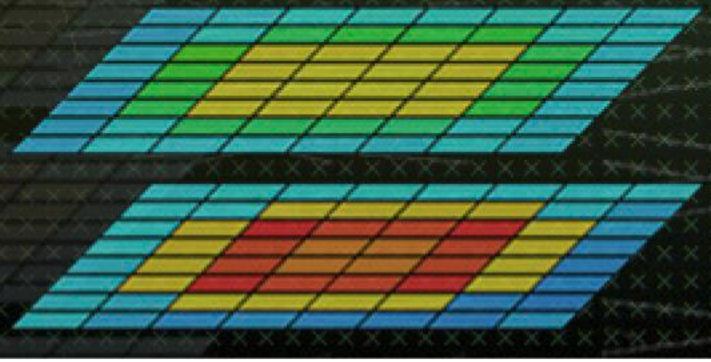
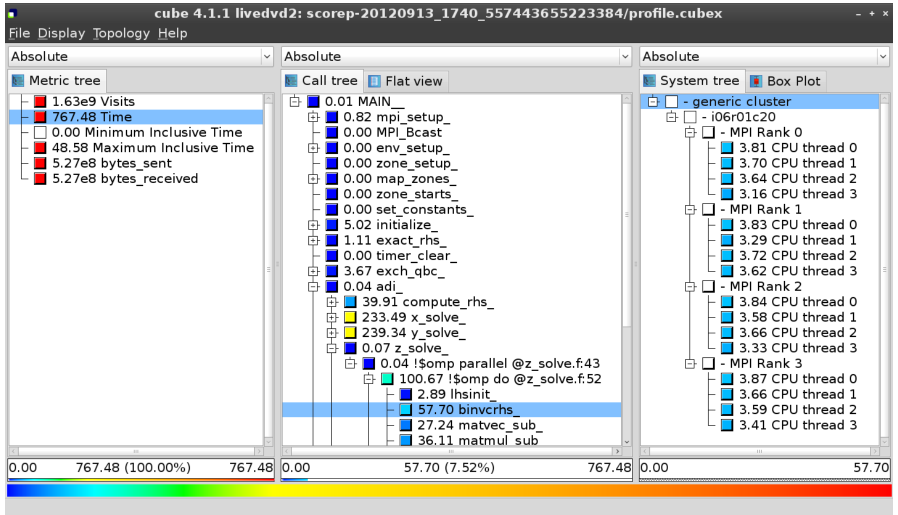


Analysis report examination with Cube

Brian Wylie
Jülich Supercomputing Centre

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 desktop or laptop
  - Latest release: Cube v4.5 (May 2020)


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
```

```
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_
```

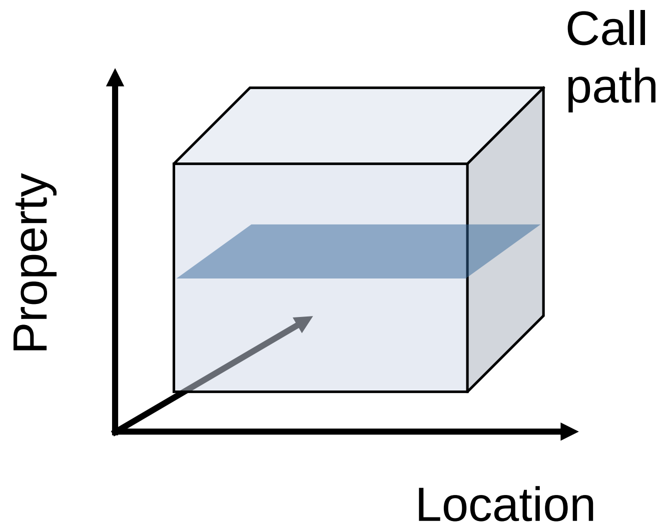
```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      3.81 CPU thread 0
      3.70 CPU thread 1
      3.64 CPU thread 2
      3.16 CPU thread 3
    - MPI Rank 1
      3.83 CPU thread 0
      3.29 CPU thread 1
      3.72 CPU thread 2
      3.62 CPU thread 3
    - MPI Rank 2
      3.84 CPU thread 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
```

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

Analysis presentation and exploration

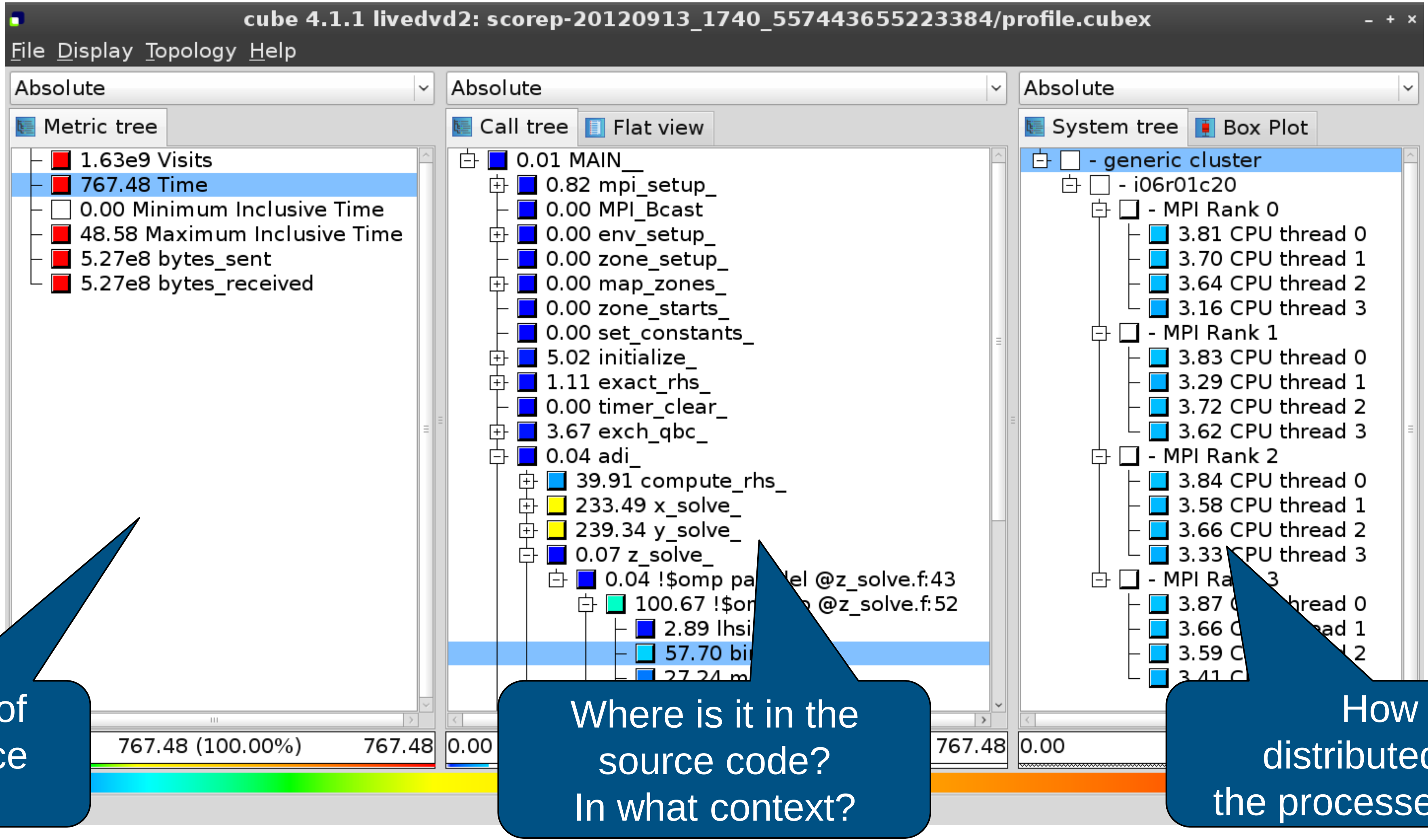
- Representation of values (severity matrix) on three hierarchical axes
  - Performance property (metric)
  - Call path (program location)
  - System location (process/thread)



- 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


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
```

```
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
```

```
- 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
```

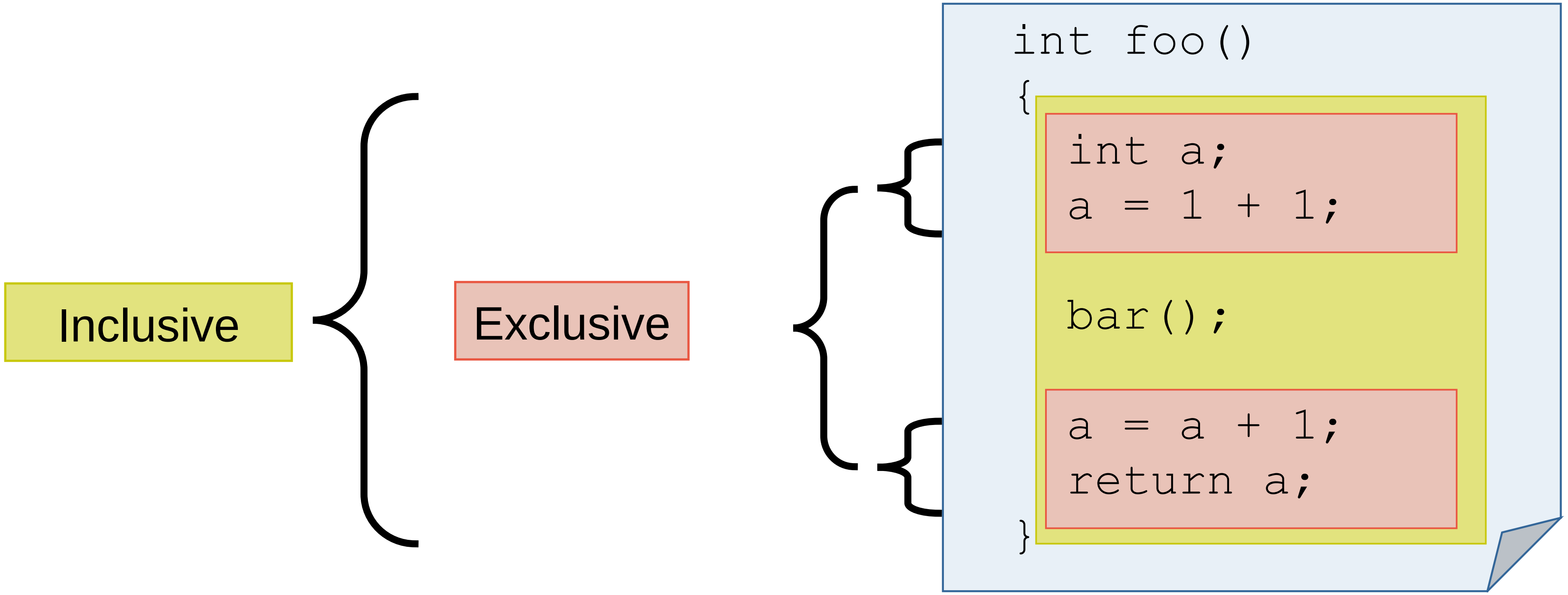
What kind of performance metric?

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

How is it distributed across the processes/threads?

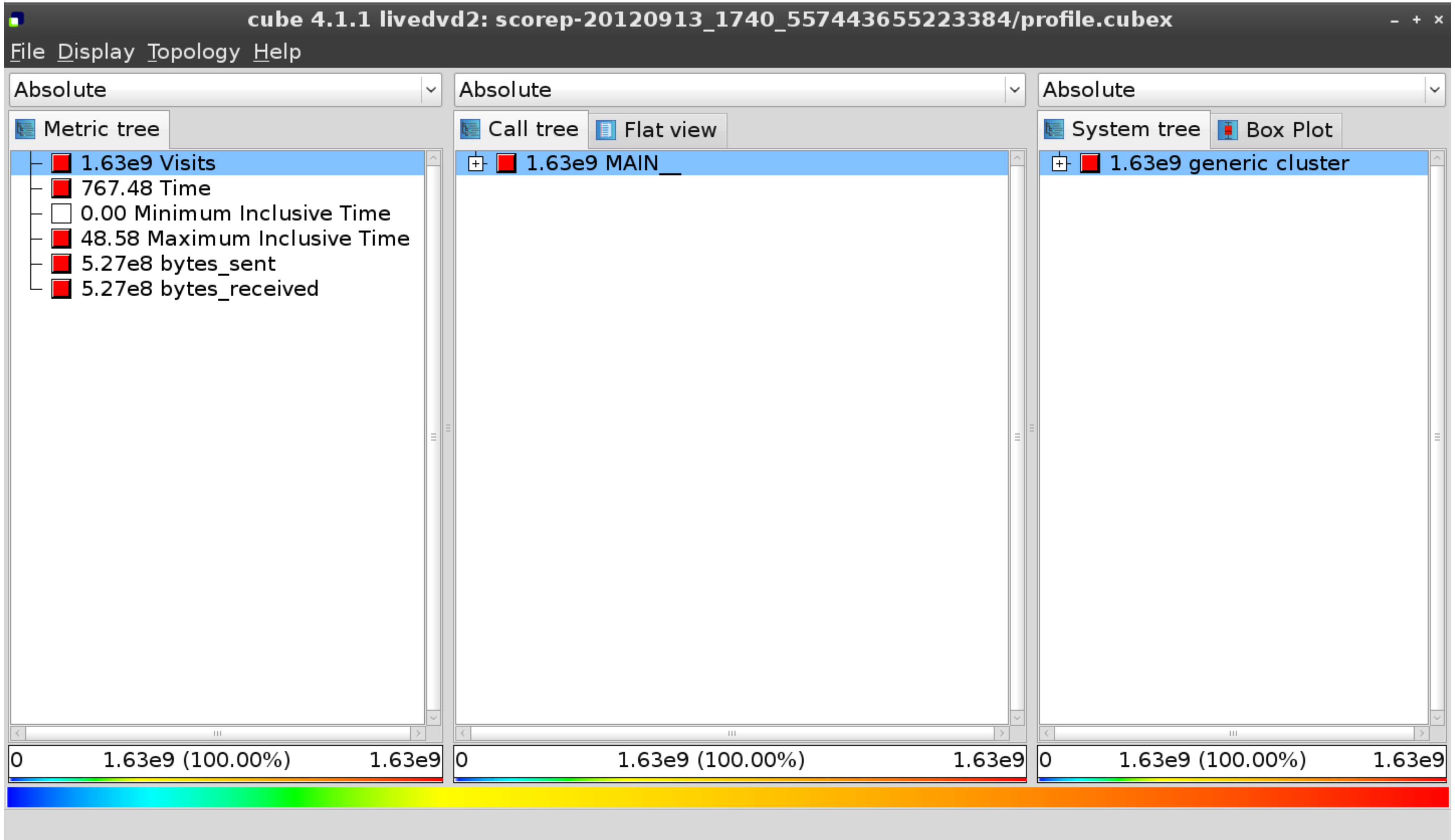
Inclusive vs. exclusive values

- 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;
}
```

Score-P analysis report exploration (opening view)



cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex
File Display Topology Help
Absolute
Metric tree
Absolute
Call tree
Flat view
Absolute
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:
- ⊞ 🟥 1.63e9 MAIN__

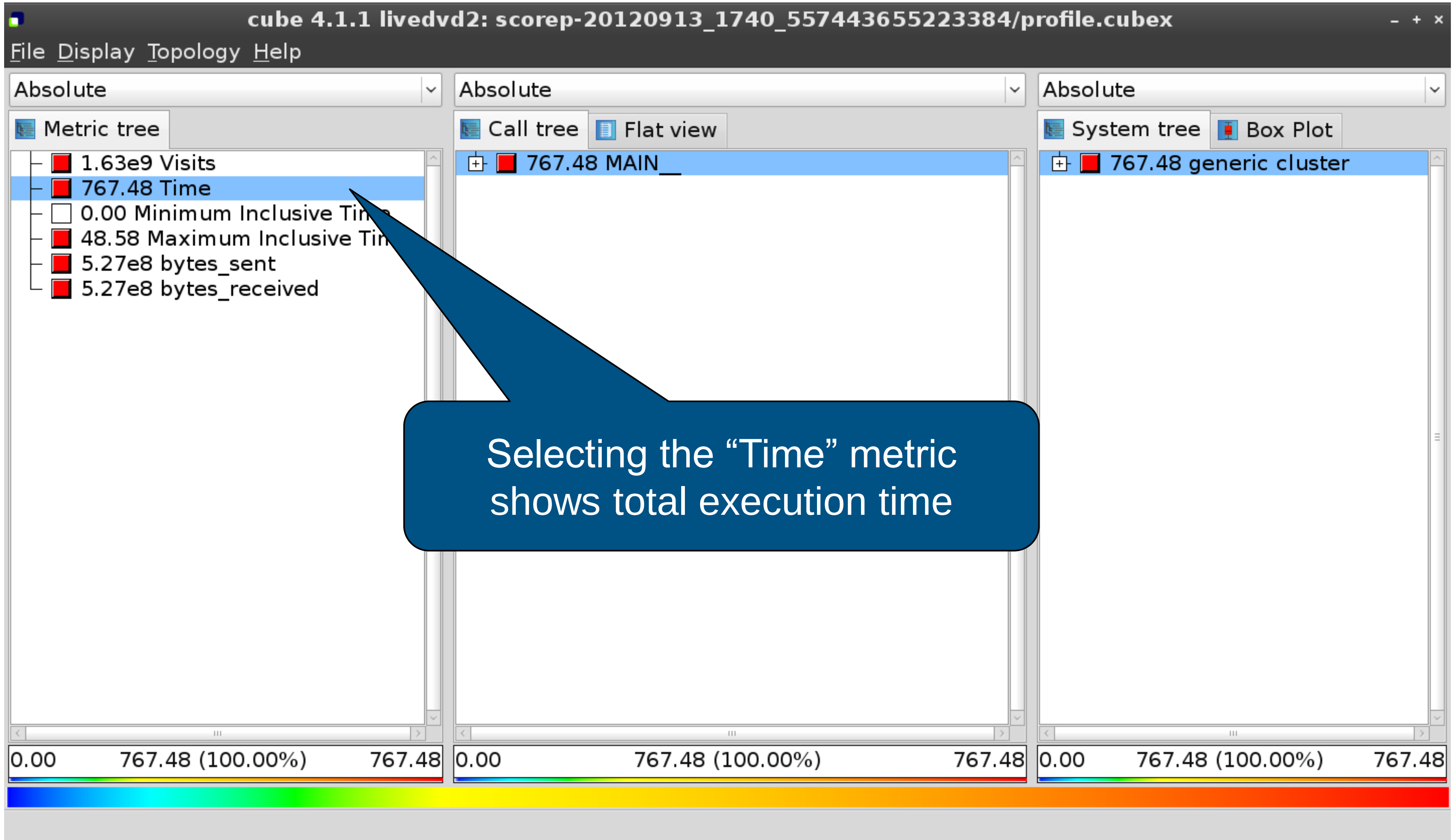
System tree:
- ⊞ 🟥 1.63e9 generic cluster

0 1.63e9 (100.00%) 1.63e9

0 1.63e9 (100.00%) 1.63e9

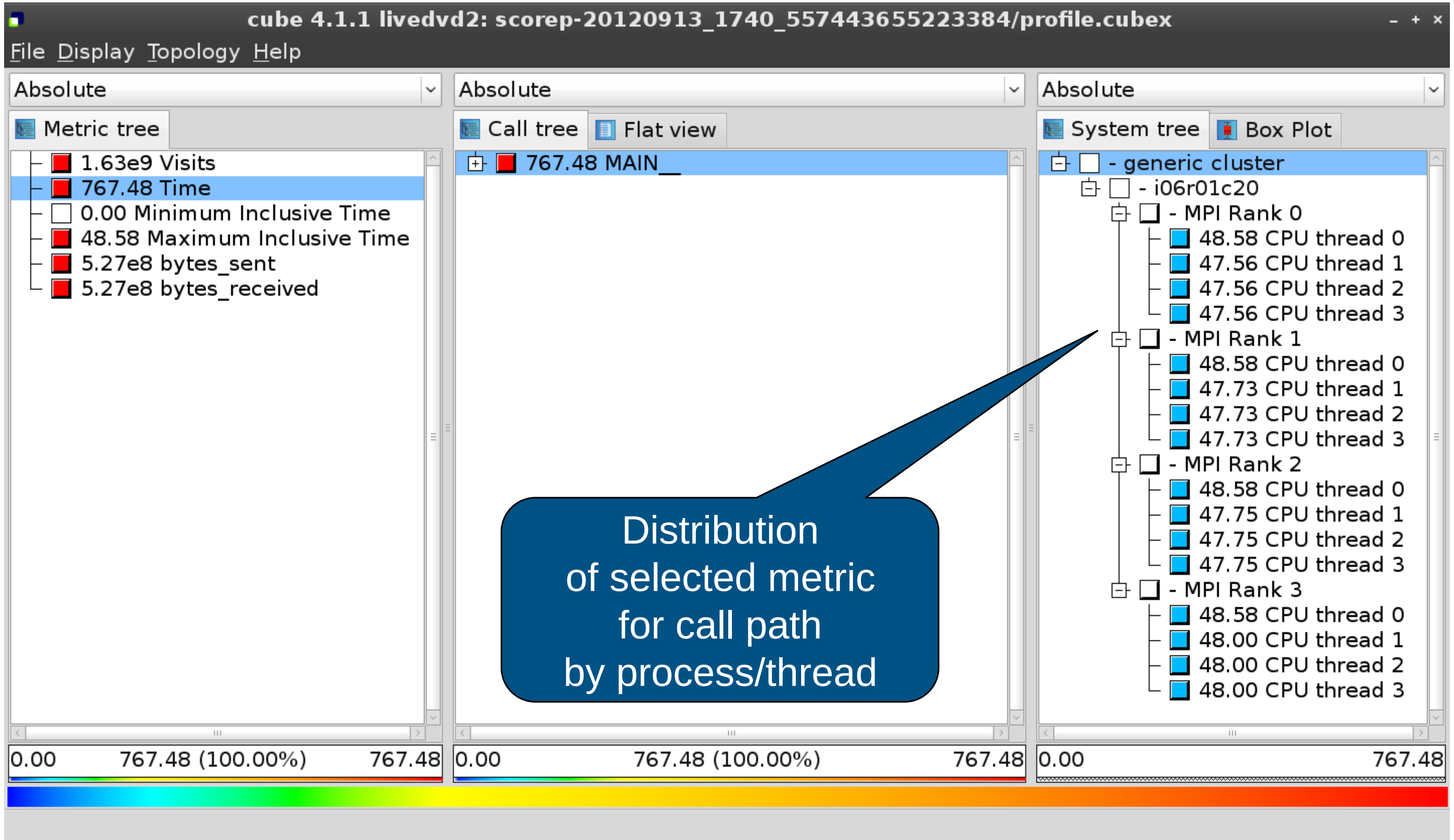
0 1.63e9 (100.00%) 1.63e9

Metric selection



Selecting the “Time” metric shows total execution time

Expanding the system tree



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

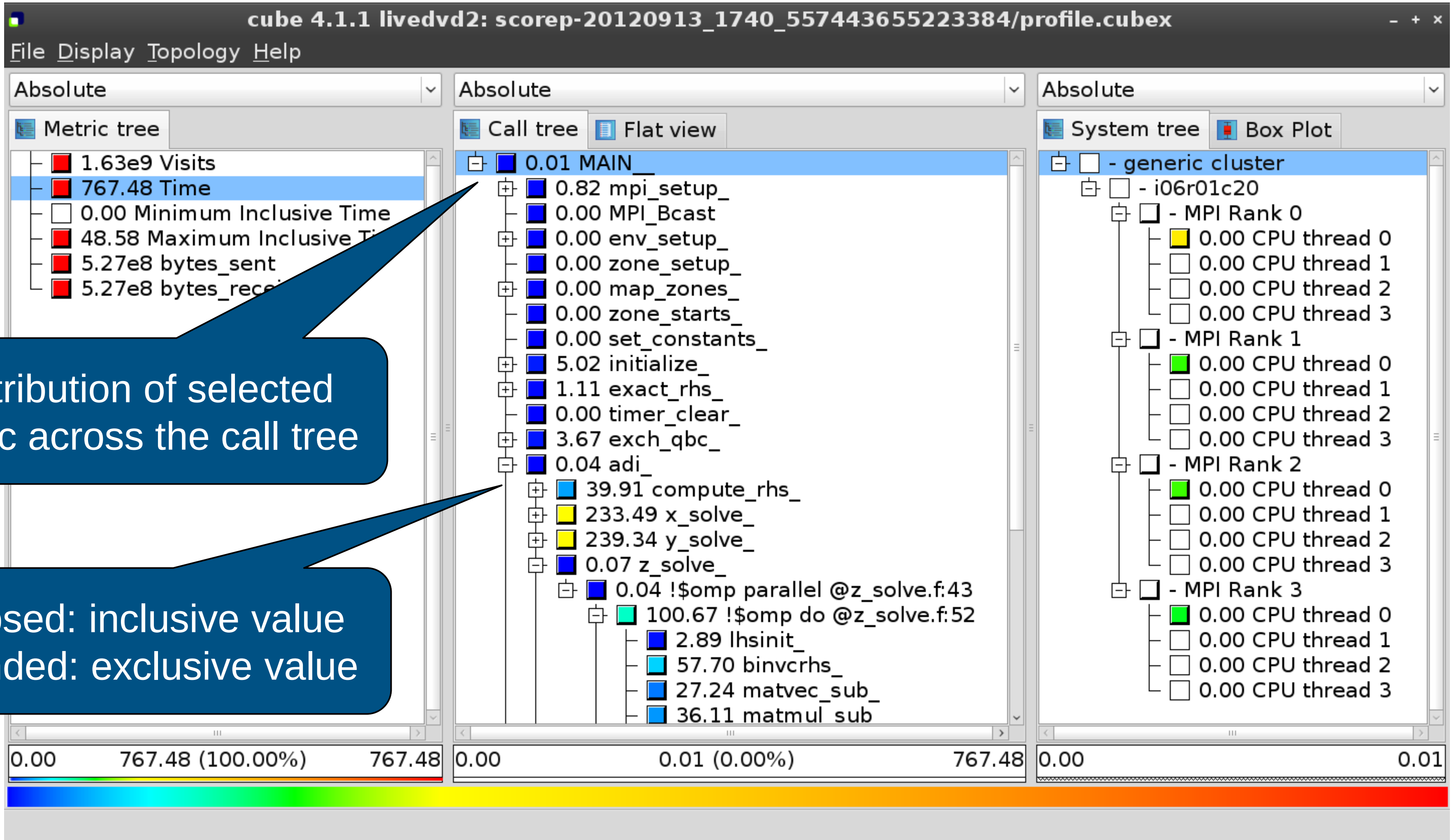
Metric tree:
- 🟥 1.63e9 Visits
- 🟥 767.48 Time
- □ 0.00 Minimum Inclusive Time
- 🟥 48.58 Maximum Inclusive Time
- 🟥 5.27e8 bytes_sent
- 🟥 5.27e8 bytes_received

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

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

```
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_
```

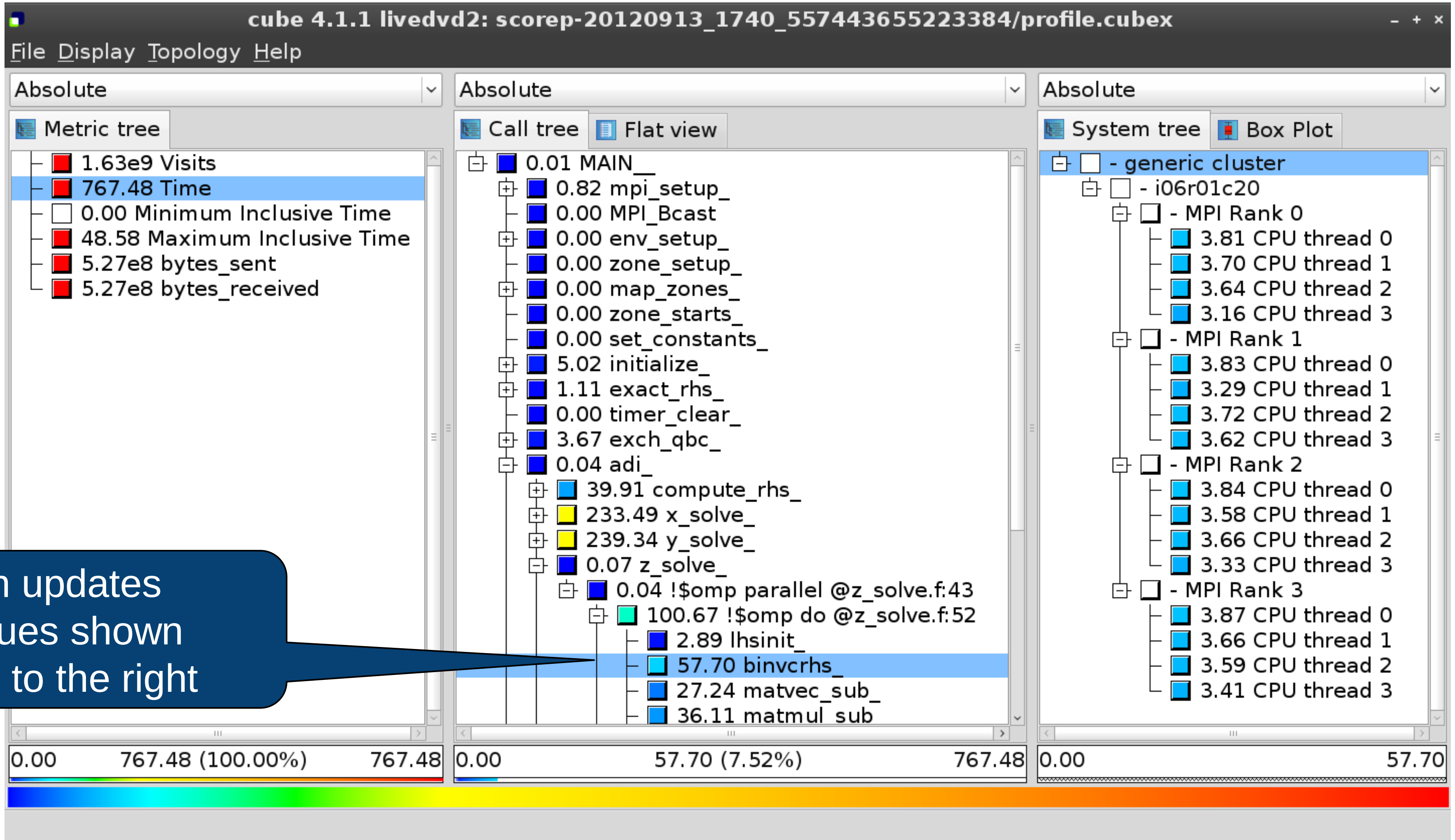
```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      0.00 CPU thread 0
      0.00 CPU thread 1
      0.00 CPU thread 2
      0.00 CPU thread 3
    - MPI Rank 1
      0.00 CPU thread 0
      0.00 CPU thread 1
      0.00 CPU thread 2
      0.00 CPU thread 3
    - MPI Rank 2
      0.00 CPU thread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

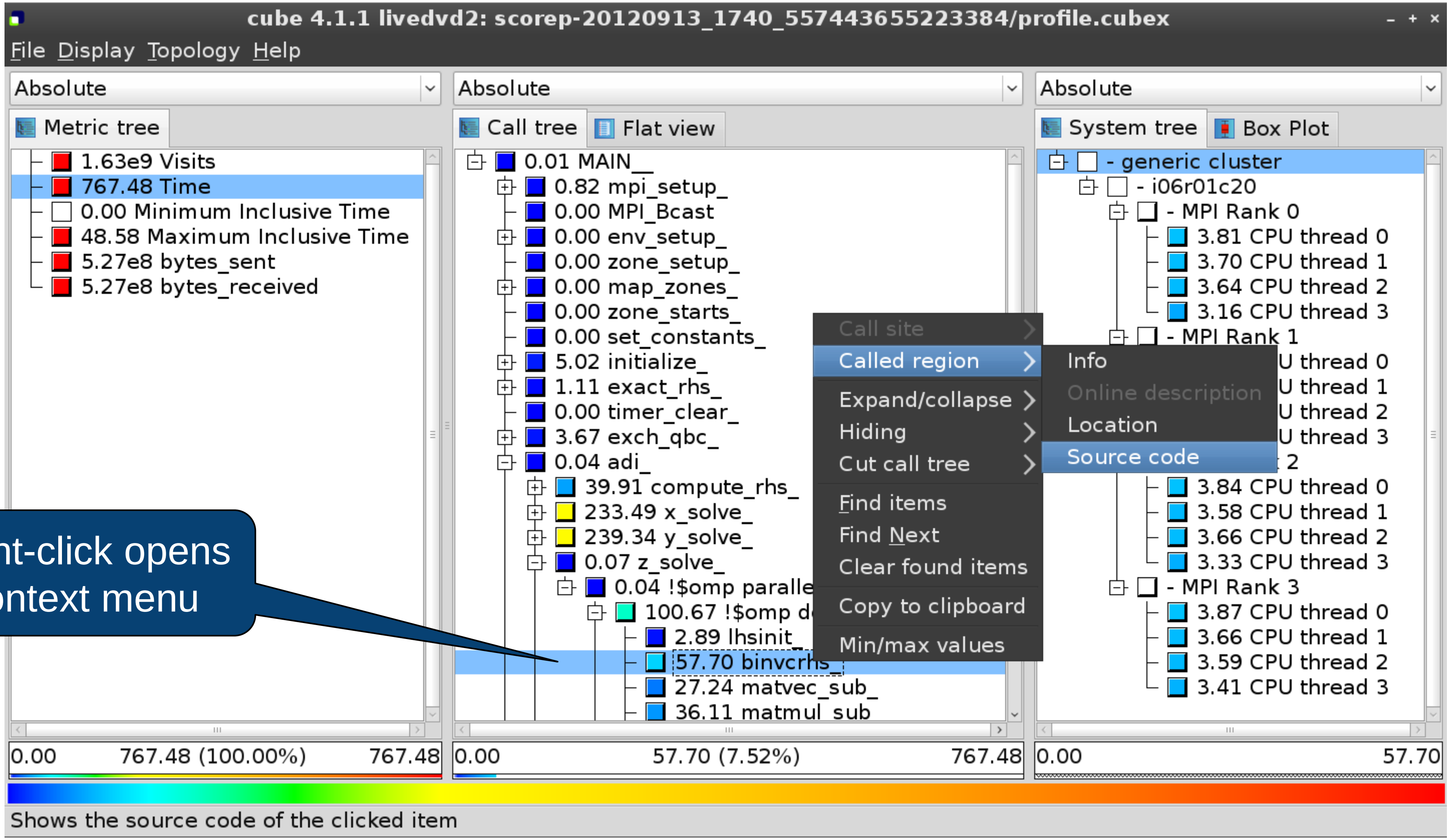


cube 4.1.1 livedvd2: scorep-20120913_1740_557443655223384/profile.cubex

```
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:
0.01 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:
- 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



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:

```
0.01 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 !$omp paralle
        100.67 !$omp d
          2.89 lhsinit_
          57.70 binvcrhs_
          27.24 matvec_sub_
          36.11 matmul_sub_
```

System tree:

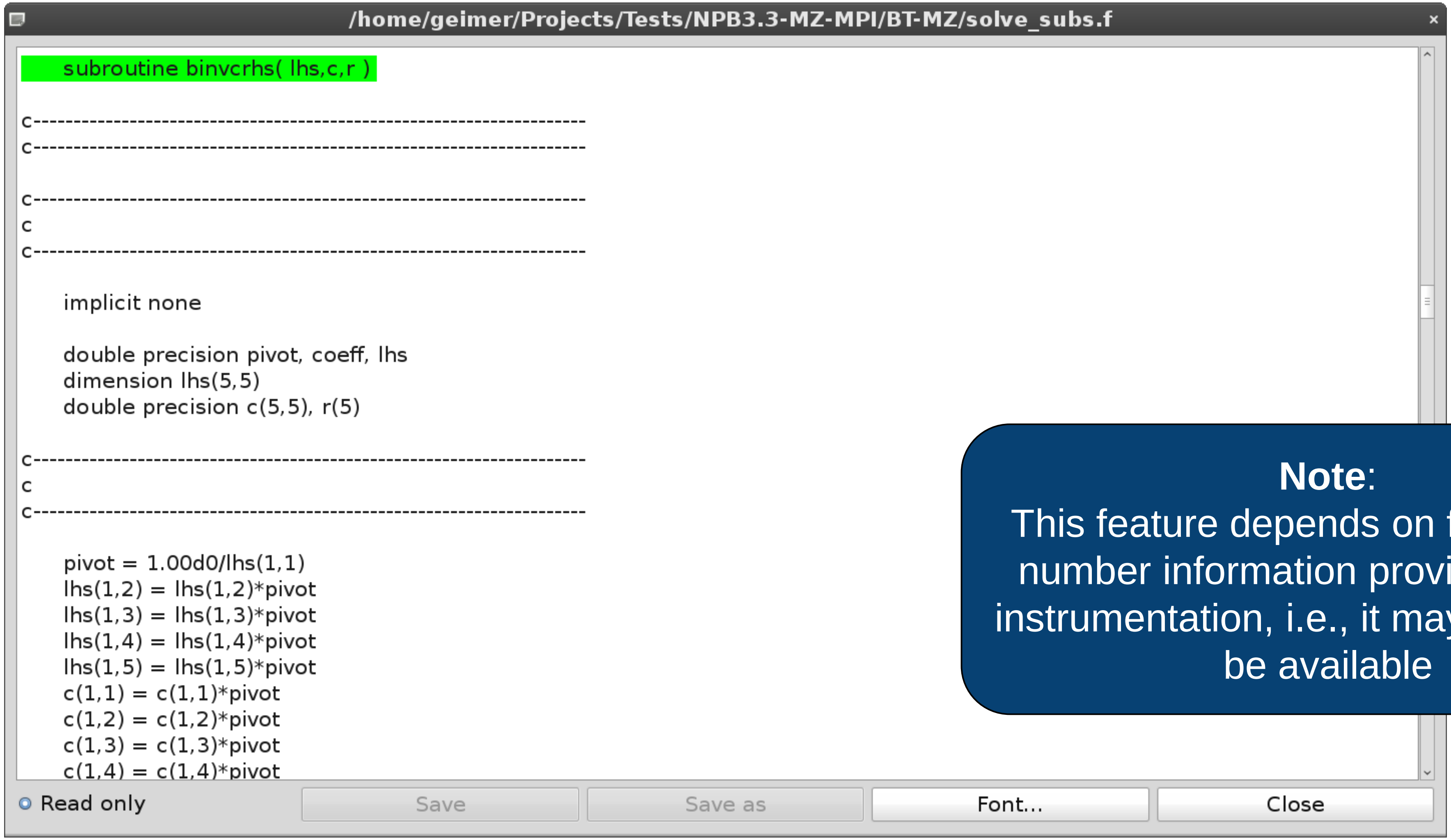
```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      3.81 CPU thread 0
      3.70 CPU thread 1
      3.64 CPU thread 2
      3.16 CPU thread 3
    - MPI Rank 1
      U thread 0
      U thread 1
      U thread 2
      U thread 3
    2
      3.84 CPU thread 0
      3.58 CPU thread 1
      3.66 CPU 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
```

Shows the source code of the clicked item

Right-click opens context menu

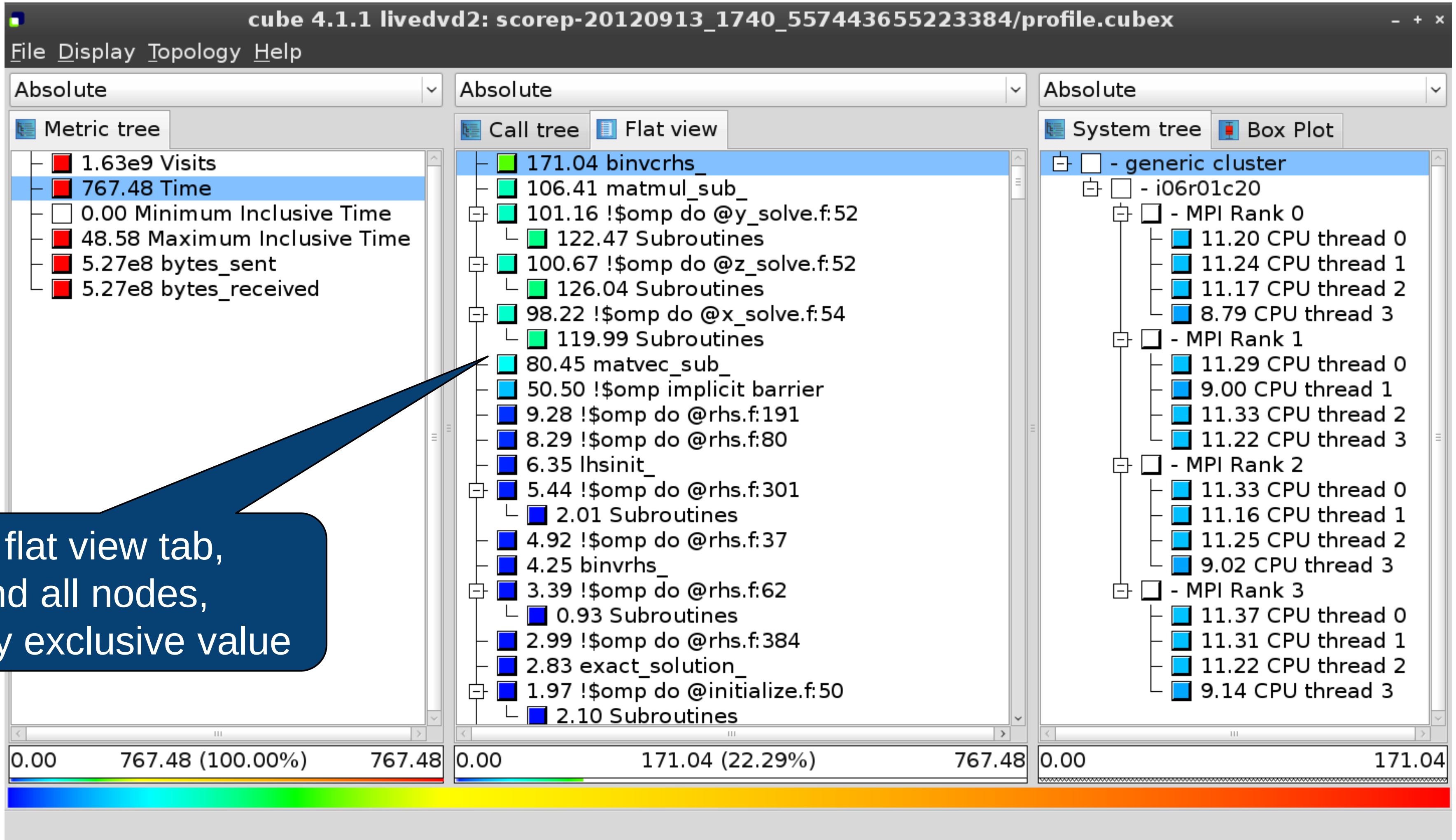
Source-code view


/home/geimer/Projects/Tests/NPB3.3-MZ-MPI/BT-MZ/solve_subs.f
×
○ Read only
Save
Save as
Font...
Close

```
      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
```

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
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
```

Flat view:

```
171.04 binvcrhs_
106.41 matmul_sub_
101.16 !$omp do @y_solve.f:52
  122.47 Subroutines
100.67 !$omp do @z_solve.f:52
  126.04 Subroutines
98.22 !$omp do @x_solve.f:54
  119.99 Subroutines
80.45 matvec_sub_
50.50 !$omp implicit barrier
9.28 !$omp do @rhs.f:191
8.29 !$omp do @rhs.f:80
6.35 lhsinit_
5.44 !$omp do @rhs.f:301
  2.01 Subroutines
4.92 !$omp do @rhs.f:37
4.25 binvrhs_
3.39 !$omp do @rhs.f:62
  0.93 Subroutines
2.99 !$omp do @rhs.f:384
2.83 exact_solution_
1.97 !$omp do @initialize.f:50
  2.10 Subroutines
```

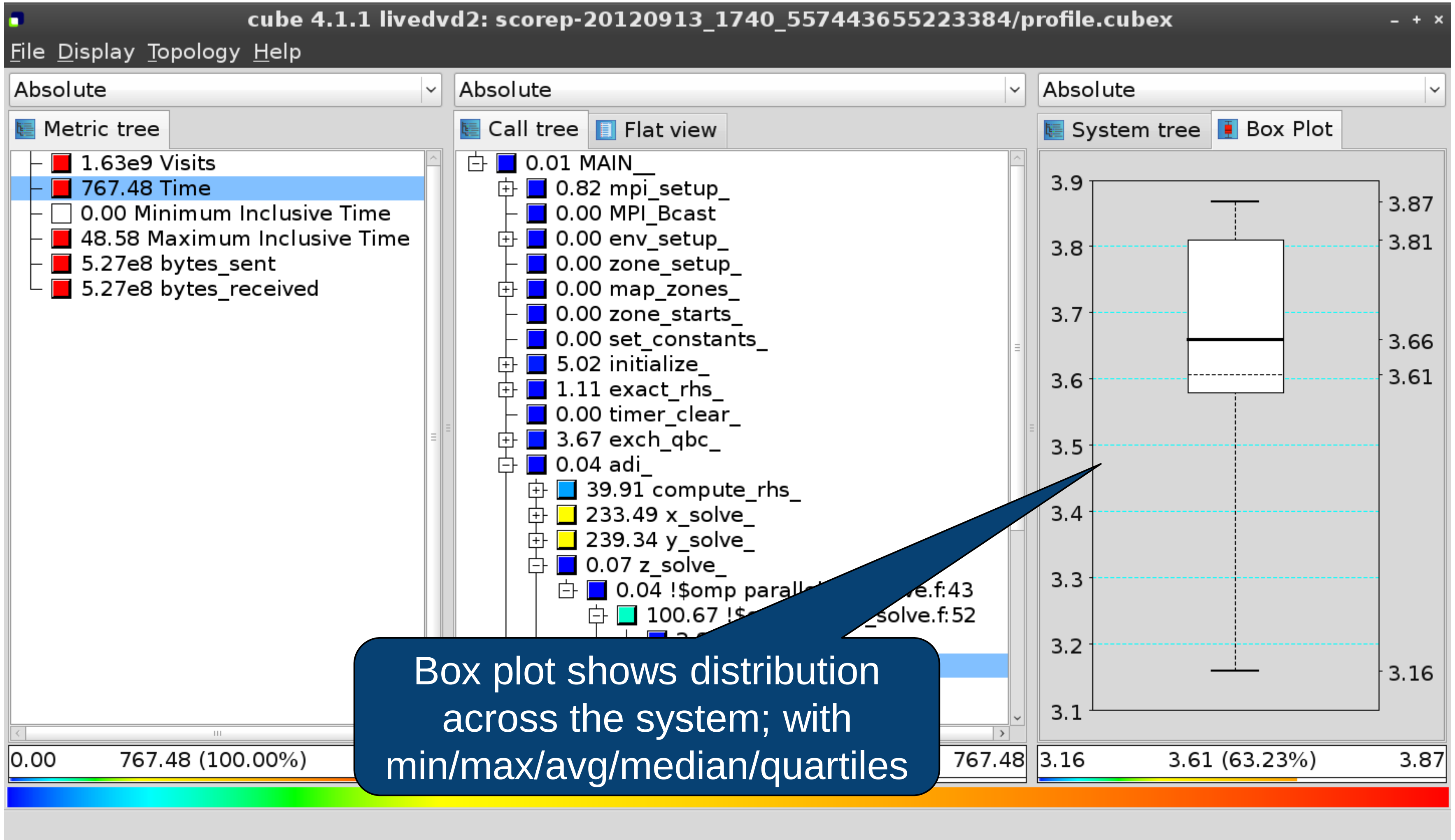
System tree:

```
- generic cluster
  - i06r01c20
    - MPI Rank 0
      11.20 CPU thread 0
      11.24 CPU thread 1
      11.17 CPU thread 2
      8.79 CPU thread 3
    - MPI Rank 1
      11.29 CPU thread 0
      9.00 CPU thread 1
      11.33 CPU thread 2
      11.22 CPU thread 3
    - MPI Rank 2
      11.33 CPU thread 0
      11.16 CPU thread 1
      11.25 CPU thread 2
      9.02 CPU thread 3
    - MPI Rank 3
      11.37 CPU thread 0
      11.31 CPU thread 1
      11.22 CPU thread 2
      9.14 CPU thread 3
```

```
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

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:

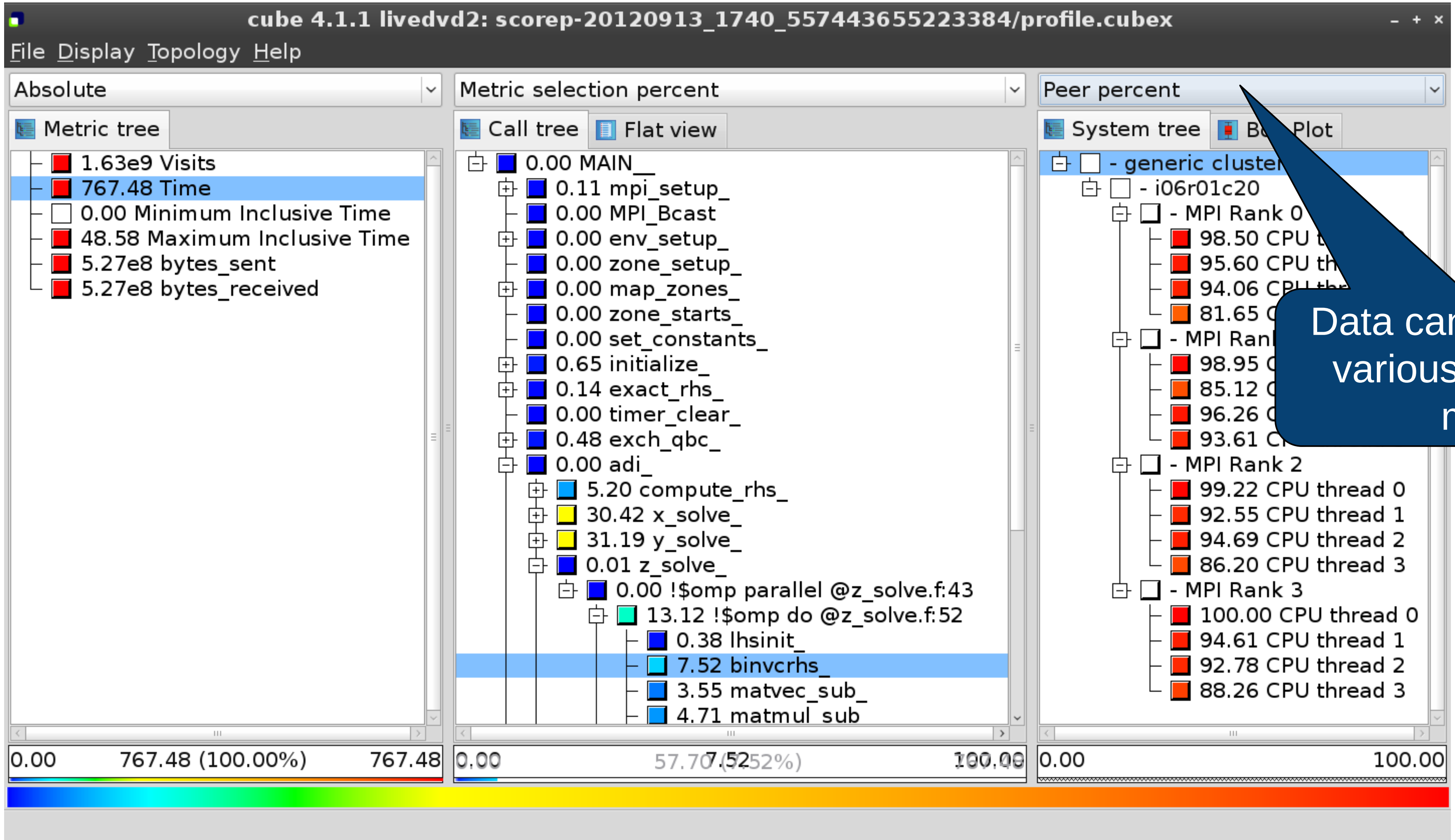
```
⊟ 0.01 MAIN__
  ⊞ 0.82 mpi_setup_
  ├ 0.00 MPI_Bcast
  ⊞ 0.00 env_setup_
  ├ 0.00 zone_setup_
  ⊞ 0.00 map_zones_
  ├ 0.00 zone_starts_
  ├ 0.00 set_constants_
  ⊞ 5.02 initialize_
  ⊞ 1.11 exact_rhs_
  ├ 0.00 timer_clear_
  ⊞ 3.67 exch_qbc_
  ⊟ 0.04 adi_
    ⊞ 39.91 compute_rhs_
    ⊞ 233.49 x_solve_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

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

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 Ran
      - 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

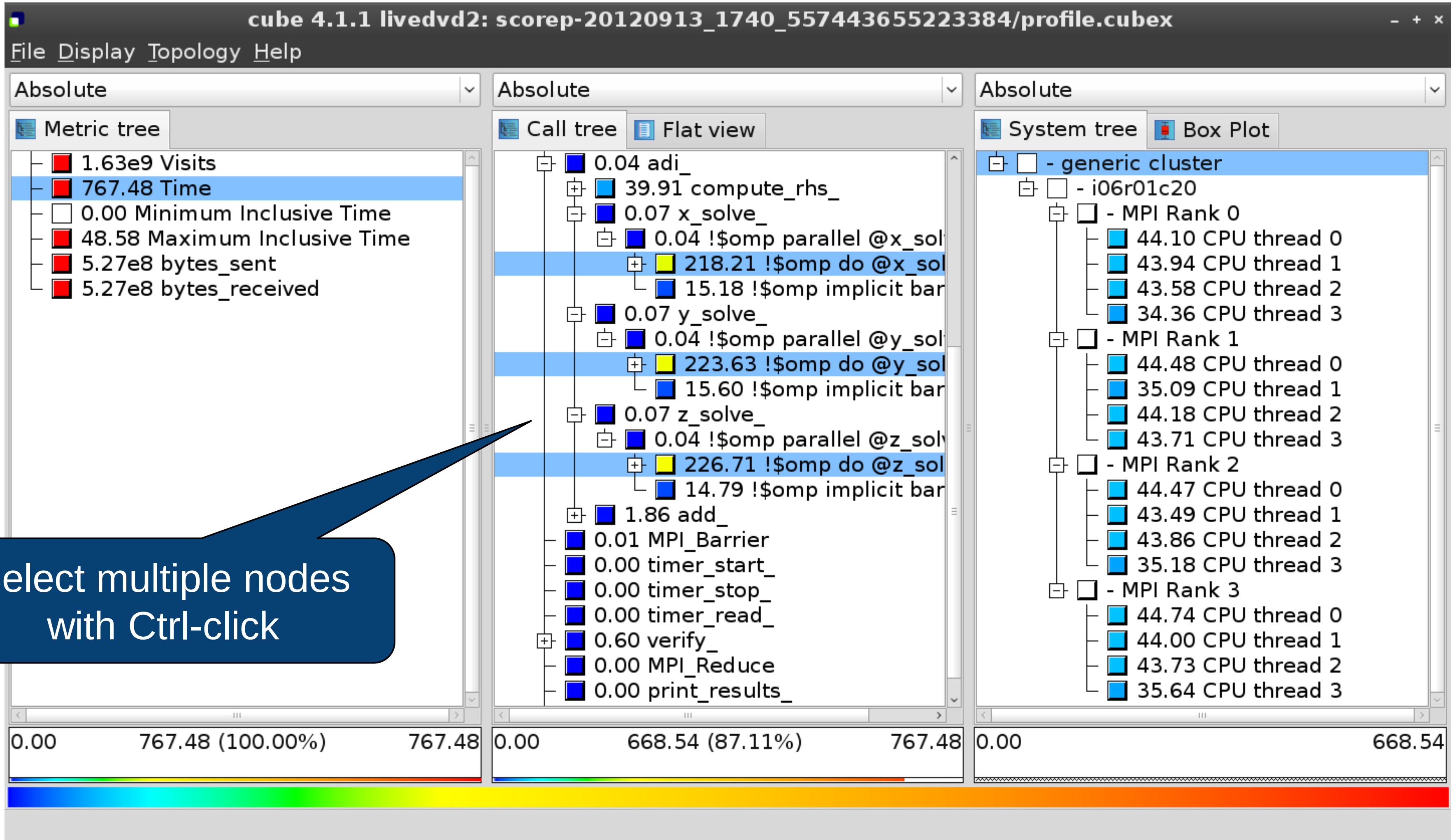
0.00 767.48 (100.00%) 767.48 | 0.00 57.70 (7.52%) 7.52 100.00 | 0.00 100.00

Data can be shown in various percentage 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



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

```
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
```

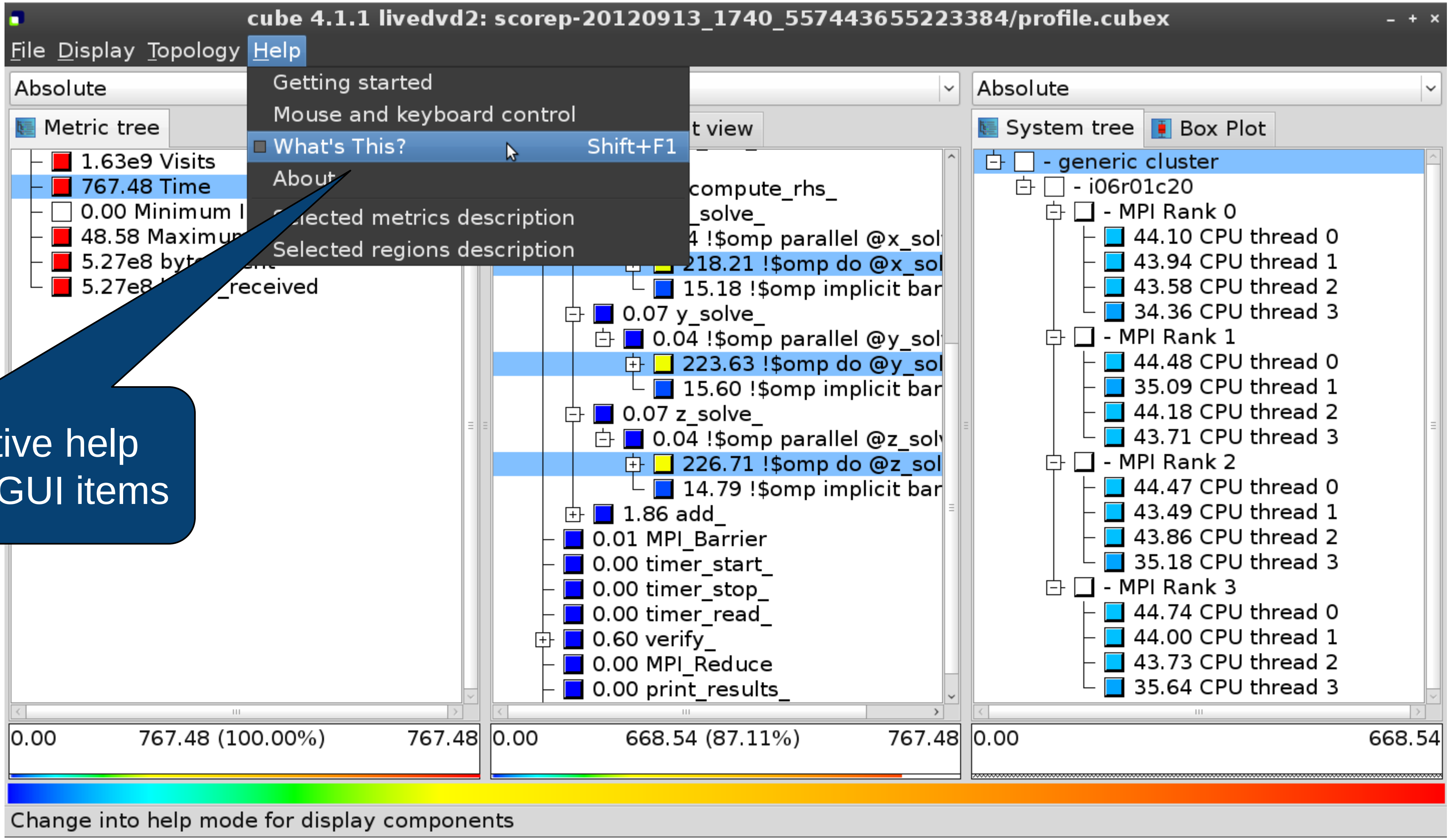
```
Call tree
0.04 adi_
  39.91 compute_rhs_
  0.07 x_solve_
    0.04 !$omp parallel @x_sol
      218.21 !$omp do @x_sol
      15.18 !$omp implicit bar
  0.07 y_solve_
    0.04 !$omp parallel @y_sol
      223.63 !$omp do @y_sol
      15.60 !$omp implicit bar
  0.07 z_solve_
    0.04 !$omp parallel @z_sol
      226.71 !$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
- 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
Absolute
Metric tree
t view
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

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

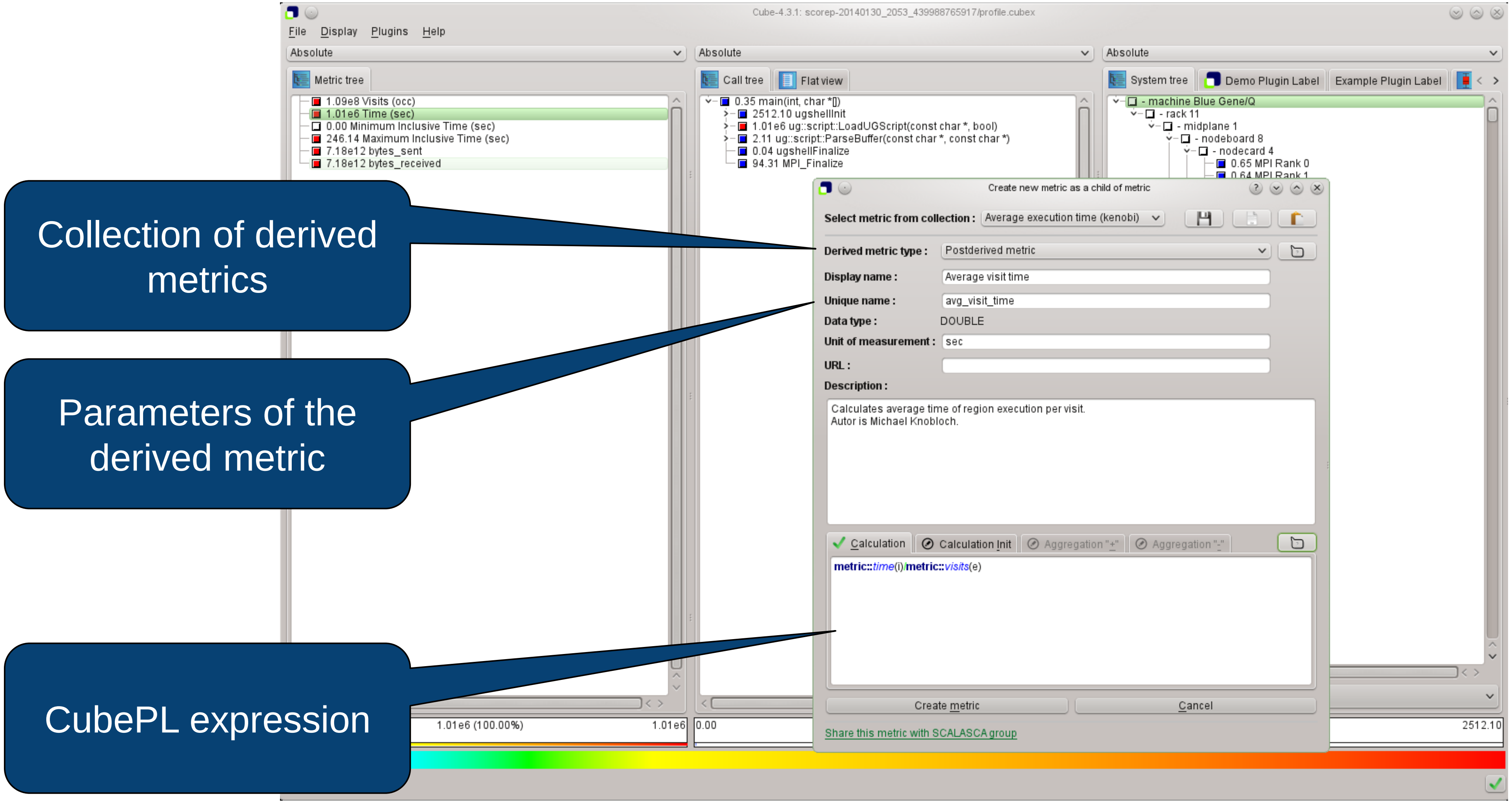
- Examples:
  - "Average execution time": Postderived metric with expression

    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
```

1.01e6 (100.00%) 1.01e6 0.00 2512.10

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.

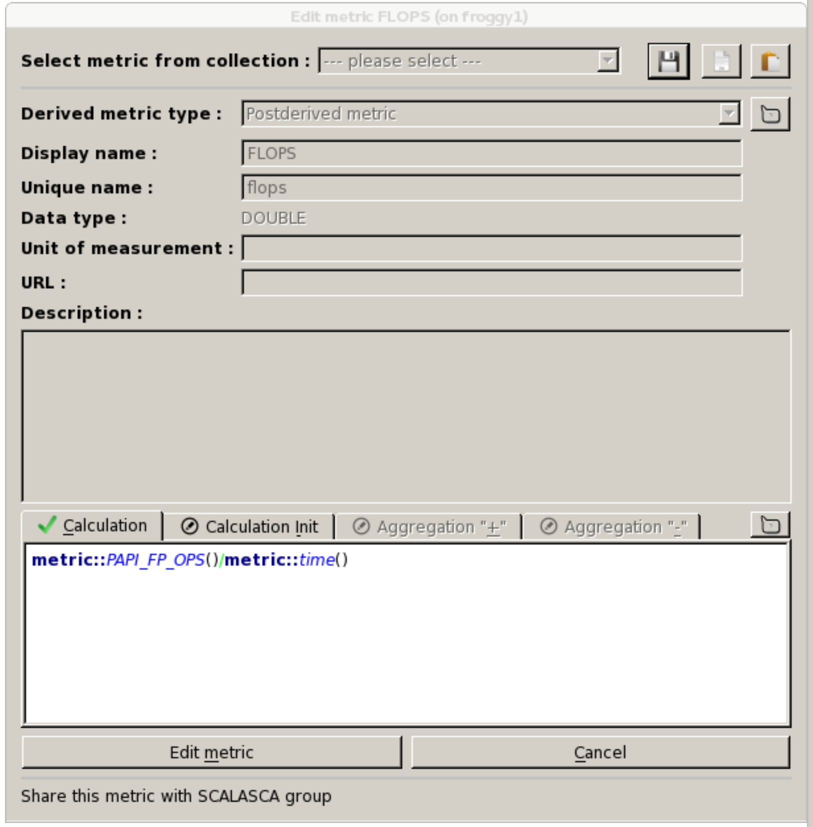
```
metric::time(i)/metric::visits(e)
```

Collection of derived metrics

Parameters of the derived metric

CubePL expression

Example: FLOPS based on PAPI_FP_OPS and time



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

Derived metric type : Postderived metric

Display name : FLOPS

Unique name : flops

Data type : DOUBLE

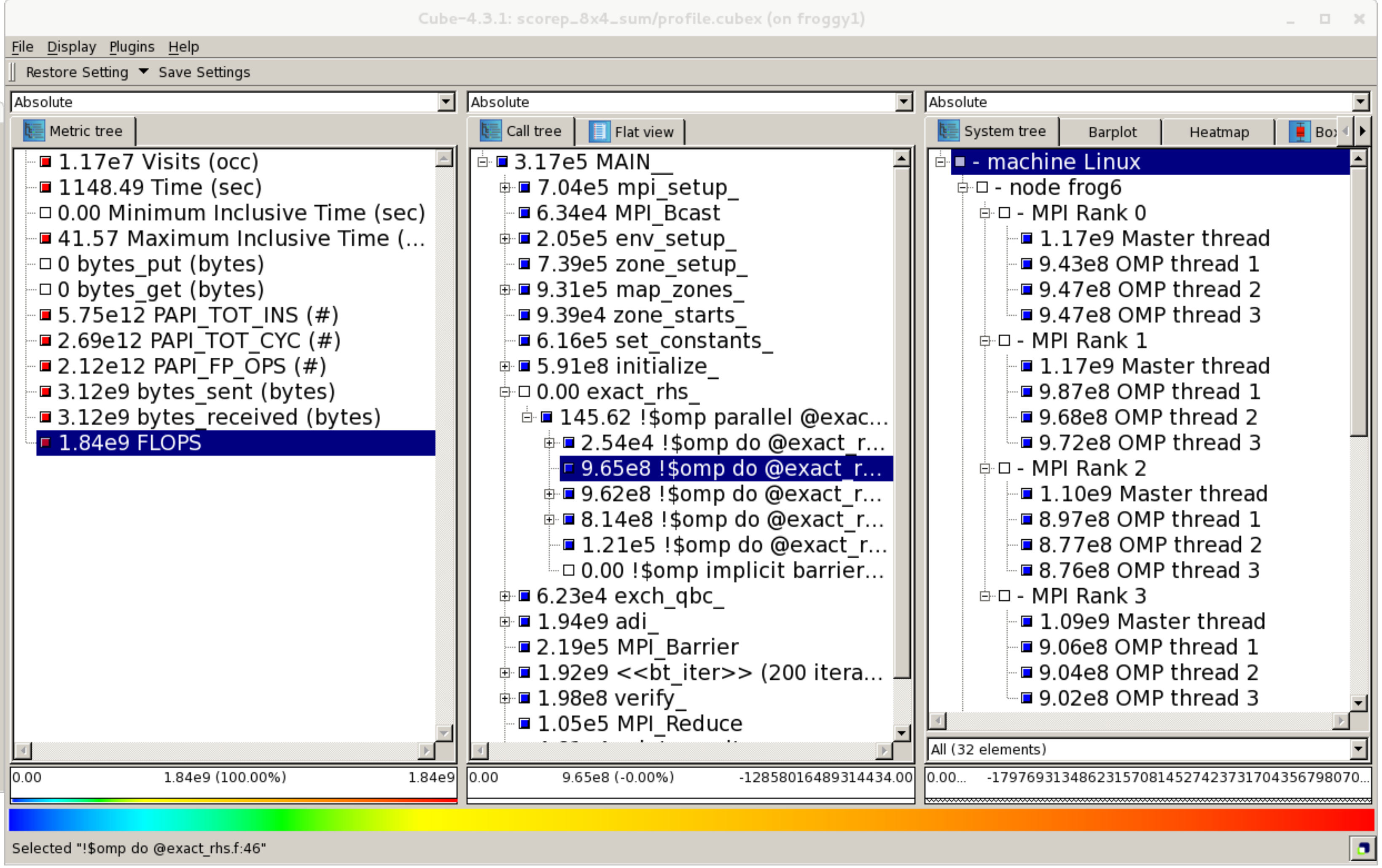
Unit of measurement :

URL :

Description :

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

Share this metric with SCALASCA group


Cube-4.3.1: scorep_8x4_sum/profile.cubex (on froggy1)
File Display Plugins Help
Restore Setting Save Settings
Absolute
Absolute
Absolute
Metric tree
Call tree
Flat view
System tree
Barplot
Heatmap
Box

```
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_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

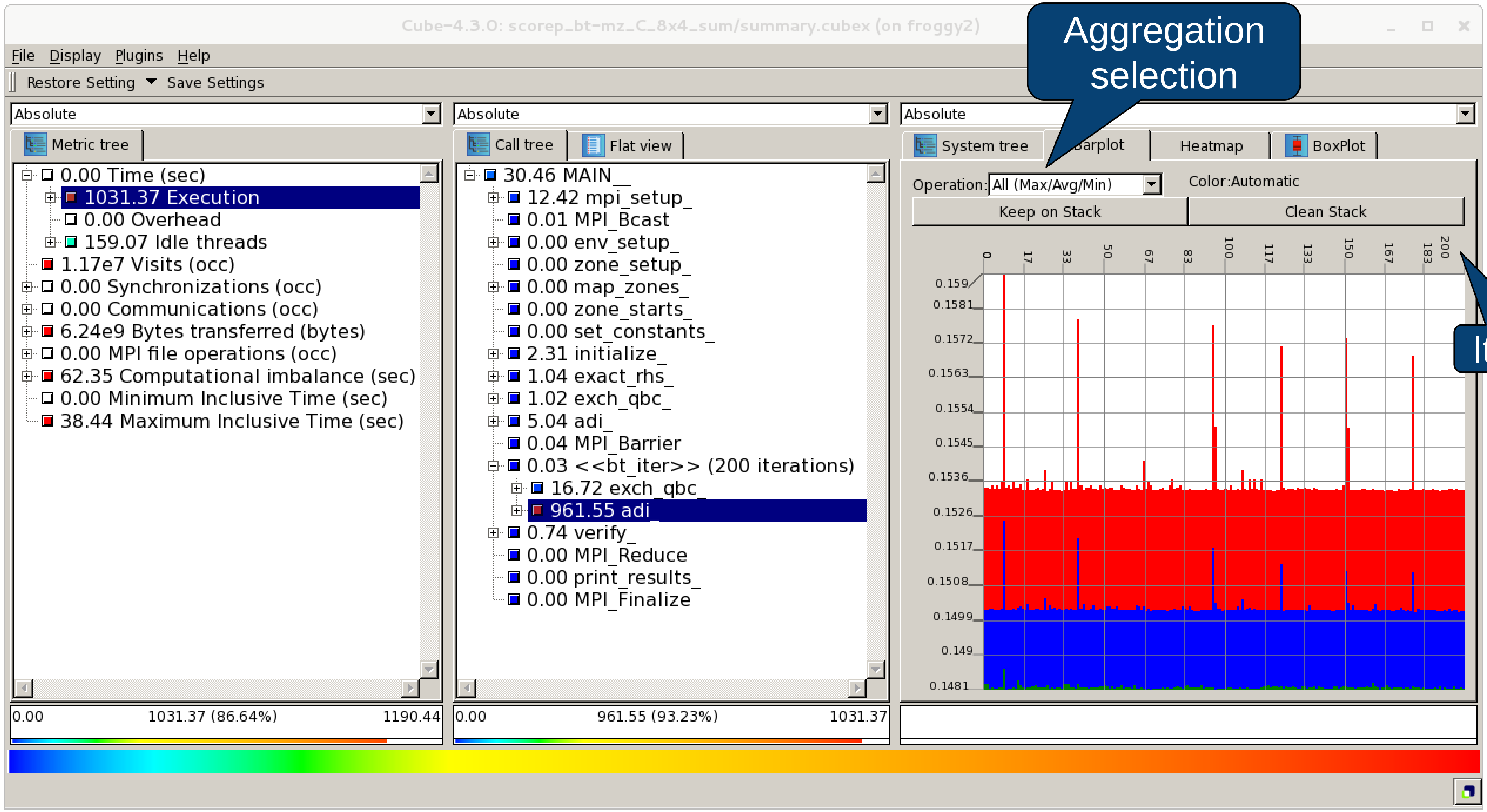
  ➢ Useful for checking results for specific iterations

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



Cube-4.3.0: scorep_bt-mz_C_8x4_sum/summary.cubex (on froggy2)

File Display Plugins Help

Restore Setting ▾ Save Settings

Absolute | Absolute | Absolute

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)
```

Call tree:

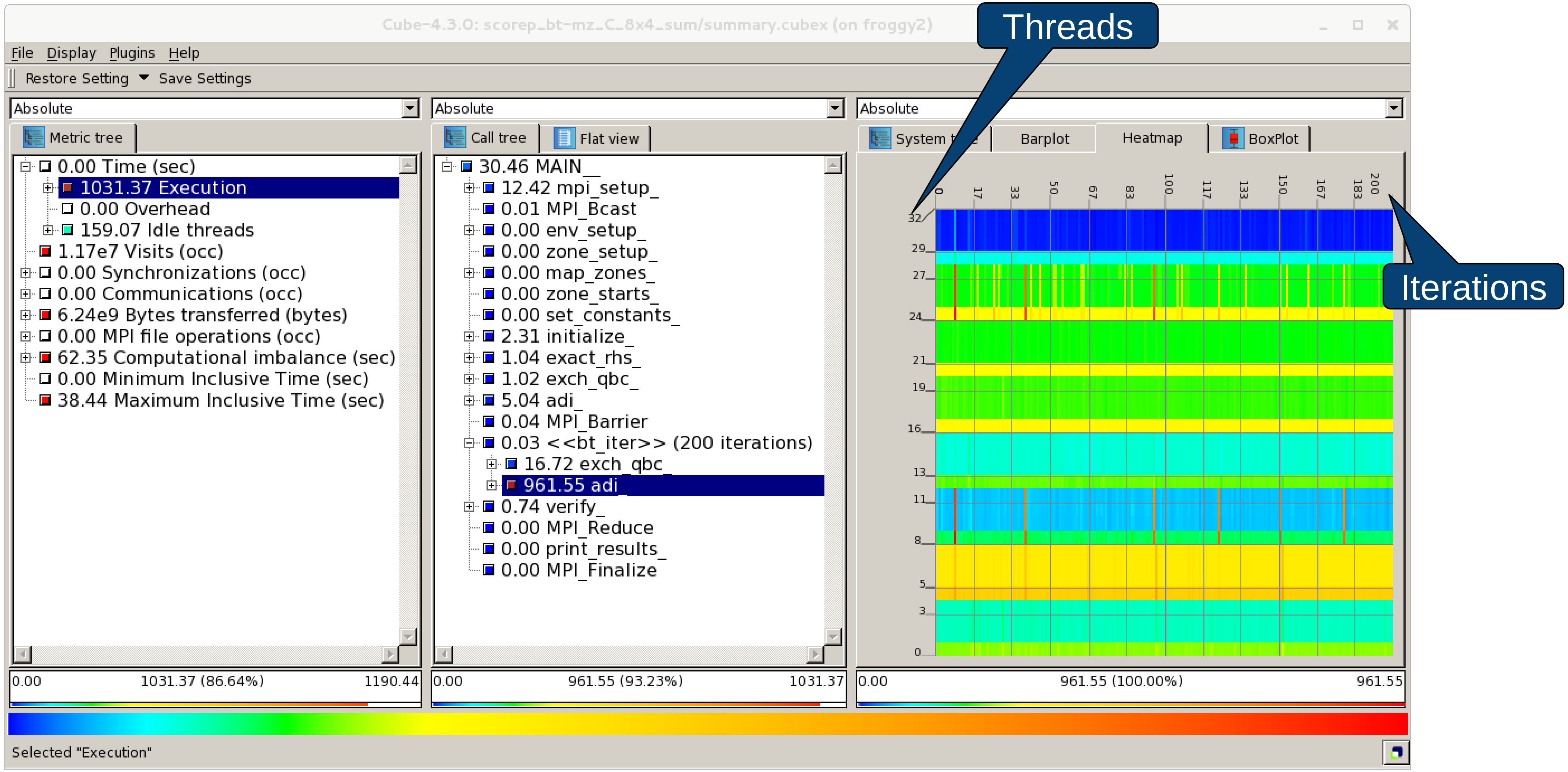
```
⊟ ■ 30.46 MAIN__
   ⊞ ■ 12.42 mpi_setup_
     ■ 0.01 MPI_Bcast
   ⊞ ■ 0.00 env_setup_
     ■ 0.00 zone_setup_
   ⊞ ■ 0.00 map_zones_
     ■ 0.00 zone_starts_
     ■ 0.00 set_constants_
   ⊞ ■ 2.31 initialize_
   ⊞ ■ 1.04 exact_rhs_
   ⊞ ■ 1.02 exch_qbc_
   ⊞ ■ 5.04 adi_
     ■ 0.04 MPI_Barrier
   ⊟ ■ 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 1031.37 (86.64%) 1190.44

0.00 961.55 (93.23%) 1031.37

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

Iteration profiling: Heatmap



Cube-4.3.0: scorep_bt-mz_C_8x4_sum/summary.cubex (on froggy2)

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)

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 1031.37 (86.64%) 1190.44

0.00 961.55 (93.23%) 1031.37

0.00 961.55 (100.00%) 961.55

Selected "Execution"

Threads

Iterations

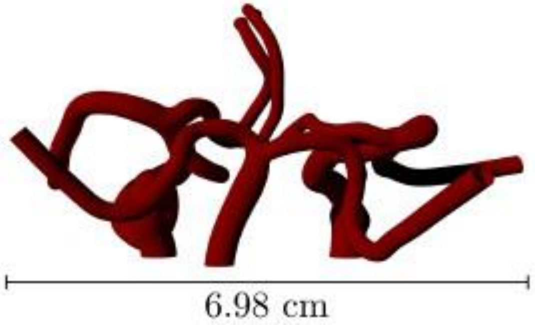
Case study HemeLB

arm
FAU FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
Lawrence Livermore National Laboratory
RWTHAACHEN UNIVERSITY
TECHNISCHE UNIVERSITÄT DRESDEN
UNIVERSITÉ DE VERSAILLES ST-QUENTIN-EN-YVELINES
Universität Stuttgart
BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación
JÜLICH Forschungszentrum
lrz Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities
TECHNISCHE UNIVERSITÄT DARMSTADT
TUM Technische Universität München
O UNIVERSITY OF OREGON
THE UNIVERSITY of TENNESSEE

HemeLB (SuperMUC-NG: no GPUs)

CompBioMed

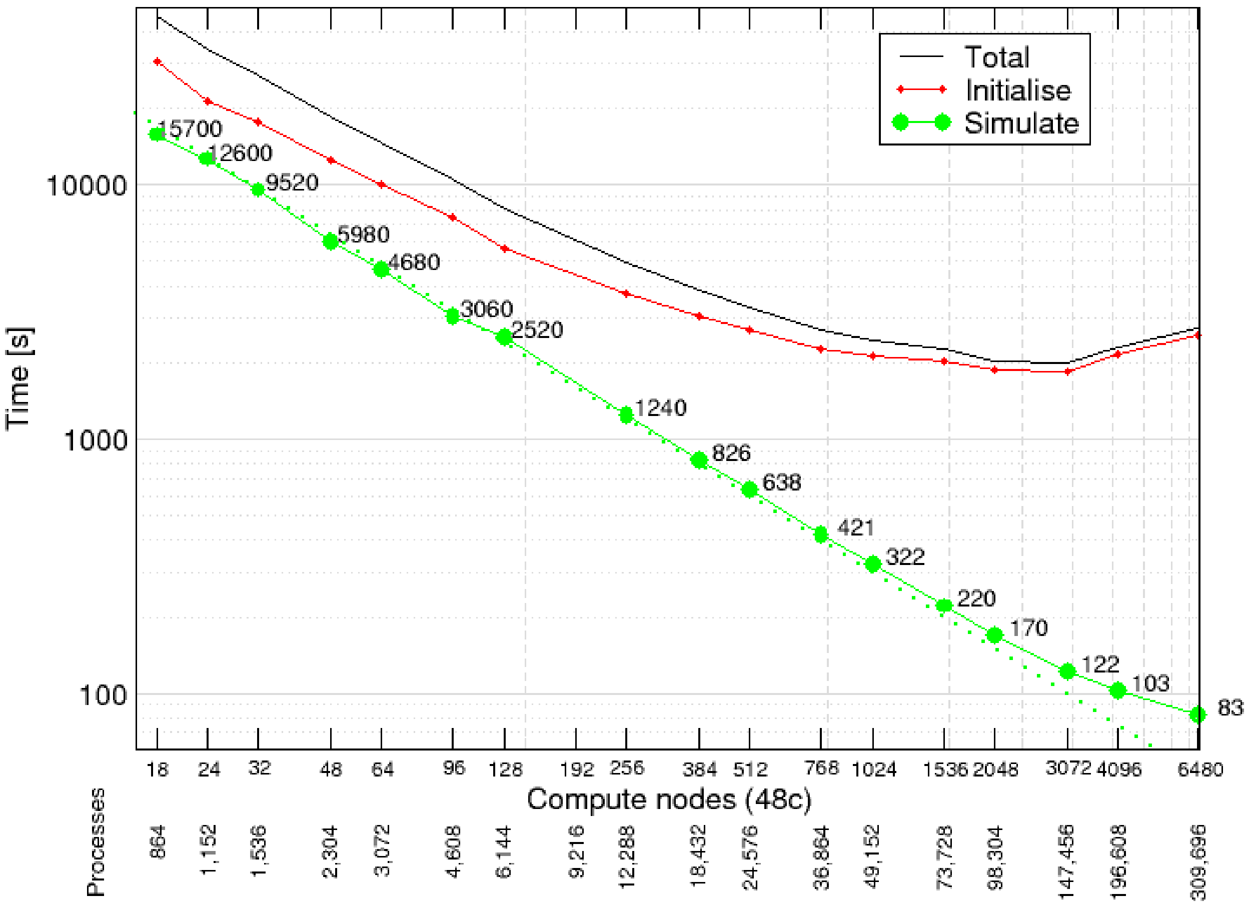
- 3D macroscopic blood flow in human arterial system developed by UC London (UK)
  - lattice-Boltzmann method tracking fluid particles on a lattice grid with complex boundary conditions
  - exascale flagship application of EU H2020 HPC Centre of Excellence for Computational Biomedicine
- HemeLB open-source code and test case: www.hemelb.org
  - 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

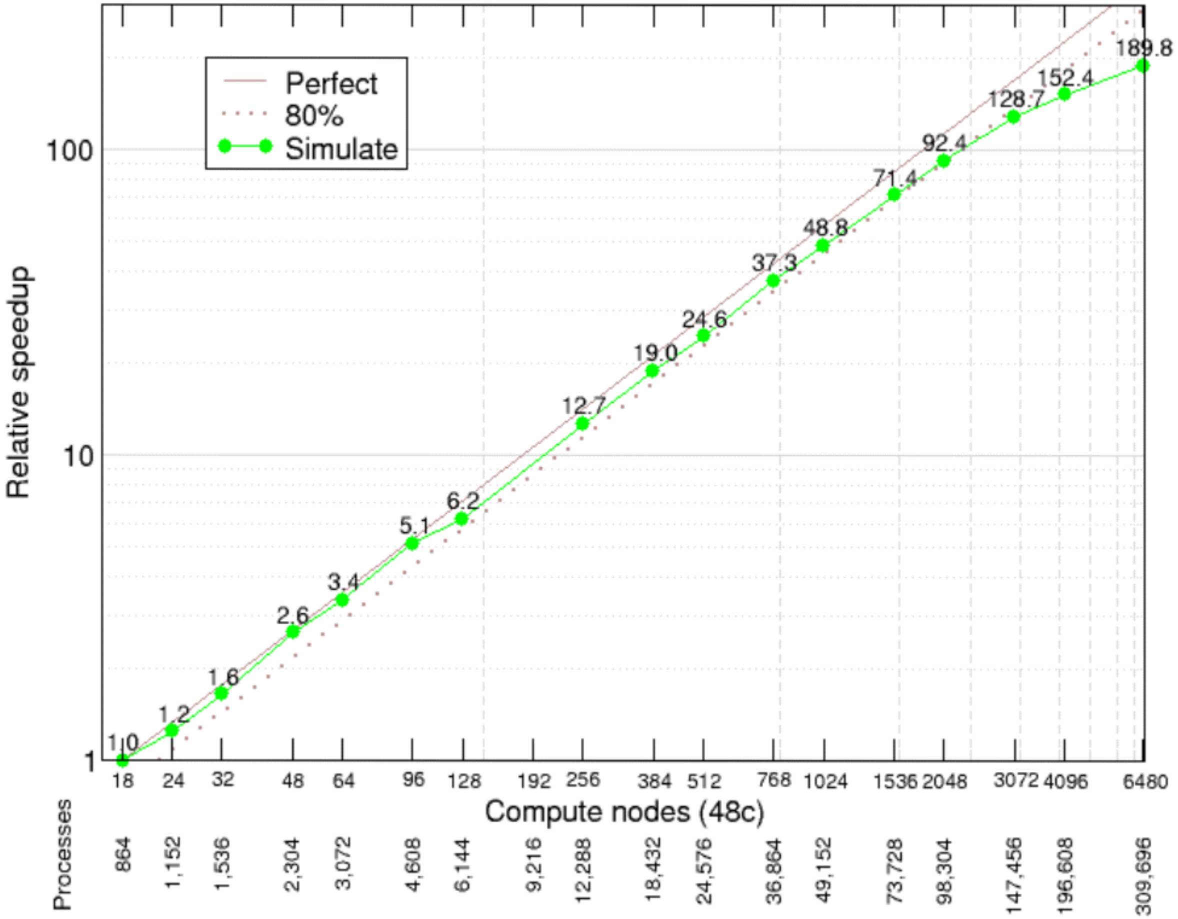


  - Focus of analysis 5,000 time-step (500μs) simulation of cerebrovascular “circle of Willis” geometry
    - 6.4μm lattice resolution (21.15 GiB): 10,154,448,502 lattice sites
- Executed on *SuperMUC-NG* Lenovo ThinkSystem SD650 (LRZ):
  - 2x 24-core Intel Xeon Platinum 8174 (‘Skylake’) @ 3.1GHz
  - 48 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***

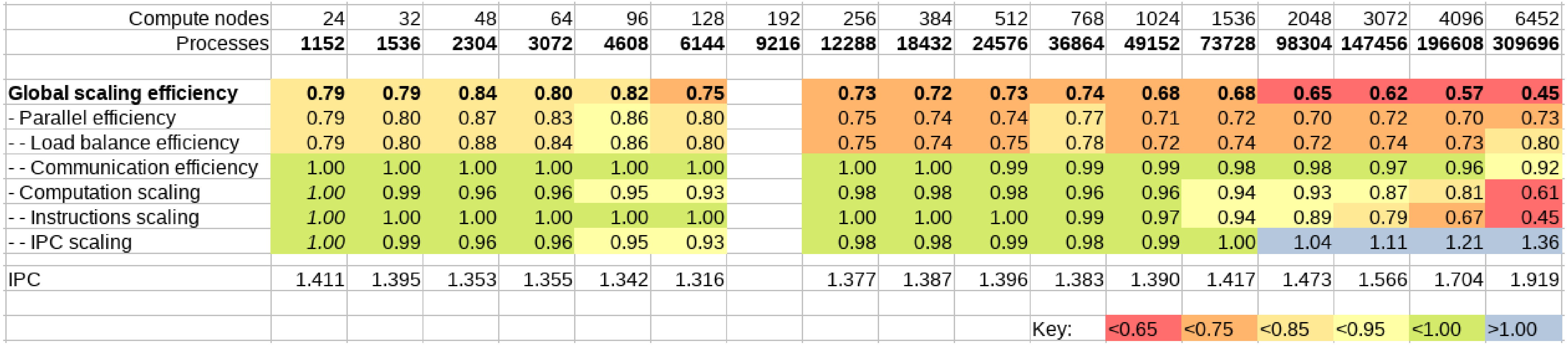
HemeLB@SNG strong scaling of FOA *RunSimulation*





[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**
Global scaling efficiency	**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]

HemeLB@SNG instrumentation & measurement

- Score-P/5.0 configured with MPIFLAGS=-DSCOREP_MPI_NO_MINI
  - don’t generate wrappers for `MPI_Comm_rank` & `MPI_Comm_size`
- HemeLB instrumentation
  - application dependencies built without modification (or instrumentation)
  - `src/main.cc` annotated with SCOREP_RECORDING_OFF/SCOREP_RECORDING_ON macros
    - to pause measurement recording during initialization
  - configured using CXX=scorep-icpc with
    - SCOREP_WRAPPER_INSTRUMENTER_FLAGS=“--user --mpp=mpi --thread=none --nomemory”
    - SCOREP_WRAPPER_COMPILER_FLAGS=“-tcollect-filter=<path_to_file>”
      - disable Intel compiler instrumentation apart from `main` routine and key classes such as `SimulationMaster`
- HemeLB execution configuration
  - SLURM `--ear=off` to enable ‘performance’ profile of processor and access to hardware counters
  - SCOREP_DEVELOPMENT_MEMORY_STATS=aggregated # report Score-P memory usage
  - SCOREP_METRIC_PAPI=PAPI_TOT_INS,PAPI_TOT_CYC,PAPI_REF_CYC,PAPI_RES_STL
  - SCOREP_TIMER=gettimeofday # use globally synchronized clock
  - SCOREP_TOTAL_MEMORY=200MB # as determined from Score-P memory usage stats

HemeLB (JUWELS-Volta)

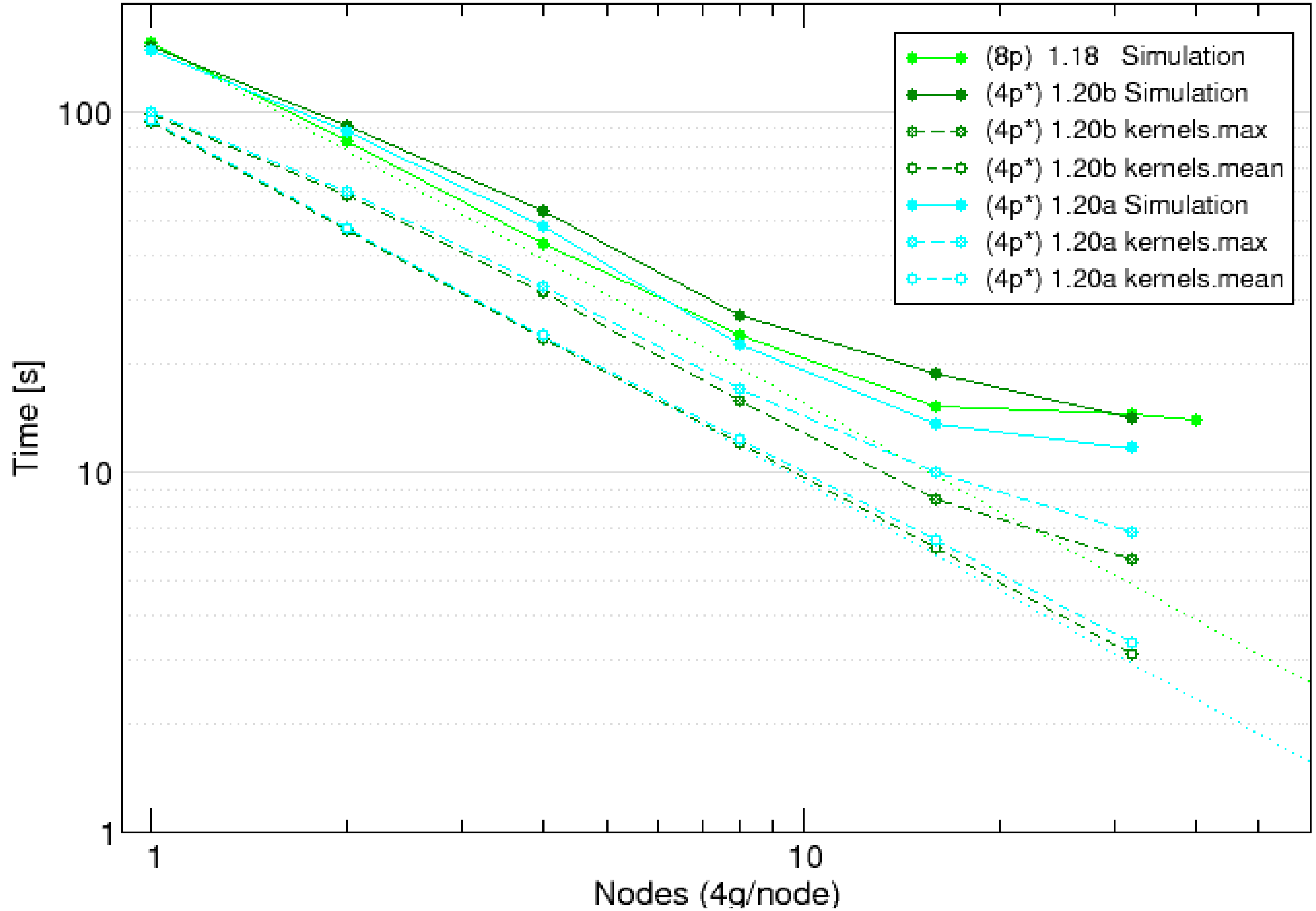
CompBioMed

- 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
  - 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 100μs) 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***

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
Simulation time [s]	147.87	88.38	48.13	22.66	13.68	11.67
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

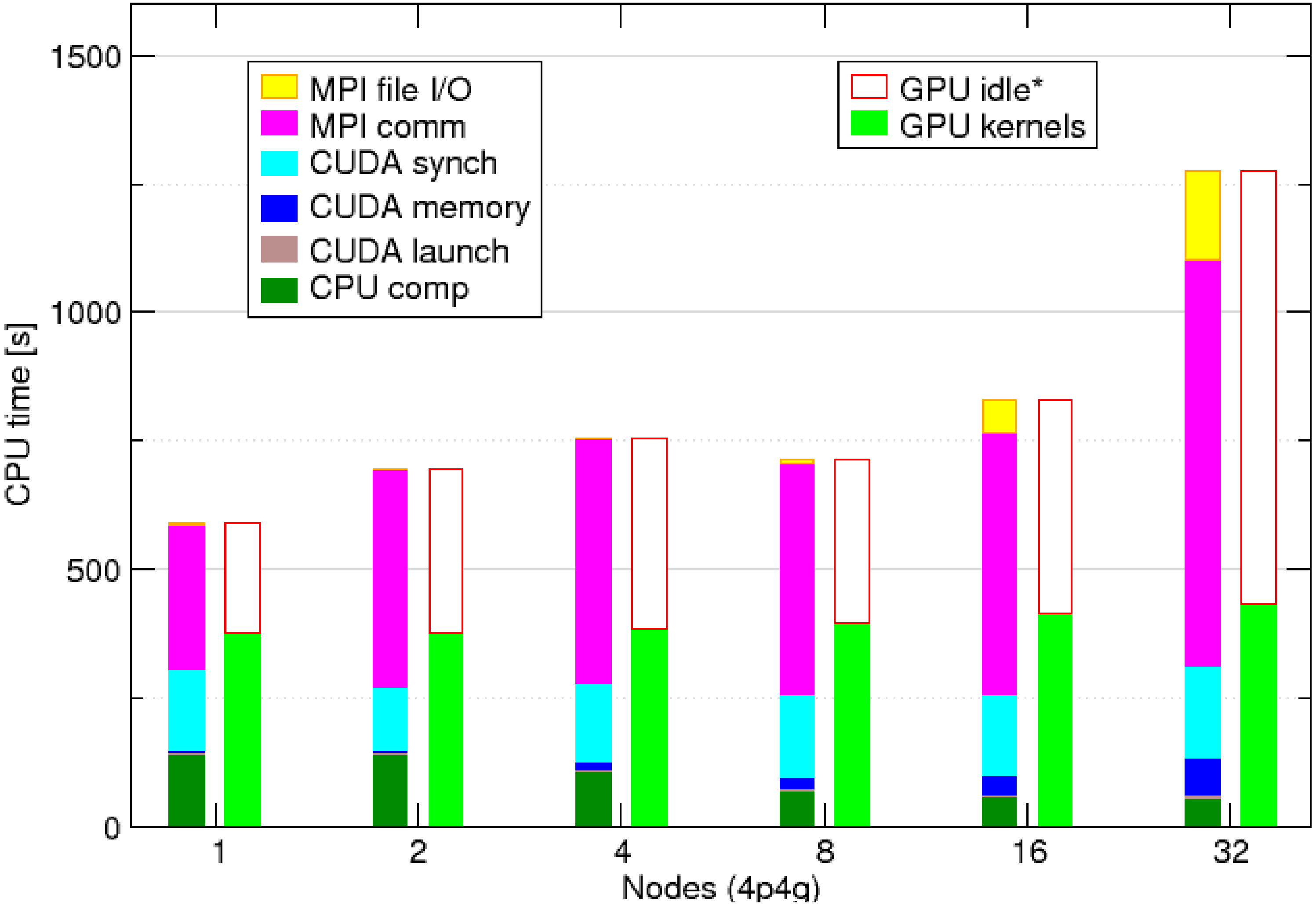
Key:
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0

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]

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

HemeLB@JUWELS-Volta instrumentation & measurement

- Score-P/6.0 instrumentation
  - CMake: CUDACXX=scorep-nvcc (no instrumentation of CXX)
  - SCOREP_WRAPPER_COMPILER_FLAGS="--relocatable-device=true –c”
  - SCOREP_WRAPPER_INSTRUMENTER_FLAGS= "--cuda --mpp=mpi --thread=none --instrument-filter=hemelb.filt"
    - hemelb.filt specifying patterns to exclude most source modules and include only routines of particular interest

- Scalasca/2.5 runtime measurement configuration
  - SCAN_TRACE_ANALYZER=none # CUDA streams not supported
  - SCOREP_CUDA_ENABLE=runtime,memcpy,kernel,sync,flushatexit
  - SCOREP_CUDA_BUFFER=10MB
  - SCOREP_MPI_ENABLE_GROUPS=coll,env,io,p2p,rma,topo,xnonblock # no ‘cg’ group
  - SCOREP_TIMER=gettimeofday # use globally synchronized clock
  - SCOREP_TOTAL_MEMORY=64MB # as determined from Score-P memory usage stats

Cube: Further information

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