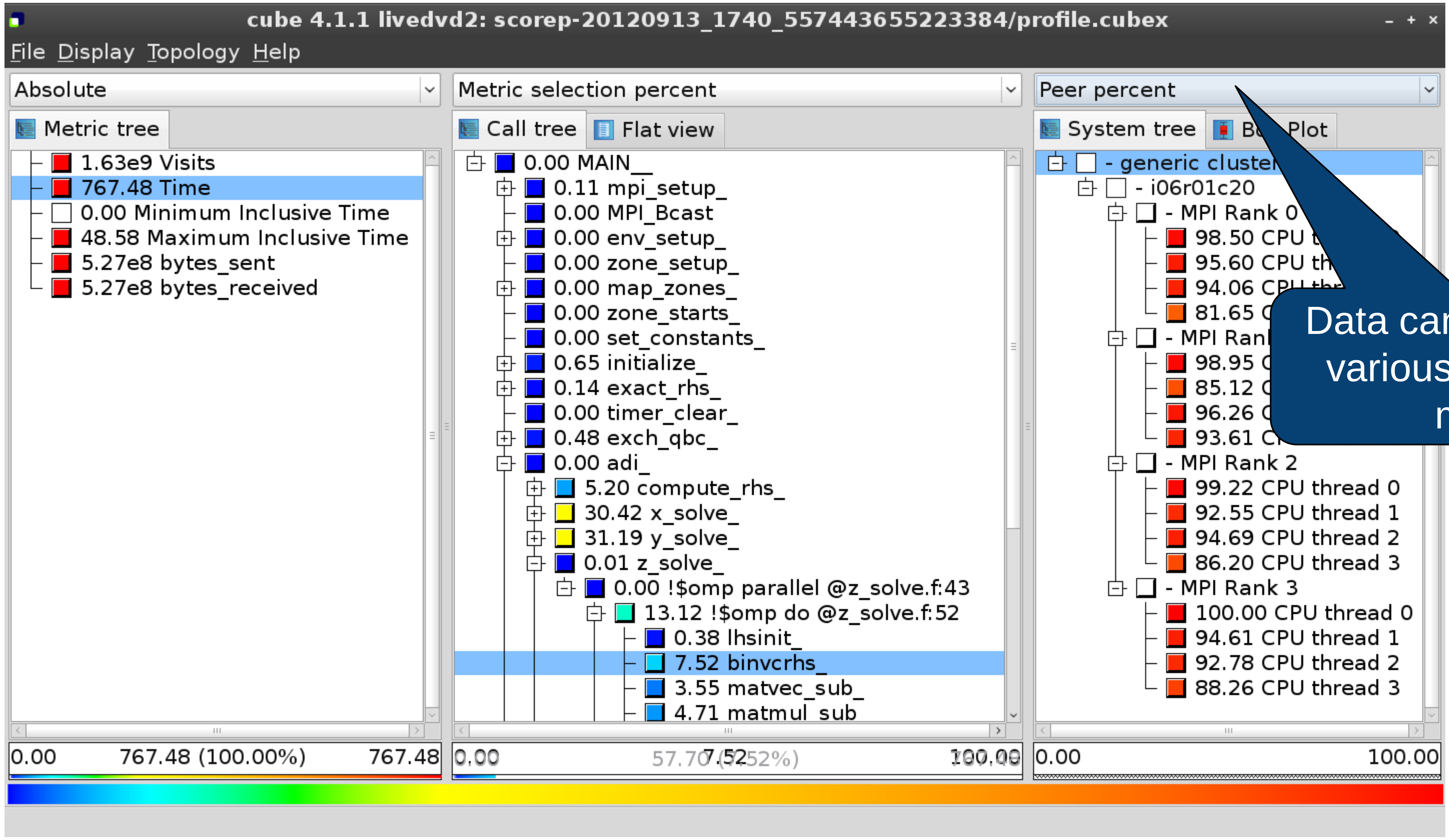
Call tree | Flat view
```
0.01 MAIN__
  0.82 mpi_setup_
  0.00 MPI_Bcast
  0.00 env_setup_
  0.00 zone_setup_
  0.00 map_zones_
  0.00 zone_starts_
  0.00 set_constants_
  5.02 initialize_
  1.11 exact_rhs_
  0.00 timer_clear_
  3.67 exch_qbc_
  0.04 adi_
    39.91 compute_rhs_
    233.49 x_solve_
    239.34 y_solve_
    0.07 z_solve_
      0.04 !$omp parall      e.f:43
        100.67 !$          _solve.f:52
```

System tree | Box Plot

0.00 767.48 (100.00%) | 767.48 | 3.16 3.61 (63.23%) 3.87

Box plot shows distribution across the system; with min/max/avg/median/quartiles

Alternative display modes



cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex

File Display Topology Help

Absolute | Metric selection percent | Peer percent

Metric tree:
- 1.63e9 Visits
- 767.48 Time
- 0.00 Minimum Inclusive Time
- 48.58 Maximum Inclusive Time
- 5.27e8 bytes_sent
- 5.27e8 bytes_received

Call tree:
```
0.00 MAIN__
  0.11 mpi_setup_
  0.00 MPI_Bcast
  0.00 env_setup_
  0.00 zone_setup_
  0.00 map_zones_
  0.00 zone_starts_
  0.00 set_constants_
  0.65 initialize_
  0.14 exact_rhs_
  0.00 timer_clear_
  0.48 exch_qbc_
  0.00 adi_
    5.20 compute_rhs_
    30.42 x_solve_
    31.19 y_solve_
    0.01 z_solve_
      0.00 !$omp parallel @z_solve.f:43
        13.12 !$omp do @z_solve.f:52
          0.38 lhsinit_
          7.52 binvcrhs_
          3.55 matvec_sub_
          4.71 matmul_sub
```

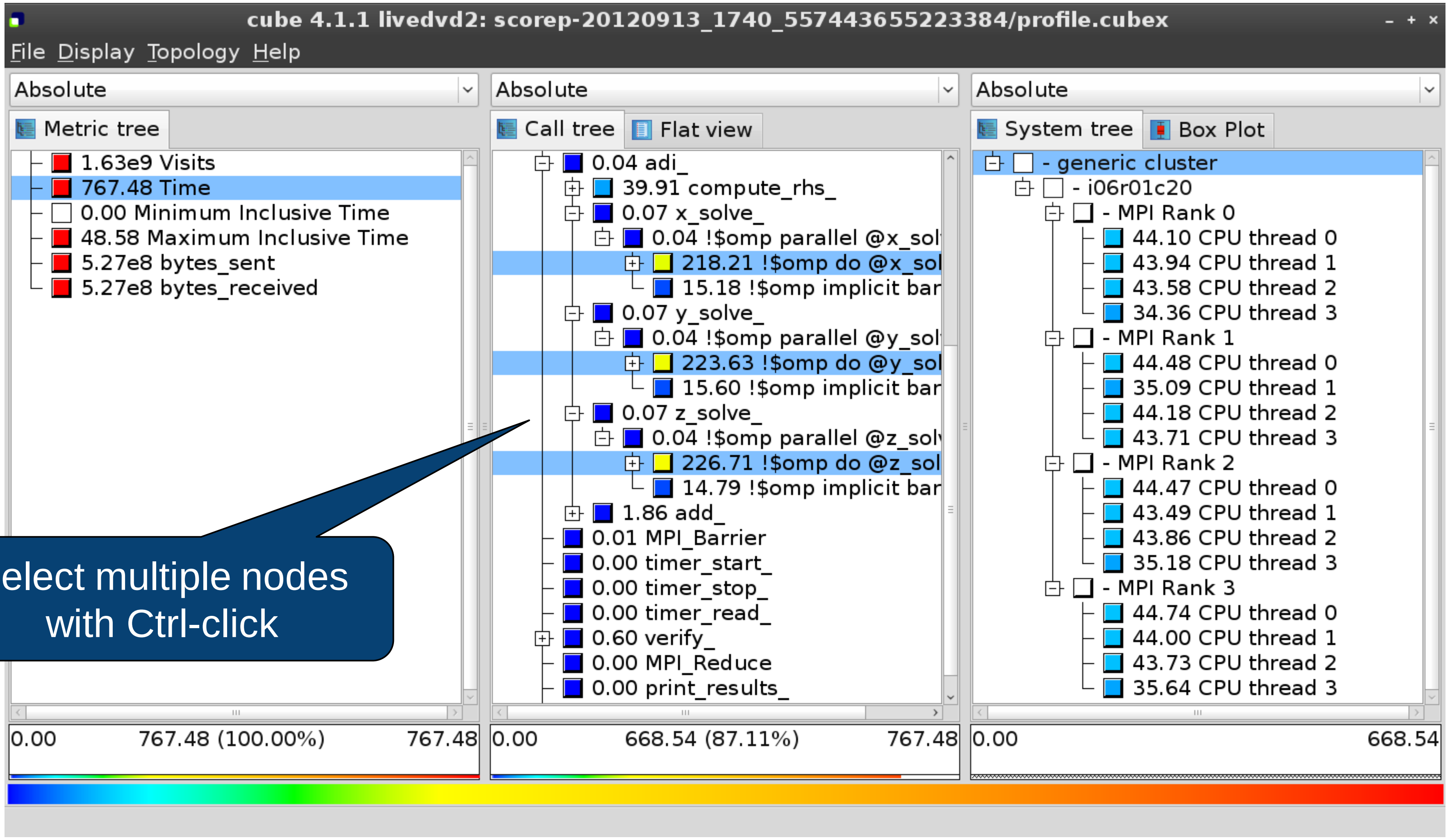
System tree:
```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      98.50 CPU t
      95.60 CPU th
      94.06 CPU thr
      81.65 C
    - MPI Rank
      98.95 C
      85.12 C
      96.26 C
      93.61 C
    - MPI Rank 2
      99.22 CPU thread 0
      92.55 CPU thread 1
      94.69 CPU thread 2
      86.20 CPU thread 3
    - MPI Rank 3
      100.00 CPU thread 0
      94.61 CPU thread 1
      92.78 CPU thread 2
      88.26 CPU thread 3
```

0.00 767.48 (100.00%) 767.48 | 0.00 57.70 7.52 (13.52%) 100.00 | 0.00 100.00

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



cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex

File Display Topology Help

Absolute | Absolute | Absolute

Metric tree:
```
1.63e9 Visits
767.48 Time
0.00 Minimum Inclusive Time
48.58 Maximum Inclusive Time
5.27e8 bytes_sent
5.27e8 bytes_received
```

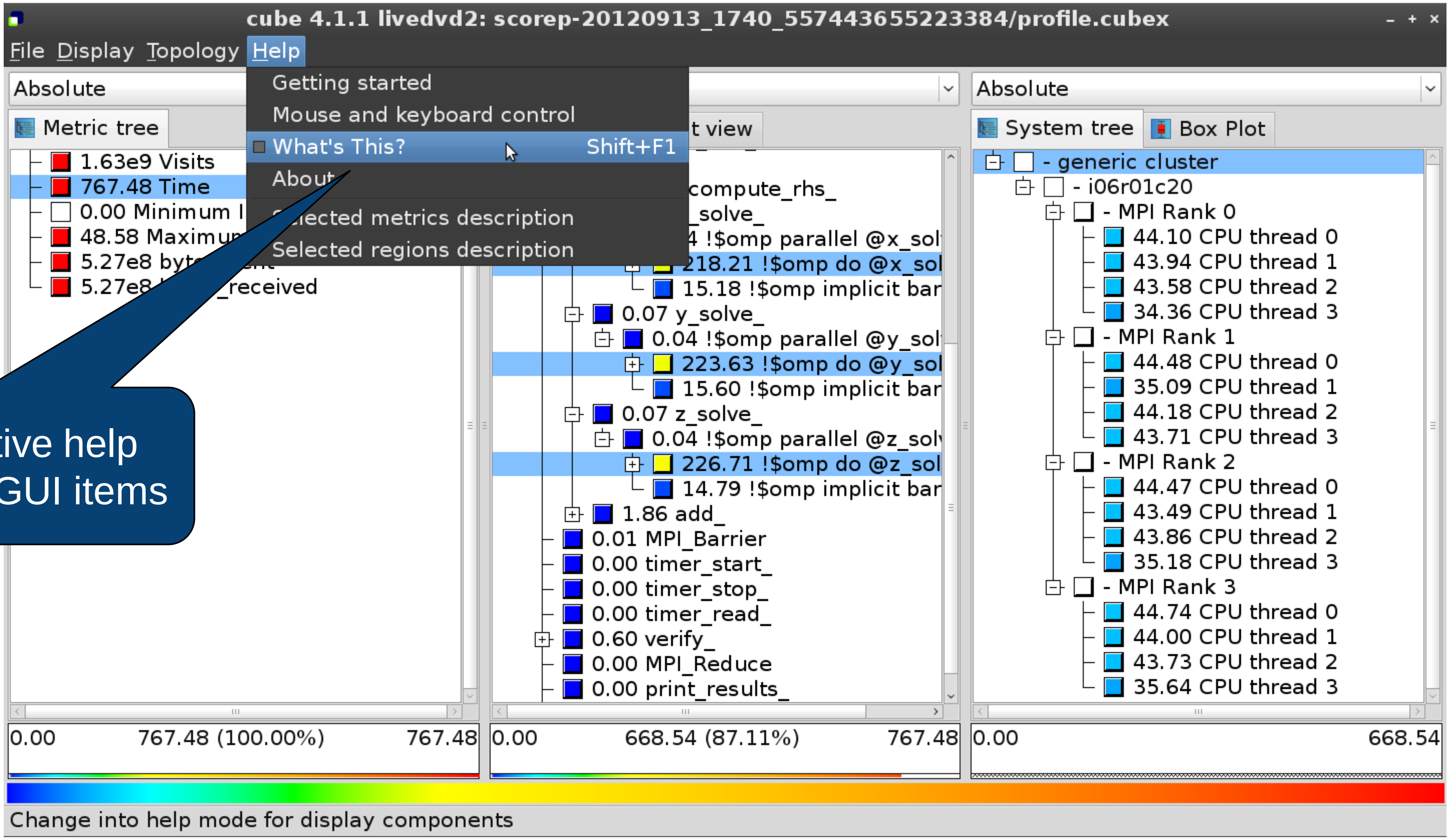
Call tree | Flat view:
```
0.04 adi_
  39.91 compute_rhs_
  0.07 x_solve_
    0.04 !$omp parallel @x_sol
      218.21 !$omp do @x_sol
      15.18 !$omp implicit bar
  0.07 y_solve_
    0.04 !$omp parallel @y_sol
      223.63 !$omp do @y_sol
      15.60 !$omp implicit bar
  0.07 z_solve_
    0.04 !$omp parallel @z_sol
      226.71 !$omp do @z_sol
      14.79 !$omp implicit bar
  1.86 add_
0.01 MPI_Barrier
0.00 timer_start_
0.00 timer_stop_
0.00 timer_read_
0.60 verify_
0.00 MPI_Reduce
0.00 print_results_
```

System tree | Box Plot:
```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      44.10 CPU thread 0
      43.94 CPU thread 1
      43.58 CPU thread 2
      34.36 CPU thread 3
    - MPI Rank 1
      44.48 CPU thread 0
      35.09 CPU thread 1
      44.18 CPU thread 2
      43.71 CPU thread 3
    - MPI Rank 2
      44.47 CPU thread 0
      43.49 CPU thread 1
      43.86 CPU thread 2
      35.18 CPU thread 3
    - MPI Rank 3
      44.74 CPU thread 0
      44.00 CPU thread 1
      43.73 CPU thread 2
      35.64 CPU thread 3
```

```
0.00   767.48 (100.00%)   767.48 | 0.00   668.54 (87.11%)   767.48 | 0.00   668.54
```

Select multiple nodes with Ctrl-click

Context-sensitive help


cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex
File Display Topology Help
Getting started
Mouse and keyboard control
What's This? Shift+F1
About
Selected metrics description
Selected regions description
Absolute
Metric tree
System tree
Box Plot

```
1.63e9 Visits
767.48 Time
0.00 Minimum I
48.58 Maximum
5.27e8 byt
5.27e8 received
```

```
compute_rhs_
solve_
4 !$omp parallel @x_sol
218.21 !$omp do @x_sol
15.18 !$omp implicit bar
0.07 y_solve_
0.04 !$omp parallel @y_sol
223.63 !$omp do @y_sol
15.60 !$omp implicit bar
0.07 z_solve_
0.04 !$omp parallel @z_sol
226.71 !$omp do @z_sol
14.79 !$omp implicit bar
1.86 add_
0.01 MPI_Barrier
0.00 timer_start_
0.00 timer_stop_
0.00 timer_read_
0.60 verify_
0.00 MPI_Reduce
0.00 print_results_
```

```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      44.10 CPU thread 0
      43.94 CPU thread 1
      43.58 CPU thread 2
      34.36 CPU thread 3
    - MPI Rank 1
      44.48 CPU thread 0
      35.09 CPU thread 1
      44.18 CPU thread 2
      43.71 CPU thread 3
    - MPI Rank 2
      44.47 CPU thread 0
      43.49 CPU thread 1
      43.86 CPU thread 2
      35.18 CPU thread 3
    - MPI Rank 3
      44.74 CPU thread 0
      44.00 CPU thread 1
      43.73 CPU thread 2
      35.64 CPU thread 3
```

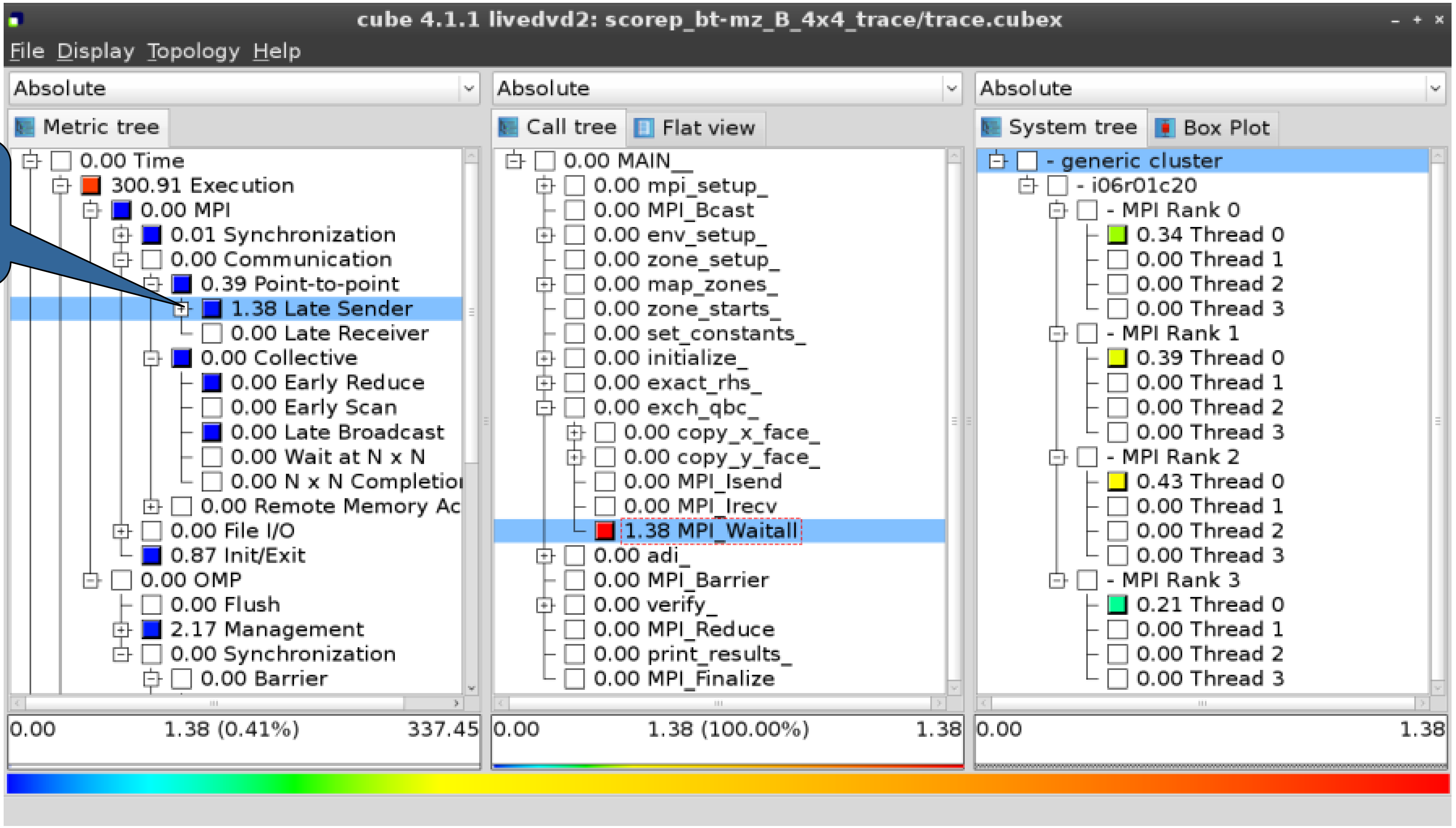
```
0.00    767.48 (100.00%)    767.48
0.00    668.54 (87.11%)     767.48
0.00                        668.54
```

Change into help mode for display components

Context-sensitive help available for all GUI items

Post-processed trace analysis report

Additional trace-based metrics in metric hierarchy

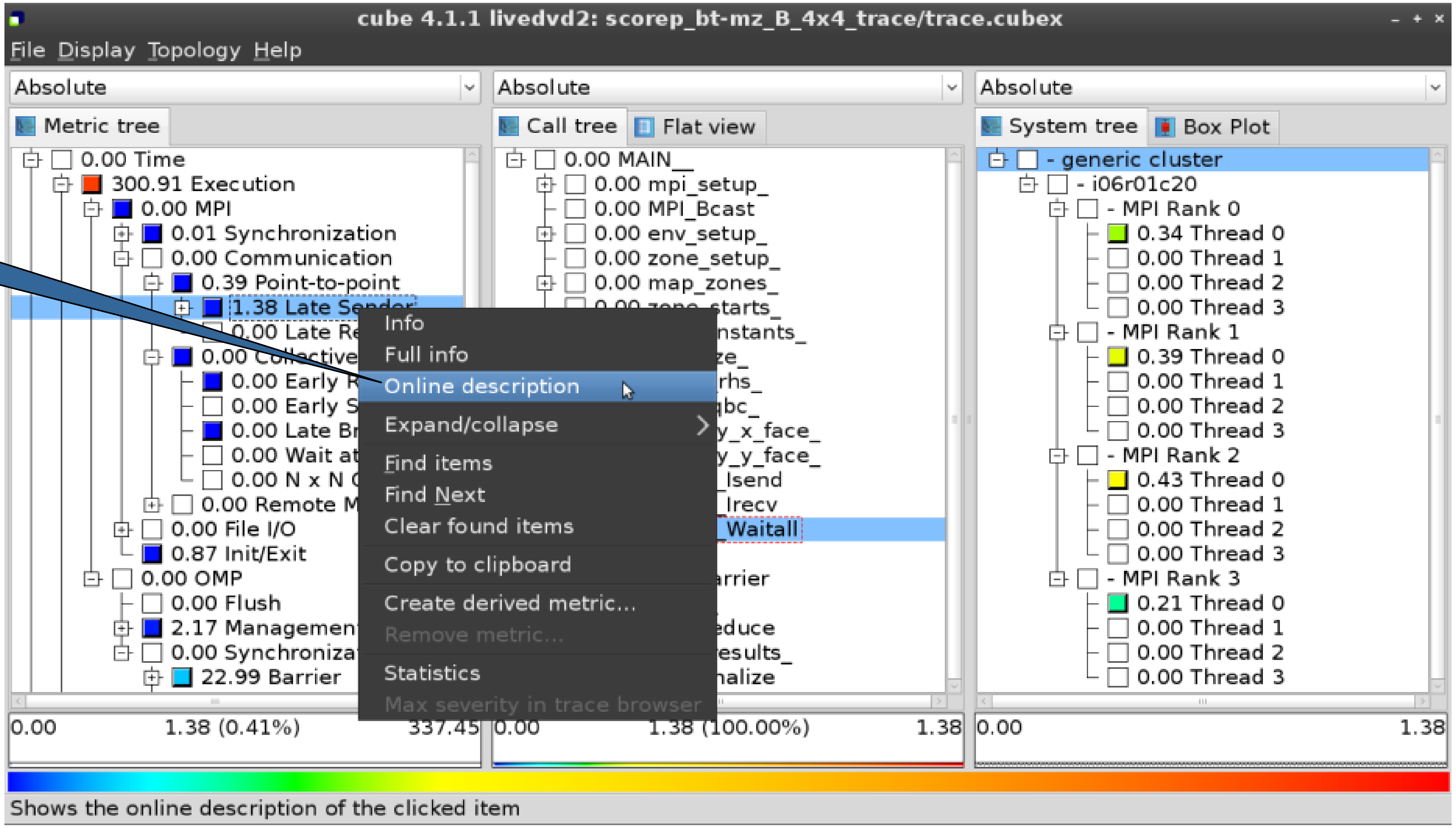


cube 4.1.1 livedvd2: scorep_bt-mz_B_4x4_trace/trace.cubex

```
Metric tree                         Call tree                      System tree
0.00 Time                           0.00 MAIN__                    - generic cluster
  300.91 Execution                    0.00 mpi_setup_                - i06r01c20
    0.00 MPI                          0.00 MPI_Bcast                   - MPI Rank 0
      0.01 Synchronization            0.00 env_setup_                    0.34 Thread 0
      0.00 Communication              0.00 zone_setup_                   0.00 Thread 1
        0.39 Point-to-point           0.00 map_zones_                    0.00 Thread 2
          1.38 Late Sender            0.00 zone_starts_                  0.00 Thread 3
          0.00 Late Receiver          0.00 set_constants_              - MPI Rank 1
        0.00 Collective               0.00 initialize_                   0.39 Thread 0
          0.00 Early Reduce           0.00 exact_rhs_                    0.00 Thread 1
          0.00 Early Scan             0.00 exch_qbc_                     0.00 Thread 2
          0.00 Late Broadcast           0.00 copy_x_face_                0.00 Thread 3
          0.00 Wait at N x N            0.00 copy_y_face_              - MPI Rank 2
          0.00 N x N Completion         0.00 MPI_Isend                   0.43 Thread 0
        0.00 Remote Memory Ac           0.00 MPI_Irecv                   0.00 Thread 1
      0.00 File I/O                     1.38 MPI_Waitall                 0.00 Thread 2
      0.87 Init/Exit                  0.00 adi_                          0.00 Thread 3
    0.00 OMP                          0.00 MPI_Barrier                 - MPI Rank 3
      0.00 Flush                      0.00 verify_                       0.21 Thread 0
      2.17 Management                 0.00 MPI_Reduce                    0.00 Thread 1
      0.00 Synchronization            0.00 print_results_                0.00 Thread 2
        0.00 Barrier                  0.00 MPI_Finalize                  0.00 Thread 3

0.00   1.38 (0.41%)   337.45   0.00   1.38 (100.00%)   1.38   0.00   1.38
```

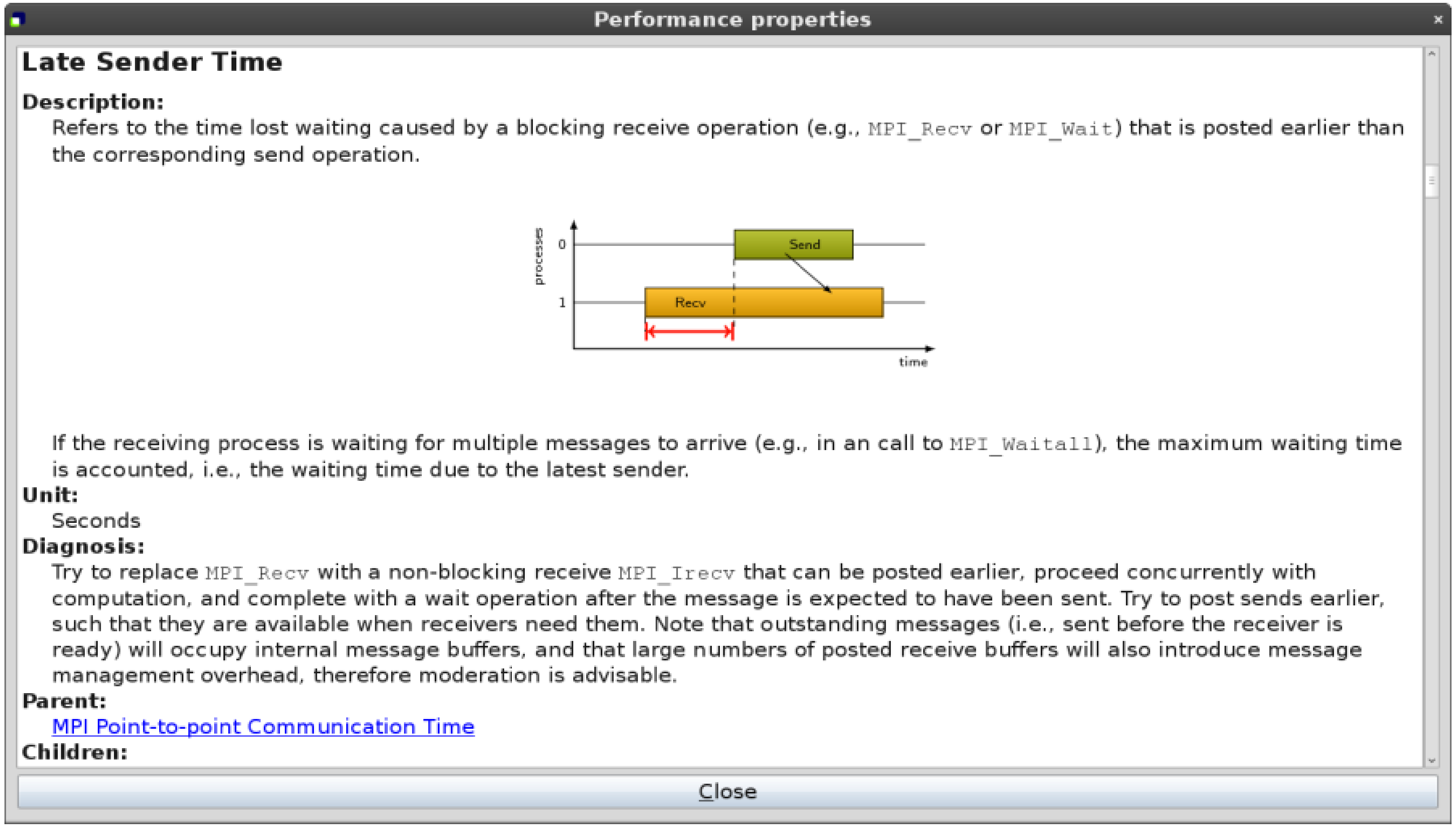
Online metric description

Access online metric description via context menu



Shows the online description of the clicked item

Online metric description

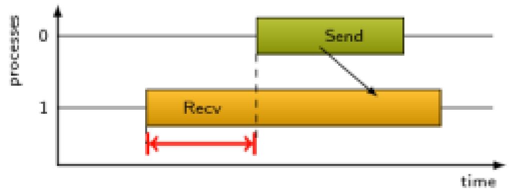


Performance properties

Late Sender Time

Description:

Refers to the time lost waiting caused by a blocking receive operation (e.g., `MPI_Recv` or `MPI_Wait`) that is posted earlier than the corresponding send operation.



If the receiving process is waiting for multiple messages to arrive (e.g., in an call to `MPI_Waitall`), the maximum waiting time is accounted, i.e., the waiting time due to the latest sender.

Unit:

Seconds

Diagnosis:

Try to replace `MPI_Recv` with a non-blocking receive `MPI_Irecv` that can be posted earlier, proceed concurrently with computation, and complete with a wait operation after the message is expected to have been sent. Try to post sends earlier, such that they are available when receivers need them. Note that outstanding messages (i.e., sent before the receiver is ready) will occupy internal message buffers, and that large numbers of posted receive buffers will also introduce message management overhead, therefore moderation is advisable.

Parent:

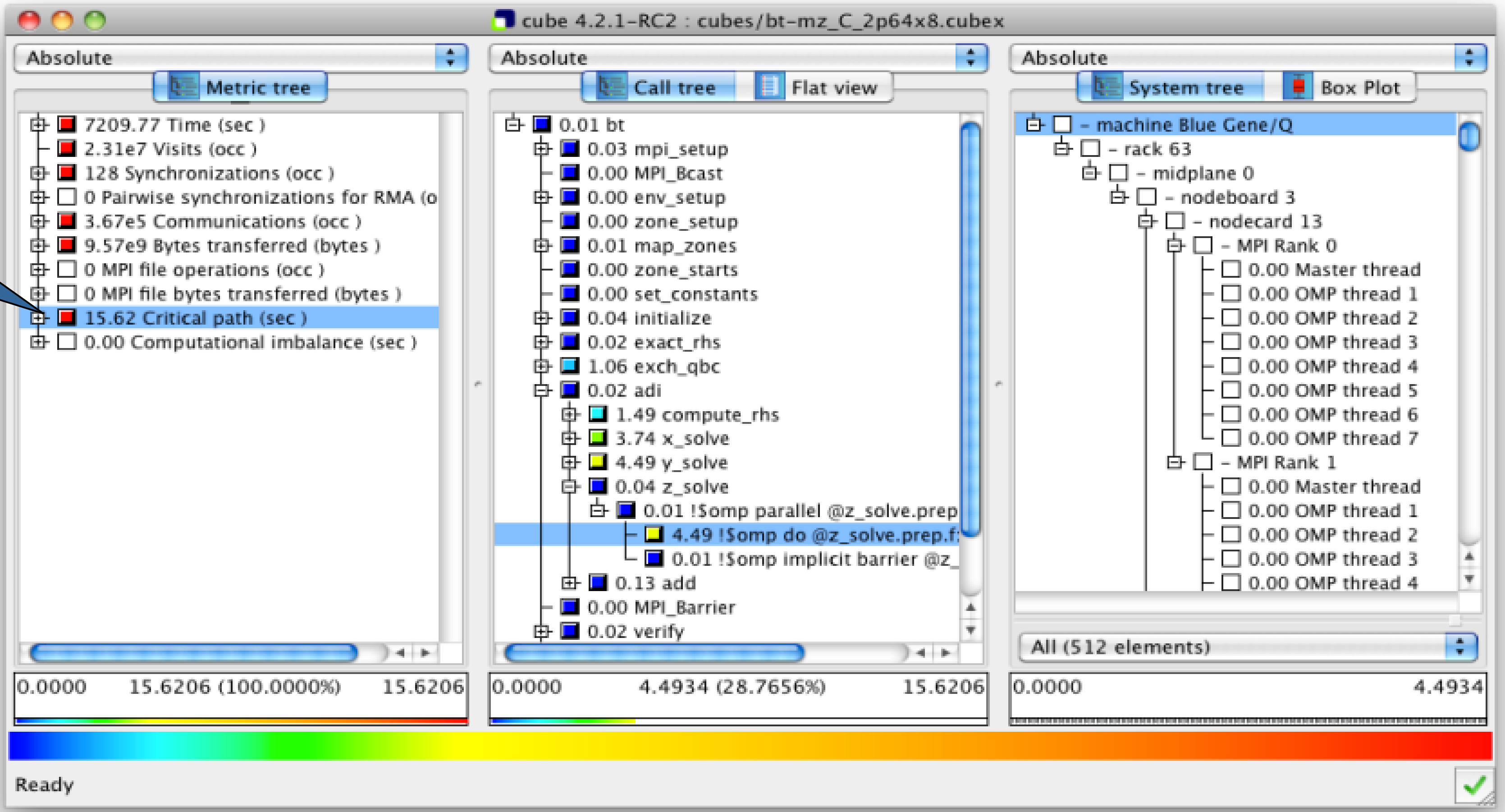
MPI Point-to-point Communication Time

Children:

Close

Critical-path analysis

Critical-path profile shows wall-clock time impact



cube 4.2.1-RC2 : cubes/bt-mz_C_2p64x8.cubex

```
7209.77 Time (sec )
2.31e7 Visits (occ )
128 Synchronizations (occ )
0 Pairwise synchronizations for RMA (o
3.67e5 Communications (occ )
9.57e9 Bytes transferred (bytes )
0 MPI file operations (occ )
0 MPI file bytes transferred (bytes )
15.62 Critical path (sec )
0.00 Computational imbalance (sec )
```

```
0.01 bt
  0.03 mpi_setup
  0.00 MPI_Bcast
  0.00 env_setup
  0.00 zone_setup
  0.01 map_zones
  0.00 zone_starts
  0.00 set_constants
  0.04 initialize
  0.02 exact_rhs
  1.06 exch_qbc
  0.02 adi
    1.49 compute_rhs
    3.74 x_solve
    4.49 y_solve
    0.04 z_solve
      0.01 !$omp parallel @z_solve.prep
        4.49 !$omp do @z_solve.prep.f
        0.01 !$omp implicit barrier @z_
    0.13 add
  0.00 MPI_Barrier
  0.02 verify
```

```
- machine Blue Gene/Q
  - rack 63
    - midplane 0
      - nodeboard 3
        - nodecard 13
          - 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
          - MPI Rank 1
            0.00 Master thread
            0.00 OMP thread 1
            0.00 OMP thread 2
            0.00 OMP thread 3
            0.00 OMP thread 4
```

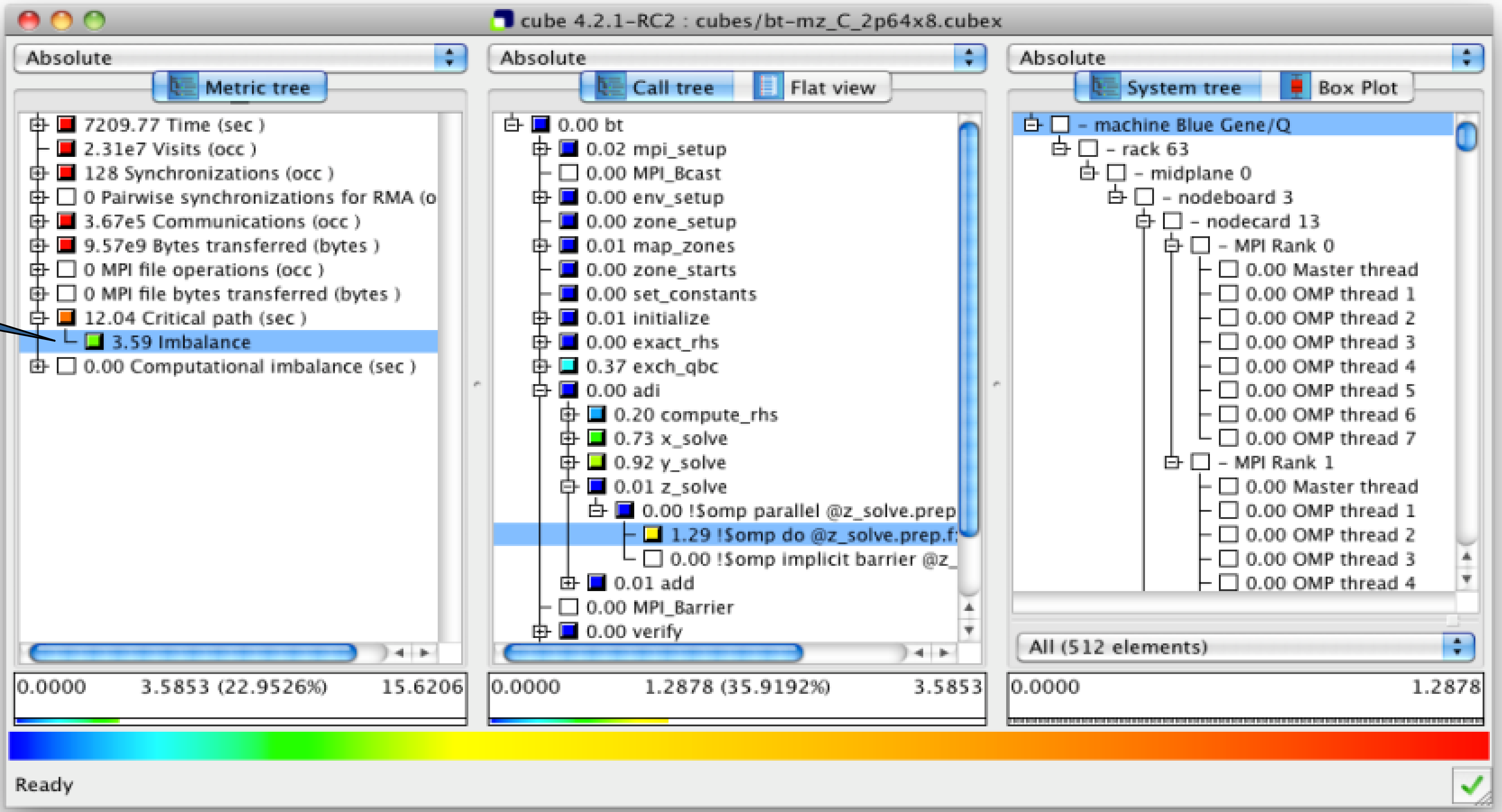
All (512 elements)

```
0.0000    15.6206 (100.0000%)    15.6206
0.0000    4.4934 (28.7656%)      15.6206
0.0000                           4.4934
```

Ready

Critical-path analysis

Critical-path imbalance highlights inefficient parallelism



cube 4.2.1-RC2 : cubes/bt-mz_C_2p64x8.cubex

Absolute | Metric tree

```
7209.77 Time (sec )
2.31e7 Visits (occ )
128 Synchronizations (occ )
0 Pairwise synchronizations for RMA (o
3.67e5 Communications (occ )
9.57e9 Bytes transferred (bytes )
0 MPI file operations (occ )
0 MPI file bytes transferred (bytes )
12.04 Critical path (sec )
  3.59 Imbalance
0.00 Computational imbalance (sec )
```

0.0000   3.5853 (22.9526%)   15.6206

Absolute | Call tree | Flat view

```
0.00 bt
  0.02 mpi_setup
  0.00 MPI_Bcast
  0.00 env_setup
  0.00 zone_setup
  0.01 map_zones
  0.00 zone_starts
  0.00 set_constants
  0.01 initialize
  0.00 exact_rhs
  0.37 exch_qbc
  0.00 adi
    0.20 compute_rhs
    0.73 x_solve
    0.92 y_solve
    0.01 z_solve
      0.00 !$omp parallel @z_solve.prep
        1.29 !$omp do @z_solve.prep.f
        0.00 !$omp implicit barrier @z_
    0.01 add
  0.00 MPI_Barrier
  0.00 verify
```

0.0000   1.2878 (35.9192%)   3.5853

Absolute | System tree | Box Plot

```
- machine Blue Gene/Q
  - rack 63
    - midplane 0
      - nodeboard 3
        - nodecard 13
          - 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
          - MPI Rank 1
            0.00 Master thread
            0.00 OMP thread 1
            0.00 OMP thread 2
            0.00 OMP thread 3
            0.00 OMP thread 4
```

All (512 elements)

0.0000   1.2878

Ready

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

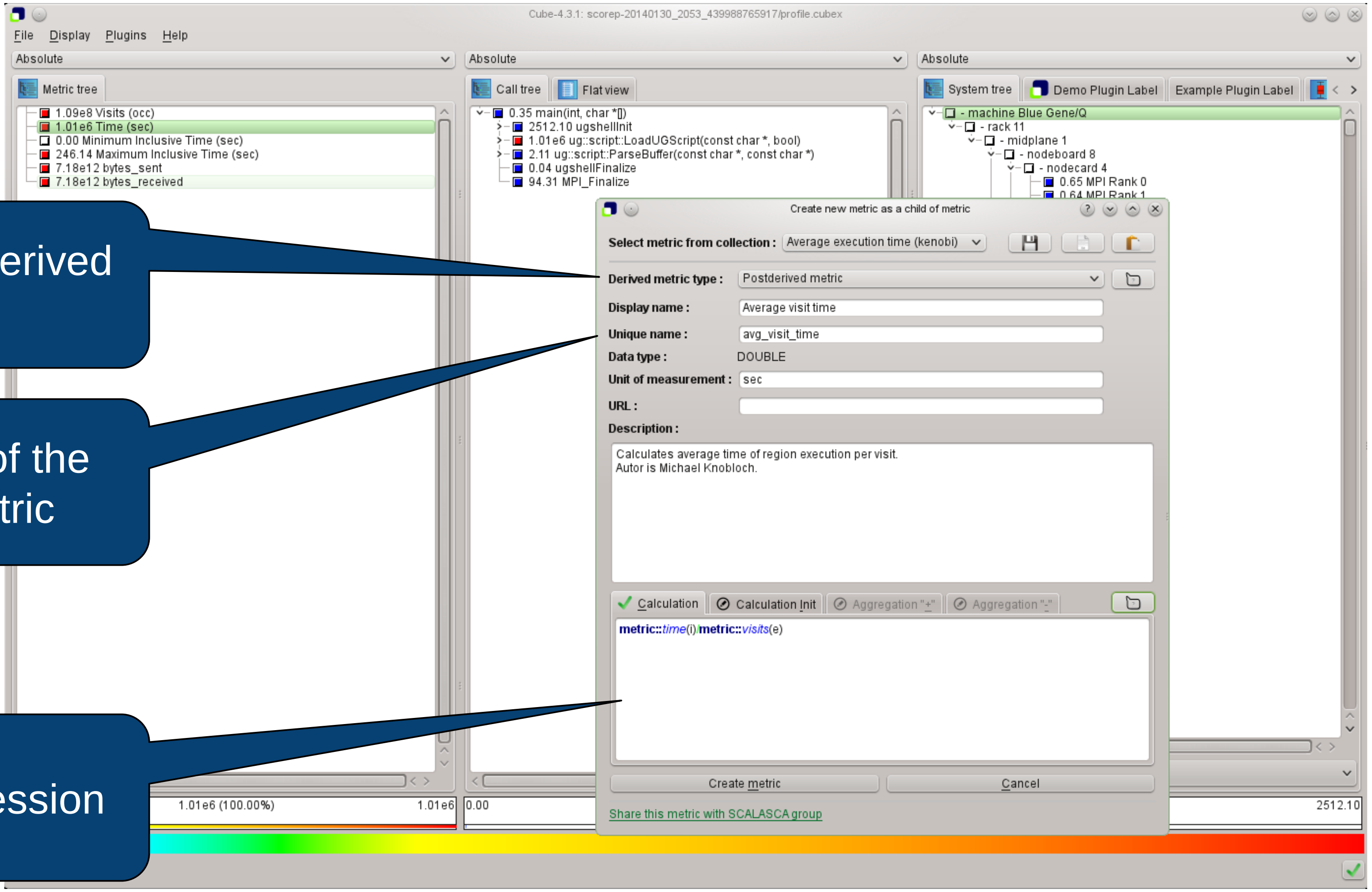
- Examples:
  - "Average execution time": Postderived metric with expression

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

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

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

Derived metrics in Cube GUI



```
1.09e8 Visits (occ)
1.01e6 Time (sec)
0.00 Minimum Inclusive Time (sec)
246.14 Maximum Inclusive Time (sec)
7.18e12 bytes_sent
7.18e12 bytes_received
```

```
0.35 main(int, char *[])
  2512.10 ugshellInit
  1.01e6 ug::script::LoadUGScript(const char *, bool)
  2.11 ug::script::ParseBuffer(const char *, const char *)
  0.04 ugshellFinalize
  94.31 MPI_Finalize
```

```
- machine Blue Gene/Q
  - rack 11
    - midplane 1
      - nodeboard 8
        - nodecard 4
          0.65 MPI Rank 0
          0.64 MPI Rank 1
```

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 :	
Description :	Calculates average time of region execution per visit. Autor is Michael Knobloch.

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

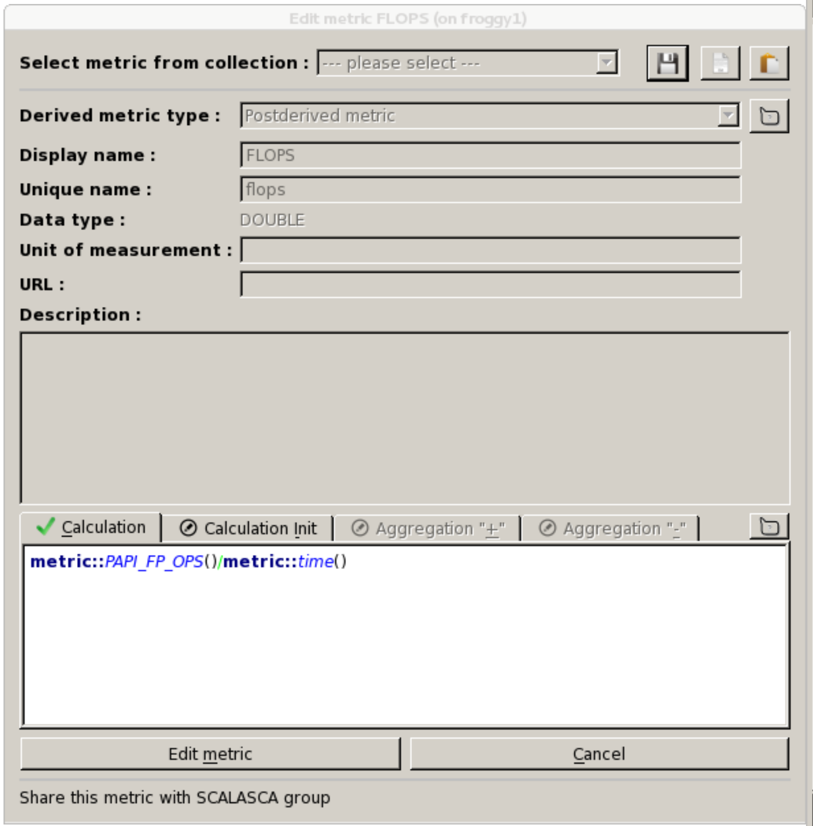
1.01e6 (100.00%) 1.01e6 0.00 2512.10

Collection of derived metrics

Parameters of the derived metric

CubePL expression

Example: FLOPS based on PAPI_FP_OPS and time



Edit metric FLOPS (on froggy1)

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

Derived metric type : Postderived metric

Display name : FLOPS

Unique name : flops

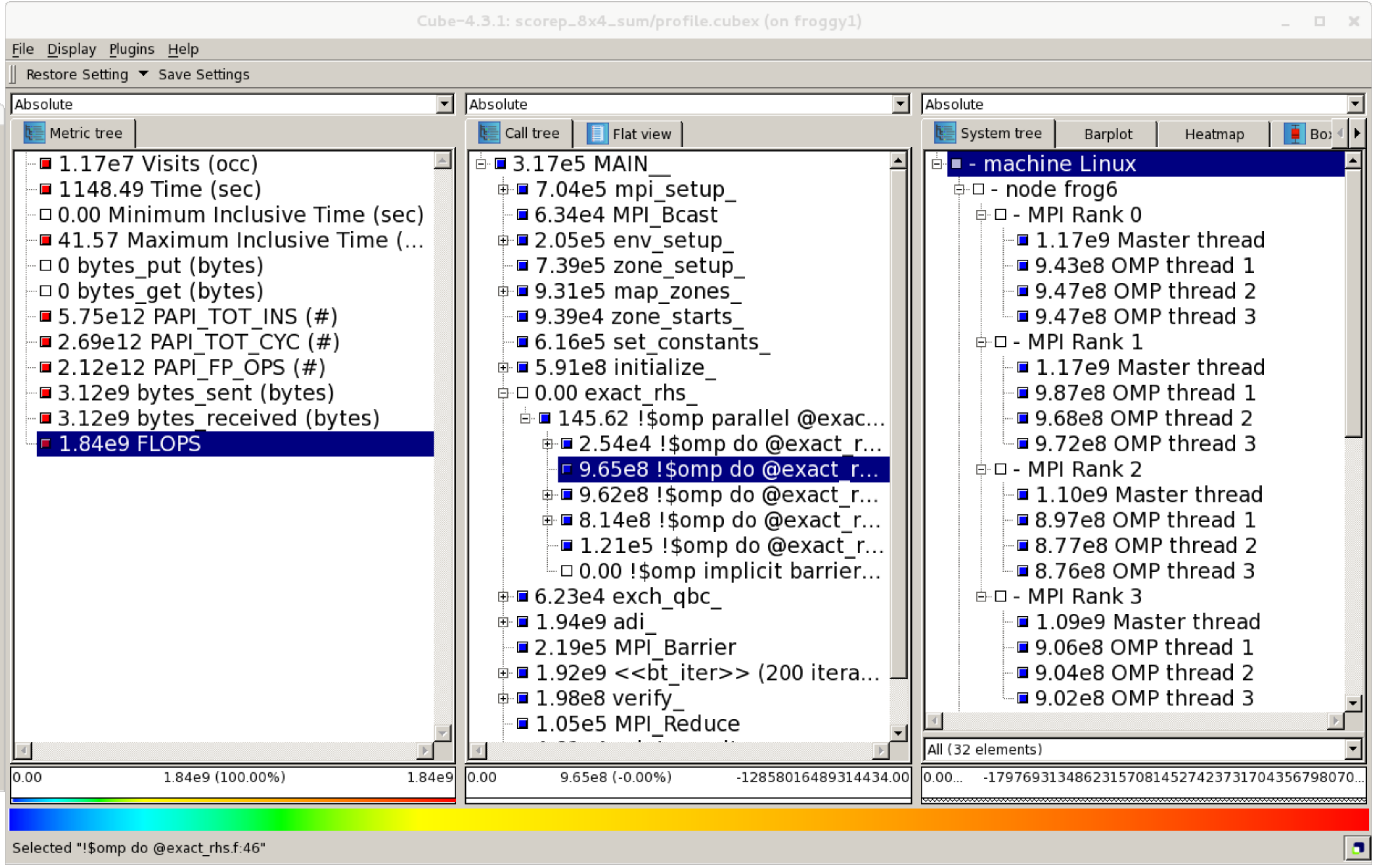
Data type : DOUBLE

Unit of measurement :

URL :

Description :

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



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

```
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
```

```
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
```

```
- 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_B_mic15p30x4_sum/profile.cubex
Writing cut.cubex... done.
```

- Calculating difference of two reports

```
% cube_diff  scorep_bt-mz_B_mic15p30x4_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

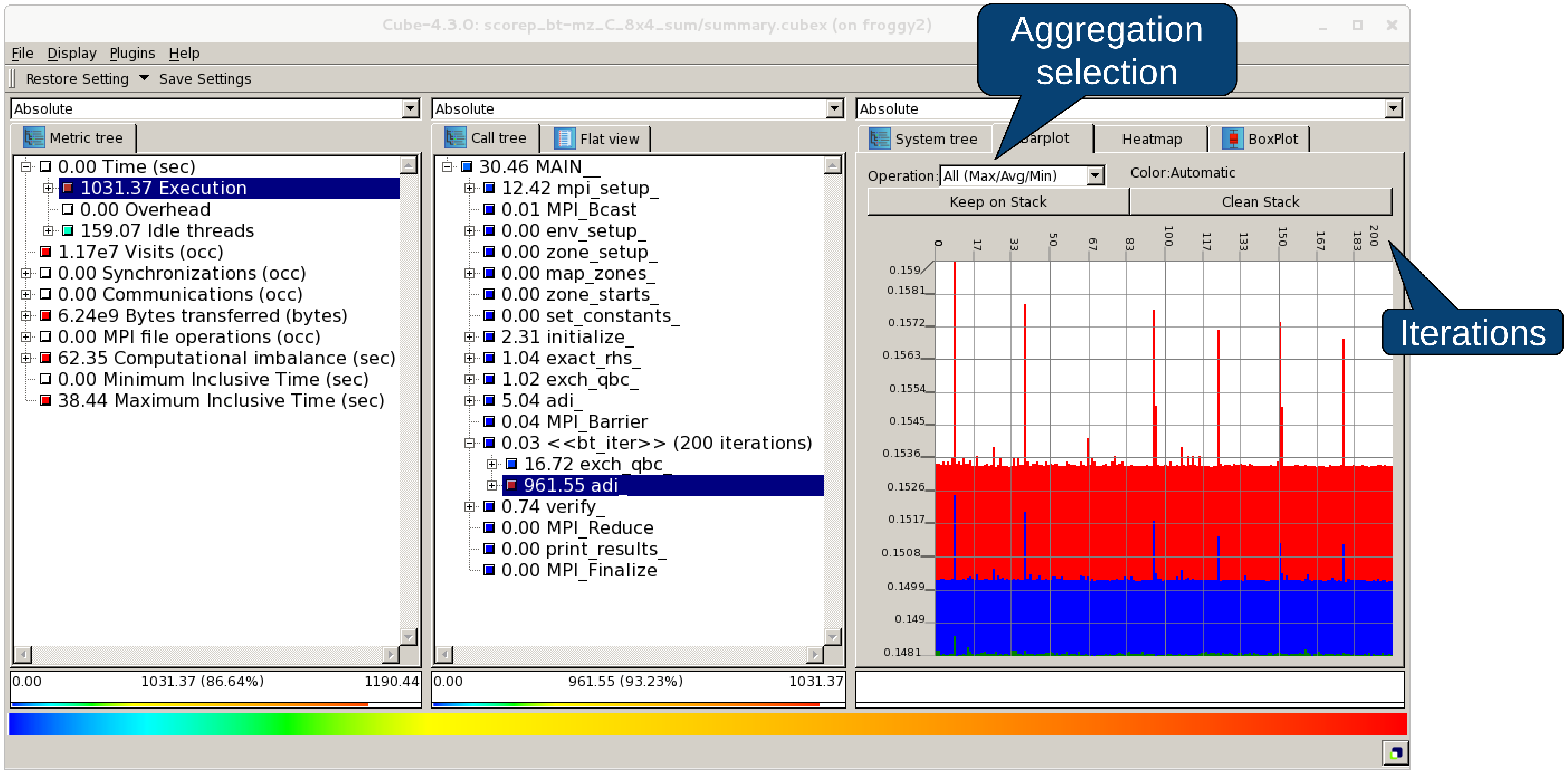
➢Useful for checking results for specific iterations

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



Operation: All (Max/Avg/Min)
Color:Automatic

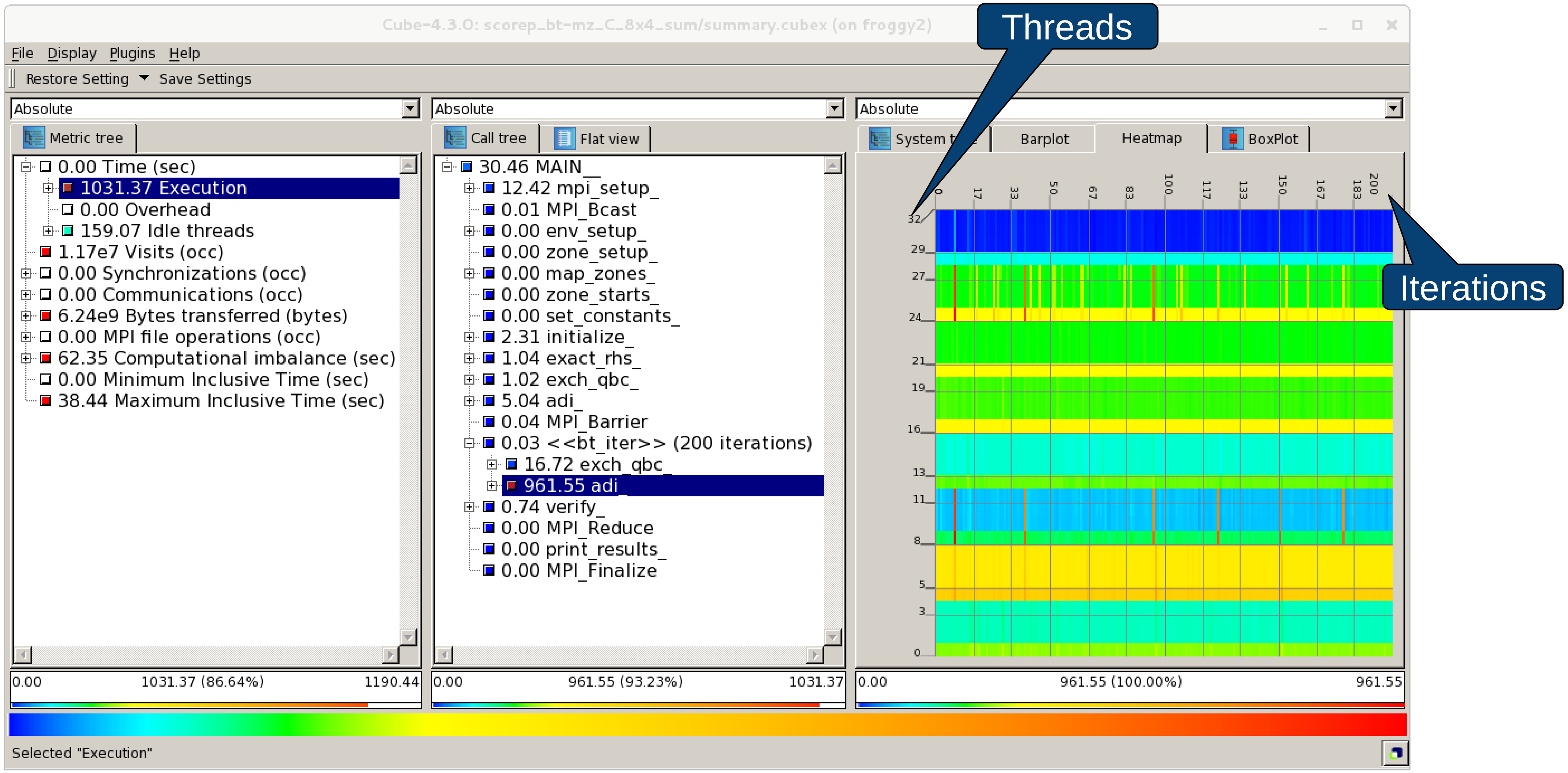
Metric tree:
- 0.00 Time (sec)
  - 1031.37 Execution
  - 0.00 Overhead
  - 159.07 Idle threads
- 1.17e7 Visits (occ)
- 0.00 Synchronizations (occ)
- 0.00 Communications (occ)
- 6.24e9 Bytes transferred (bytes)
- 0.00 MPI file operations (occ)
- 62.35 Computational imbalance (sec)
- 0.00 Minimum Inclusive Time (sec)
- 38.44 Maximum Inclusive Time (sec)

0.00 1031.37 (86.64%) 1190.44

Call tree:
- 30.46 MAIN__
  - 12.42 mpi_setup_
  - 0.01 MPI_Bcast
  - 0.00 env_setup_
  - 0.00 zone_setup_
  - 0.00 map_zones_
  - 0.00 zone_starts_
  - 0.00 set_constants_
  - 2.31 initialize_
  - 1.04 exact_rhs_
  - 1.02 exch_qbc_
  - 5.04 adi_
  - 0.04 MPI_Barrier
  - 0.03 <<bt_iter>> (200 iterations)
    - 16.72 exch_qbc_
    - 961.55 adi_
  - 0.74 verify_
  - 0.00 MPI_Reduce
  - 0.00 print_results_
  - 0.00 MPI_Finalize

0.00 961.55 (93.23%) 1031.37

Iteration profiling: Heatmap

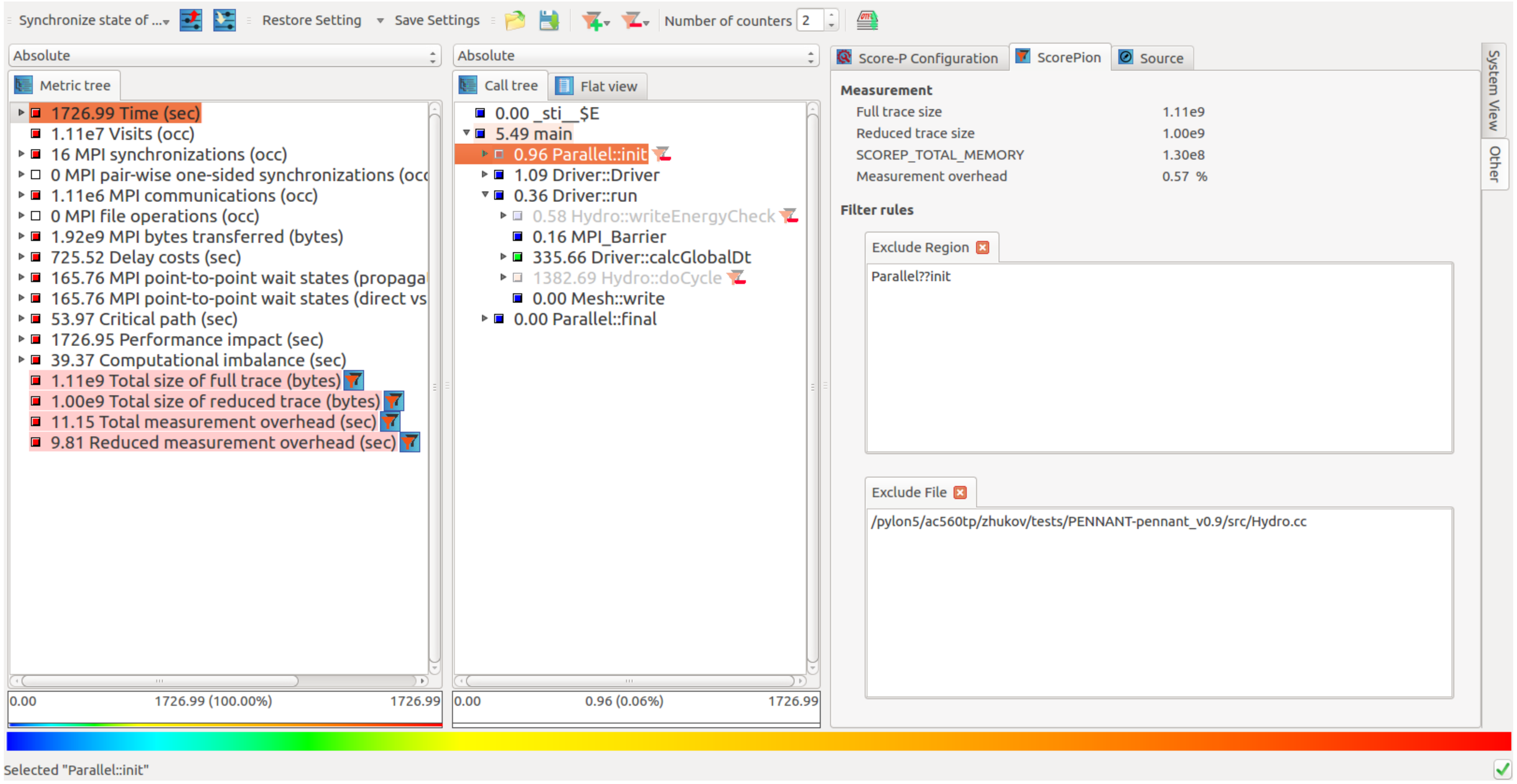


```
0.00 Time (sec)
  1031.37 Execution
    0.00 Overhead
  159.07 Idle threads
1.17e7 Visits (occ)
0.00 Synchronizations (occ)
0.00 Communications (occ)
6.24e9 Bytes transferred (bytes)
0.00 MPI file operations (occ)
62.35 Computational imbalance (sec)
0.00 Minimum Inclusive Time (sec)
38.44 Maximum Inclusive Time (sec)
```

```
30.46 MAIN__
  12.42 mpi_setup_
  0.01 MPI_Bcast
  0.00 env_setup_
  0.00 zone_setup_
  0.00 map_zones_
  0.00 zone_starts_
  0.00 set_constants_
  2.31 initialize_
  1.04 exact_rhs_
  1.02 exch_qbc_
  5.04 adi_
  0.04 MPI_Barrier
  0.03 <<bt_iter>> (200 iterations)
    16.72 exch_qbc_
    961.55 adi_
  0.74 verify_
  0.00 MPI_Reduce
  0.00 print_results_
  0.00 MPI_Finalize
```

```
0.00    1031.37 (86.64%)    1190.44
0.00    961.55 (93.23%)     1031.37
0.00    961.55 (100.00%)    961.55
Selected "Execution"
```

Score-P/Intel compiler filter creation plugin



```
1726.99 Time (sec)
1.11e7 Visits (occ)
16 MPI synchronizations (occ)
0 MPI pair-wise one-sided synchronizations (occ
1.11e6 MPI communications (occ)
0 MPI file operations (occ)
1.92e9 MPI bytes transferred (bytes)
725.52 Delay costs (sec)
165.76 MPI point-to-point wait states (propaga
165.76 MPI point-to-point wait states (direct vs
53.97 Critical path (sec)
1726.95 Performance impact (sec)
39.37 Computational imbalance (sec)
1.11e9 Total size of full trace (bytes)
1.00e9 Total size of reduced trace (bytes)
11.15 Total measurement overhead (sec)
9.81 Reduced measurement overhead (sec)
```

```
0.00 _sti__$E
5.49 main
  0.96 Parallel::init
  1.09 Driver::Driver
  0.36 Driver::run
    0.58 Hydro::writeEnergyCheck
    0.16 MPI_Barrier
    335.66 Driver::calcGlobalDt
    1382.69 Hydro::doCycle
    0.00 Mesh::write
  0.00 Parallel::final
```

0.00 1726.99 (100.00%) 1726.99

0.00 0.96 (0.06%) 1726.99

Measurement

Full trace size	1.11e9
Reduced trace size	1.00e9
SCOREP_TOTAL_MEMORY	1.30e8
Measurement overhead	0.57 %

Filter rules

Exclude Region

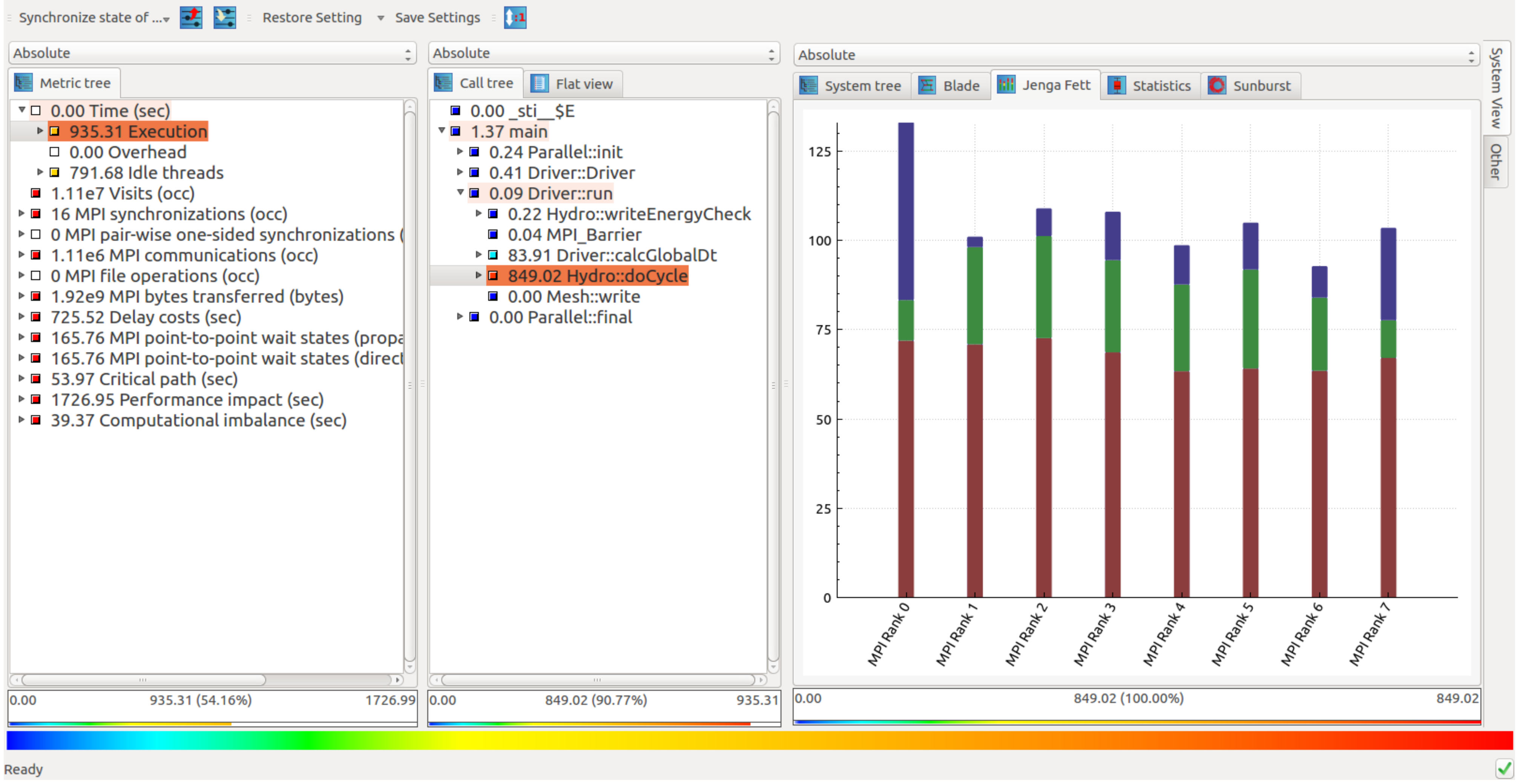
Parallel??init

Exclude File

/pylon5/ac560tp/zhukov/tests/PENNANT-pennant_v0.9/src/Hydro.cc

Selected "Parallel::init"

Metrics correlation explorer plugin



Metric tree:

```
▾ □ 0.00 Time (sec)
  ▸ ■ 935.31 Execution
    □ 0.00 Overhead
  ▸ ■ 791.68 Idle threads
  ■ 1.11e7 Visits (occ)
▸ ■ 16 MPI synchronizations (occ)
▸ □ 0 MPI pair-wise one-sided synchronizations (
▸ ■ 1.11e6 MPI communications (occ)
▸ □ 0 MPI file operations (occ)
▸ ■ 1.92e9 MPI bytes transferred (bytes)
▸ ■ 725.52 Delay costs (sec)
▸ ■ 165.76 MPI point-to-point wait states (propa
▸ ■ 165.76 MPI point-to-point wait states (direct
▸ ■ 53.97 Critical path (sec)
▸ ■ 1726.95 Performance impact (sec)
▸ ■ 39.37 Computational imbalance (sec)
```

0.00 935.31 (54.16%) 1726.99

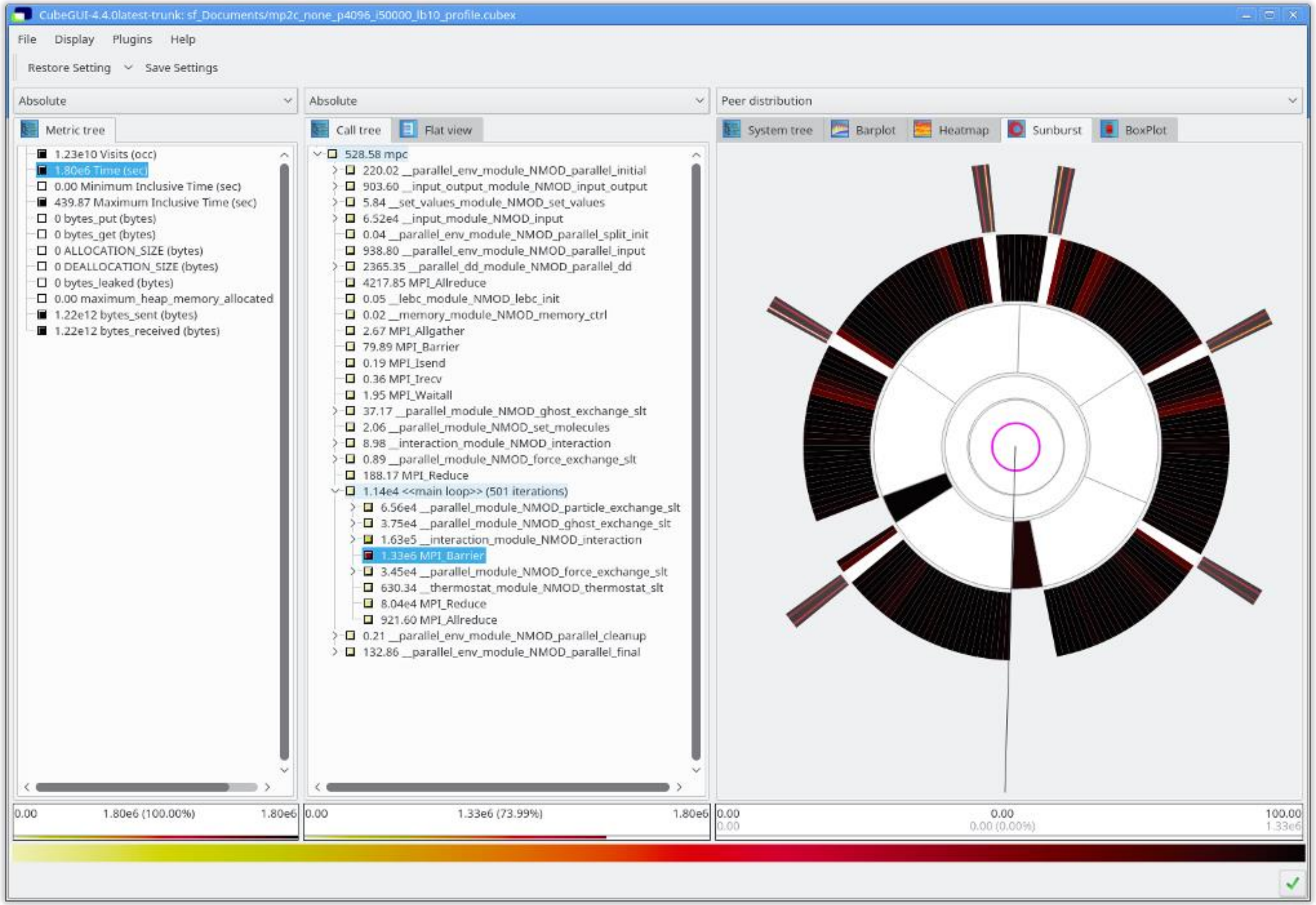
Call tree:

```
■ 0.00 _sti__$E
▾ ■ 1.37 main
  ▸ ■ 0.24 Parallel::init
  ▸ ■ 0.41 Driver::Driver
  ▾ ■ 0.09 Driver::run
    ▸ ■ 0.22 Hydro::writeEnergyCheck
      ■ 0.04 MPI_Barrier
    ▸ ■ 83.91 Driver::calcGlobalDt
    ▸ ■ 849.02 Hydro::doCycle
      ■ 0.00 Mesh::write
  ▸ ■ 0.00 Parallel::final
```

0.00 849.02 (90.77%) 935.31

0.00 849.02 (100.00%) 849.02

System sunburst plugin



CubeGUI-4.4.0latest-trunk: sf_Documents/mp2c_none_p4096_i50000_lb10_profile.cubex

File Display Plugins Help

Restore Setting Save Settings

Absolute | Absolute | Peer distribution

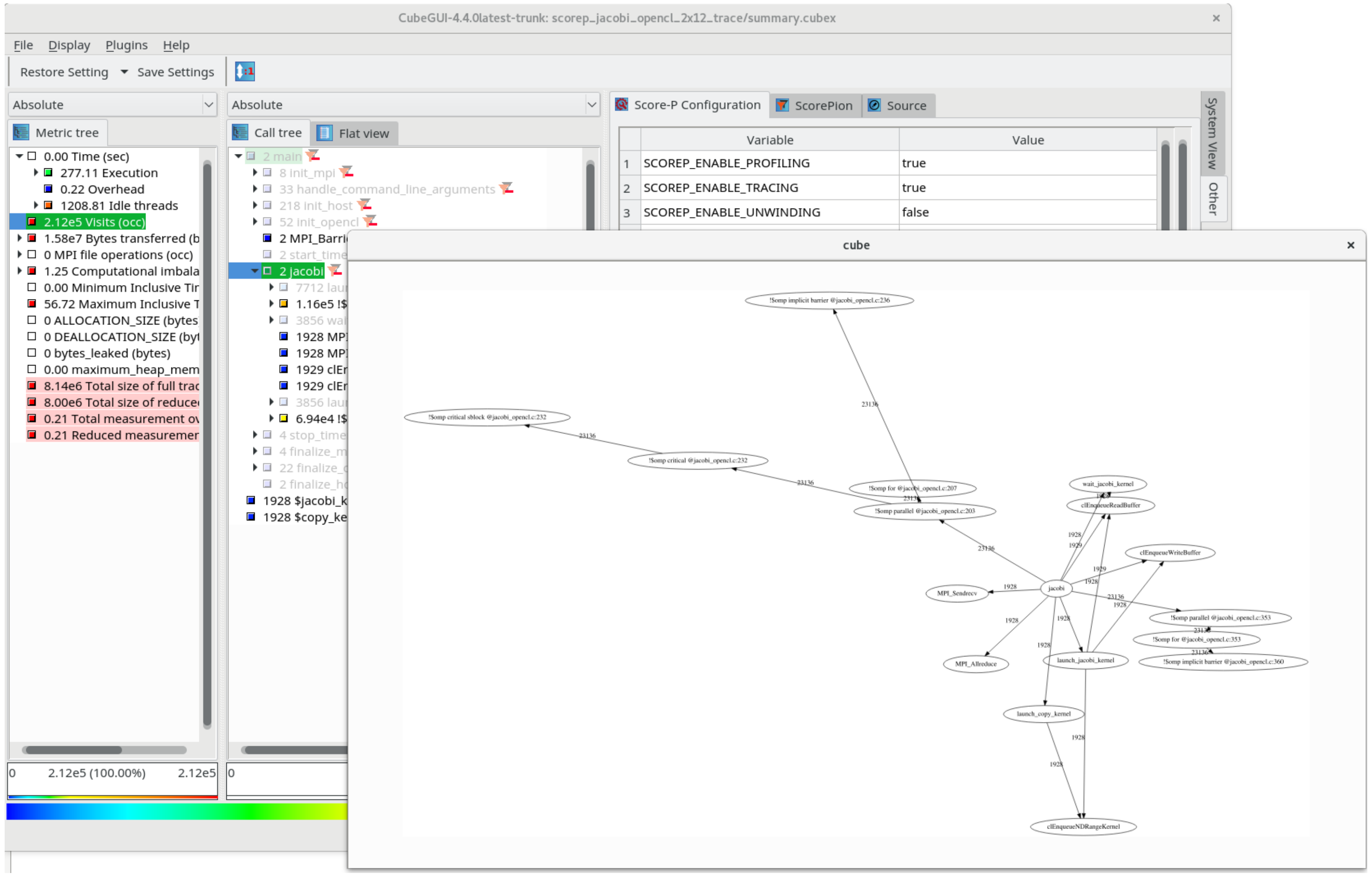
Metric tree | Call tree | Flat view | System tree | Barplot | Heatmap | Sunburst | BoxPlot

```
1.23e10 Visits (occ)
1.80e6 Time (sec)
0.00 Minimum Inclusive Time (sec)
439.87 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
1.22e12 bytes_sent (bytes)
1.22e12 bytes_received (bytes)
```

```
528.58 mpc
  220.02 __parallel_env_module_NMOD_parallel_initial
  903.60 __input_output_module_NMOD_input_output
  5.84 __set_values_module_NMOD_set_values
  6.52e4 __input_module_NMOD_input
  0.04 __parallel_env_module_NMOD_parallel_split_init
  938.80 __parallel_env_module_NMOD_parallel_input
  2365.35 __parallel_dd_module_NMOD_parallel_dd
  4217.85 MPI_Allreduce
  0.05 __lebc_module_NMOD_lebc_init
  0.02 __memory_module_NMOD_memory_ctrl
  2.67 MPI_Allgather
  79.89 MPI_Barrier
  0.19 MPI_Isend
  0.36 MPI_Irecv
  1.95 MPI_Waitall
  37.17 __parallel_module_NMOD_ghost_exchange_slt
  2.06 __parallel_module_NMOD_set_molecules
  8.98 __interaction_module_NMOD_interaction
  0.89 __parallel_module_NMOD_force_exchange_slt
  188.17 MPI_Reduce
  1.14e4 <<main loop>> (501 iterations)
    6.56e4 __parallel_module_NMOD_particle_exchange_slt
    3.75e4 __parallel_module_NMOD_ghost_exchange_slt
    1.63e5 __interaction_module_NMOD_interaction
    1.33e6 MPI_Barrier
    3.45e4 __parallel_module_NMOD_force_exchange_slt
    630.34 __thermostat_module_NMOD_thermostat_slt
    8.04e4 MPI_Reduce
    921.60 MPI_Allreduce
  0.21 __parallel_env_module_NMOD_parallel_cleanup
  132.86 __parallel_env_module_NMOD_parallel_final
```

```
0.00   1.80e6 (100.00%)   1.80e6 | 0.00   1.33e6 (73.99%)   1.80e6 | 0.00   0.00   100.00
                                                                    0.00   0.00 (0.00%)   1.33e6
```

Call graph display plugin



CubeGUI-4.4.0latest-trunk: scorep_jacobi_opencl_2x12_trace/summary.cubex

File Display Plugins Help

Restore Setting Save Settings

Absolute | Absolute

Metric tree | Call tree | Flat view

- 0.00 Time (sec)
  - 277.11 Execution
  - 0.22 Overhead
  - 1208.81 Idle threads
- 2.12e5 Visits (occ)
- 1.58e7 Bytes transferred (b
- 0 MPI file operations (occ)
- 1.25 Computational imbala
- 0.00 Minimum Inclusive Tir
- 56.72 Maximum Inclusive T
- 0 ALLOCATION_SIZE (bytes
- 0 DEALLOCATION_SIZE (byt
- 0 bytes_leaked (bytes)
- 0.00 maximum_heap_mem
- 8.14e6 Total size of full trac
- 8.00e6 Total size of reduce
- 0.21 Total measurement ov
- 0.21 Reduced measuremer

- 2 main
  - 8 init_mpi
  - 33 handle_command_line_arguments
  - 218 init_host
  - 52 init_opencl
  - 2 MPI_Barri
  - 2 start_time
  - 2 jacobi
    - 7712 lau
    - 1.16e5 !$
    - 3856 wai
    - 1928 MP
    - 1928 MP
    - 1929 clEr
    - 1929 clEr
    - 3856 lau
    - 6.94e4 !$
  - 4 stop_time
  - 4 finalize_m
  - 22 finalize_
  - 2 finalize_h
- 1928 $jacobi_k
- 1928 $copy_ke

0 2.12e5 (100.00%) 2.12e5 | 0

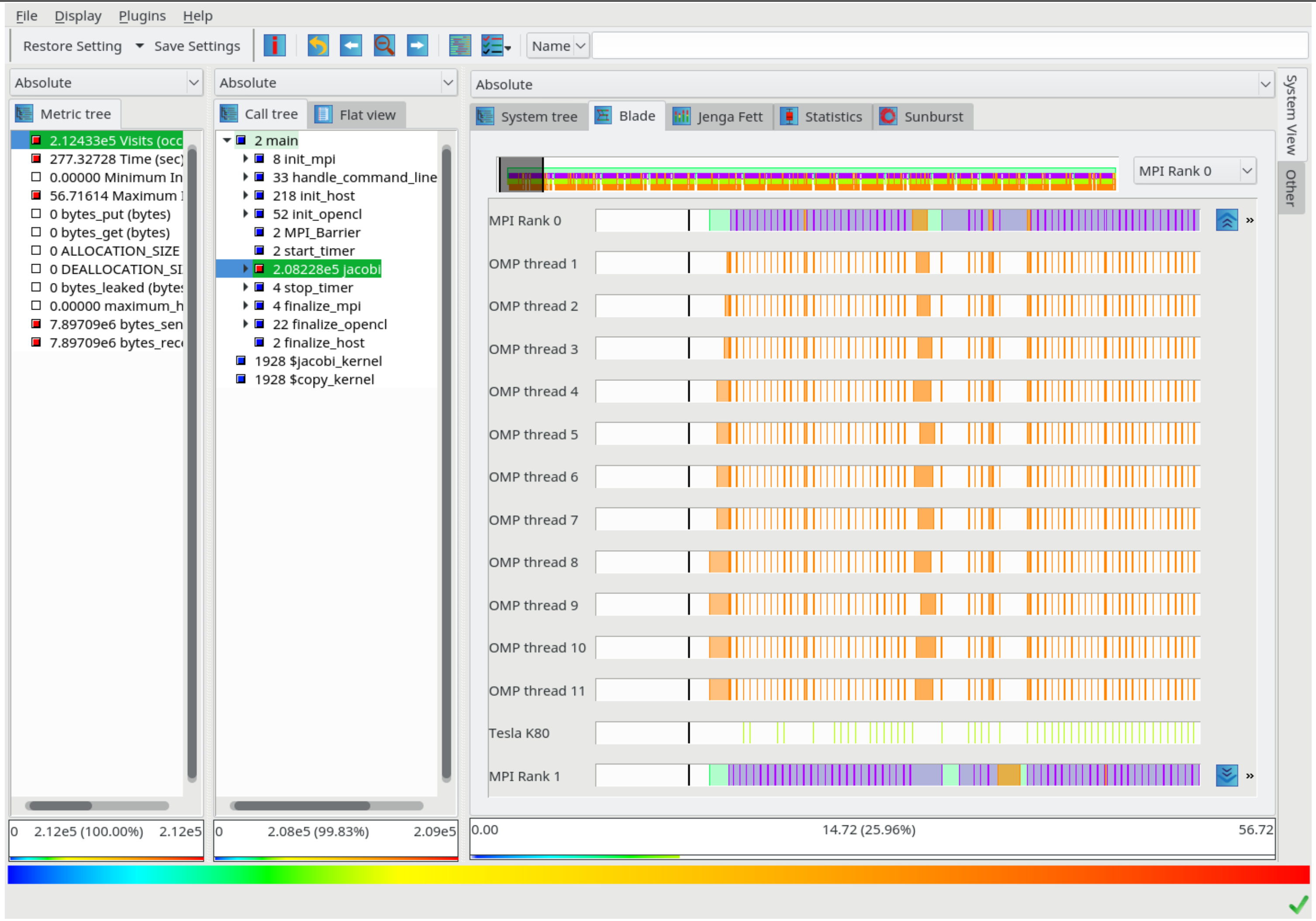
Score-P Configuration | ScorePion | Source | System View | Other

	Variable	Value
1	SCOREP_ENABLE_PROFILING	true
2	SCOREP_ENABLE_TRACING	true
3	SCOREP_ENABLE_UNWINDING	false

cube

!$omp implicit barrier @jacobi_opencl.c:236
!$omp critical sblock @jacobi_opencl.c:232
!$omp critical @jacobi_opencl.c:232
!$omp for @jacobi_opencl.c:207
!$omp parallel @jacobi_opencl.c:203
wait_jacobi_kernel
clEnqueueReadBuffer
clEnqueueWriteBuffer
MPI_Sendrecv
jacobi
!$omp parallel @jacobi_opencl.c:353
!$omp for @jacobi_opencl.c:353
!$omp implicit barrier @jacobi_opencl.c:360
MPI_Allreduce
launch_jacobi_kernel
launch_copy_kernel
clEnqueueNDRangeKernel
23136
1928
1929

Simple trace explorer plugin (experimental)

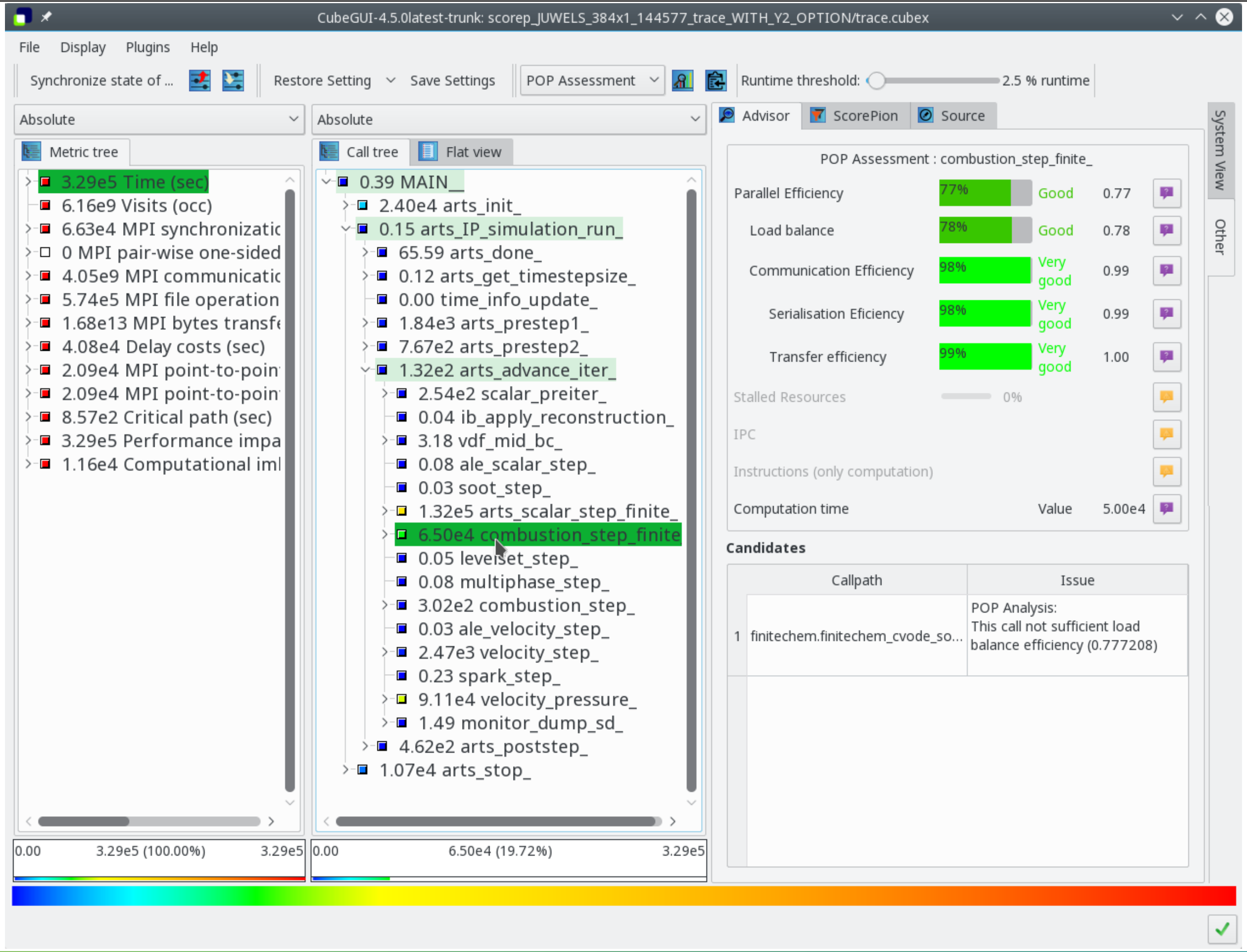


2.12433e5 Visits (occ
277.32728 Time (sec)
0.00000 Minimum In
56.71614 Maximum I
0 bytes_put (bytes)
0 bytes_get (bytes)
0 ALLOCATION_SIZE
0 DEALLOCATION_SI
0 bytes_leaked (byte
0.00000 maximum_h
7.89709e6 bytes_sen
7.89709e6 bytes_rec

2 main
8 init_mpi
33 handle_command_line
218 init_host
52 init_opencl
2 MPI_Barrier
2 start_timer
2.08228e5 jacobi
4 stop_timer
4 finalize_mpi
22 finalize_opencl
2 finalize_host
1928 $jacobi_kernel
1928 $copy_kernel

0 2.12e5 (100.00%) 2.12e5
0 2.08e5 (99.83%) 2.09e5
0.00 14.72 (25.96%) 56.72

Performance analysis plugin



CubeGUI-4.5.0latest-trunk: scorep_JUWELS_384x1_144577_trace_WITH_Y2_OPTION/trace.cubex

Metric tree:

- 3.29e5 Time (sec)
- 6.16e9 Visits (occ)
- 6.63e4 MPI synchronizatic
- 0 MPI pair-wise one-sided
- 4.05e9 MPI communicatic
- 5.74e5 MPI file operation
- 1.68e13 MPI bytes transfe
- 4.08e4 Delay costs (sec)
- 2.09e4 MPI point-to-poin
- 2.09e4 MPI point-to-poin
- 8.57e2 Critical path (sec)
- 3.29e5 Performance impa
- 1.16e4 Computational iml

Call tree:

```
0.39 MAIN__
  2.40e4 arts_init_
  0.15 arts_IP_simulation_run_
    65.59 arts_done_
    0.12 arts_get_timestepsize_
    0.00 time_info_update_
    1.84e3 arts_prestep1_
    7.67e2 arts_prestep2_
    1.32e2 arts_advance_iter_
      2.54e2 scalar_preiter_
      0.04 ib_apply_reconstruction_
      3.18 vdf_mid_bc_
      0.08 ale_scalar_step_
      0.03 soot_step_
      1.32e5 arts_scalar_step_finite_
      6.50e4 combustion_step_finite
      0.05 levelset_step_
      0.08 multiphase_step_
      3.02e2 combustion_step_
      0.03 ale_velocity_step_
      2.47e3 velocity_step_
      0.23 spark_step_
      9.11e4 velocity_pressure_
      1.49 monitor_dump_sd_
    4.62e2 arts_poststep_
  1.07e4 arts_stop_
```

0.00 3.29e5 (100.00%) 3.29e5

0.00 6.50e4 (19.72%) 3.29e5

POP Assessment : combustion_step_finite_

Parallel Efficiency	77%	Good	0.77
Load balance	78%	Good	0.78
Communication Efficiency	98%	Very good	0.99
Serialisation Eficiency	98%	Very good	0.99
Transfer efficiency	99%	Very good	1.00
Stalled Resources	0%		
IPC			
Instructions (only computation)			
Computation time		Value	5.00e4

Candidates

	Callpath	Issue
1	finitechem.finitechem_cvode_so...	POP Analysis: This call not sufficient load balance efficiency (0.777208)

Cube: Further information

- Parallel program analysis report exploration tools
  - Libraries for XML 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:
  - `cube-config --cube-dir`/share/doc/CubeGuide.pdf
- Contact:
  - mailto: scalasca@fz-juelich.de