Hands-on: *COSMA & Hamilton*
NPB-MZ-MPI / bt-mz_C.8

VI-HPS Team

Tutorial exercise objectives

- Familiarise with usage of VI-HPS tools
  - complementary tools' capabilities & interoperability
- Prepare to apply tools productively to *your* applications(s)
- Exercise is based on a small portable benchmark code
  - unlikely to have significant optimisation opportunities

- Optional (recommended) exercise extensions
  - analyse performance of alternative configurations
  - investigate effectiveness of system-specific compiler/MPI optimisations and/or placement/binding/ affinity capabilities
  - investigate scalability and analyse scalability limiters
  - compare performance on different HPC platforms
  - …

Access to COSMA

```
# Connect to the COSMA access host
% ssh -X -C user@login.cosma.dur.ac.uk
```

Access to Hamilton

```
# Connect to the Hamilton access host
% ssh -X -C user@vega.dur.ac.uk
# … then to Hamilton
% ssh -X -C hamilton2
```

- Unpack tutorial sources in your working directory, ideally on a parallel file system

```
% cd /gpfs/scratch/$USER
% wget  http://www.vi-hps.org/upload/material/general/NPB3.3-MZ-MPI.tar.gz
% tar zxvf  NPB3.3-MZ-MPI.tar.gz
% cd NPB3.3-MZ-MPI
```

- System documentation:
  - http://icc.dur.ac.uk/index.php?content=Computing/Cosma
  - https://www.dur.ac.uk/cis/local/hpc/hamilton/

Compiler and MPI modules

- Load development modules with the default Intel compiler with Intel MPI

```
% module load intel_comp/c4/2015
% module load intel_mpi/5.0.3
```

  - `mpiicc (mpicc -cc=icc)`
  - `mpiicpc (mpicxx -cxx=icpc)`
  - `mpiifort (mpif77 -f77=ifort)`, etc.

```
% module load intel/xe_2015.2
% module load intelmpi/intel/5.0.3
% module load slurm
```

Hamilton jobscripts provided for SLURM (not default SGE)

NPB-MZ-MPI Suite

- The NAS Parallel Benchmark suite (MPI+OpenMP version)
  - Available from:

    http://www.nas.nasa.gov/Software/NPB
  - 3 benchmarks in Fortran77
  - Configurable for various sizes & classes
- Move into the NPB3.3-MZ-MPI root directory

```
% ls
bin/     common/   jobscript/   Makefile   README.install    SP-MZ/
BT-MZ/   config/   LU-MZ/       README     README.tutorial   sys/
```

- Subdirectories contain source code for each benchmark
  - plus additional configuration and common code
- The provided distribution has already been configured for the tutorial, such that it is ready to "make" one or more of the benchmarks and install them into a (tool-specific) "bin" subdirectory

Building an NPB-MZ-MPI Benchmark

```
% make
 ===========================================
 =      NAS PARALLEL BENCHMARKS 3.3        =
 =      MPI+OpenMP Multi-Zone Versions     =
 =      F77                                =
 ===========================================

 To make a NAS multi-zone benchmark type

        make <benchmark-name> CLASS=<class> NPROCS=<nprocs>

 where <benchmark-name> is "bt-mz", "lu-mz", or "sp-mz"
       <class>          is "S", "W", "A" through "F"
       <nprocs>         is number of processes

 [...]

***************************************************************
* Custom build configuration is specified in config/make.def  *
* Suggested tutorial exercise configuration for HPC systems:  *
*       make bt-mz CLASS=C NPROCS=8                           *
***************************************************************
```

- Type “make” for instructions

Building an NPB-MZ-MPI Benchmark

```
% make bt-mz CLASS=C NPROCS=8
make[1]: Entering directory `BT-MZ'
make[2]: Entering directory `sys'
cc  -o setparams setparams.c -lm
make[2]: Leaving directory `sys'
../sys/setparams bt-mz 8 C
make[2]: Entering directory `../BT-MZ'
mpif77  -c  -O3 -openmp       bt.f
[…]
mpif77  -c  -O3 -openmp       mpi_setup.f
cd ../common;  mpif77  -c  -O3 -openmp        print_results.f
cd ../common;  mpif77  -c  -O3 -openmp        timers.f
mpif77  -O3 -openmp   -o ../bin/bt-mz_C.8 bt.o
 initialize.o exact_solution.o exact_rhs.o set_constants.o adi.o
 rhs.o zone_setup.o x_solve.o y_solve.o  exch_qbc.o solve_subs.o
 z_solve.o add.o error.o verify.o mpi_setup.o ../common/print_results.o
 ../common/timers.o
make[2]: Leaving directory `BT-MZ'
Built executable ../bin/bt-mz_C.8
make[1]: Leaving directory `BT-MZ'
```

- Specify the benchmark configuration
  - benchmark name: **bt-mz**, lu-mz, sp-mz
  - the number of MPI processes: NPROCS=**8**
  - the benchmark class (S, W, A, B, C, D, E): CLASS=**C**

Shortcut: `% make suite`

NPB-MZ-MPI / BT (Block Tridiagonal Solver)

- What does it do?
  - Solves a discretized version of the unsteady, compressible Navier-Stokes equations in three spatial dimensions
  - Performs 200 time-steps on a regular 3-dimensional grid
- Implemented in 20 or so Fortran77 source modules
- Uses MPI & OpenMP in combination
  - 8 processes each with 3 threads should be reasonable for 2 compute nodes of COSMA4
  - bt-mz_B.8 should run in around 15 seconds
  - bt-mz_C.8 should run in around 60 seconds

NPB-MZ-MPI / BT Reference Execution

```
% cd bin
% cp ../jobscript/cosma/run.lsf .
% less run.lsf
% bsub < run.lsf
```

```
% cd bin
% cp ../jobscript/hamilton/run.slurm .
% less run.slurm
% sbatch run.slurm
```

```
% cat run-<job_id>.out
 NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:   8 x   8
 Iterations:  200   dt:   0.000300
 Number of active processes:      8
 Total number of threads:        24  (  3.0 threads/process)

 Time step    1
 Time step   20
  [...]
 Time step  180
 Time step  200
 Verification Successful

 BT-MZ Benchmark Completed.
 Time in seconds = 58.78
```

- Copy jobscript and launch as a hybrid MPI+OpenMP application

Hint: save the benchmark output (or note the run time) to be able to refer to it later

Tutorial Exercise Steps

- Edit config/make.def to adjust build configuration
  - Modify specification of compiler/linker: MPIF77
- Make clean and then build new tool-specific executable

```
% make clean
% make bt-mz CLASS=C NPROCS=8
Built executable ../bin.scorep/bt-mz_C.8
```

- Change to the directory containing the new executable before running it with the desired tool configuration

```
% cd bin.scorep
% cp ../jobscript/cosma/scorep.lsf  .
% bsub < scorep.lsf
```

```
% cd bin.scorep
% cp ../jobscript/hamilton/scorep.slurm  .
% sbatch scorep.slurm
```

NPB-MZ-MPI / BT: config/make.def

```
#                  SITE- AND/OR PLATFORM-SPECIFIC DEFINITIONS.
#
#---------------------------------------------------------------------------

#---------------------------------------------------------------------------
# Configured for generic MPI with INTEL compiler
#---------------------------------------------------------------------------
#OPENMP  = -fopenmp      # GCC compiler
OPENMP = -openmp         # Intel compiler

...
#---------------------------------------------------------------------------
# The Fortran compiler used for MPI programs
#---------------------------------------------------------------------------
MPIF77 = mpiifort # Intel compiler

# Alternative variant to perform instrumentation
#MPIF77 = scorep --user  mpiifort

# PREP is a generic preposition macro for instrumentation preparation
#MPIF77 = $(PREP) mpiifort
...
```

Default (no instrumentation)

Hint: uncomment a compiler wrapper to do instrumentation

VI-HPS tools modules

- Load development modules with the default Intel compiler with Intel MPI

```
% module load intel_comp/c4/2015
% module load intel_mpi/5.0.3
```

  - mpiicc (mpicc -cc=icc)
  - mpiicpc (mpicxx -cxx=icpc)
  - mpiifort (mpif77 -f77=ifort), etc.

```
% module load intel/xe_2015.2
% module load intelmpi/intel/5.0.3
% module load slurm
```

Hamilton jobscripts provided for SLURM (not default SGE)

- and then VI-HPS tools

```
% module load scorep/1.4.2
% module load cube/4.3.2
% module load scalasca/2.2.1
% module load must/1.4.0
```

```
% module load scorep/impi/intel/1.4.2
% module load cube/gcc/4.3.2
% module load scalasca/impi/intel/2.2.1
% module load must/impi/intel/1.4.0
```

Hands-On Exercise:
Measuring Application Performance with Score-P

VI-HPS Team

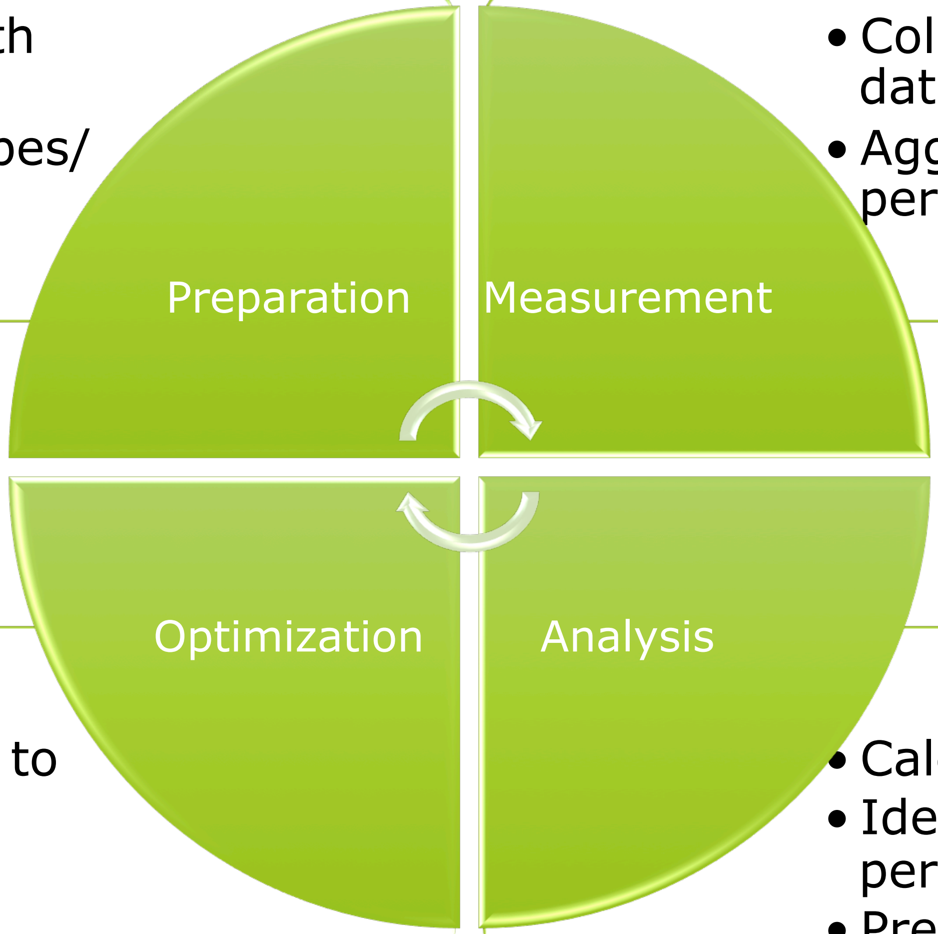
Score-P

Scalable performance measurement infrastructure for parallel codes

Performance engineering workflow

- Prepare application with symbols
- Insert extra code (probes/hooks)

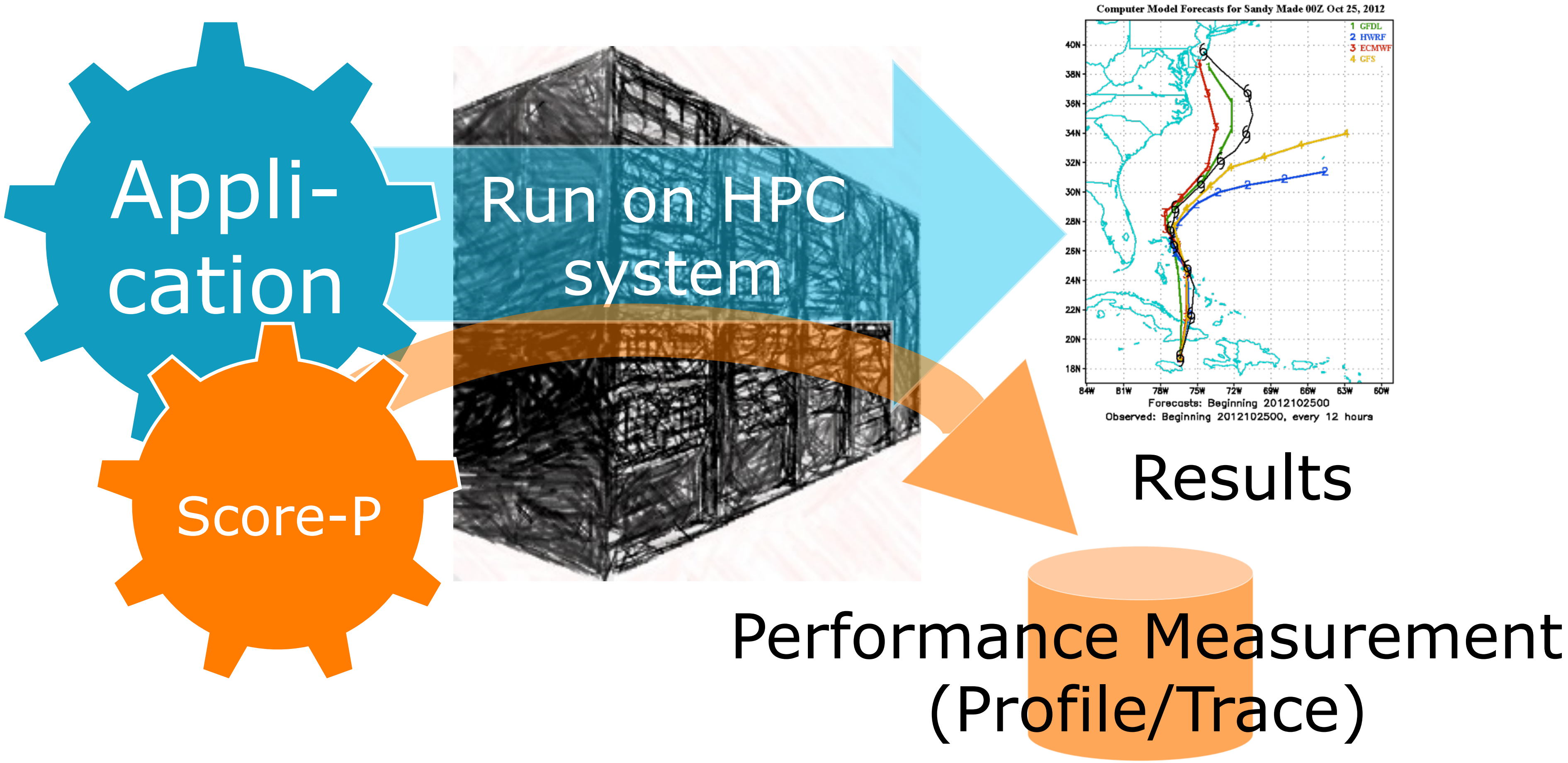
- Collection of performance data
- Aggregation of performance data



- Modifications intended to eliminate/reduce performance problem

- Calculation of metrics
- Identification of performance problems
- Presentation of results

Runtime Performance Measurement



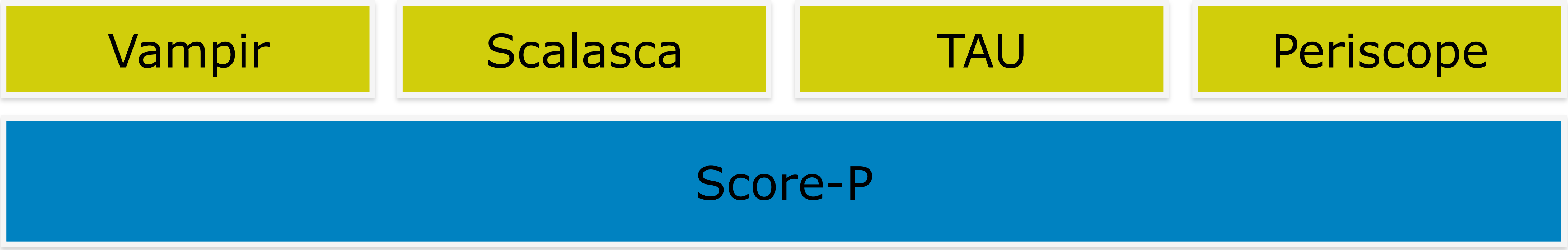
Fragmentation of Tools Landscape

- Several performance tools co-exist
  - Separate measurement systems and output formats
- Complementary features and overlapping functionality
- Redundant effort for development and maintenance
  - Limited or expensive interoperability
- Complications for user experience, support, training

Vampir	Scalasca	TAU	Periscope
VampirTrace OTF	EPILOG / CUBE	TAU native formats	Online measurement

Score-P Project Idea

- A community effort for a common infrastructure
- Developer perspective:
  - Save manpower by sharing development resources
  - Save efforts for maintenance, testing, porting, support, training
- User perspective:
  - Single learning curve
  - Single installation, fewer version updates
  - Interoperability and data exchange



Score-P Functionality

- Provide typical functionality for HPC performance tools
- Support all fundamental concepts of partner's tools

- Instrumentation (various methods)
- Flexible measurement without re-compilation:
  - Basic and advanced profile generation
  - Event trace recording
  - Online access to profiling data

- MPI/SHMEM, OpenMP/Pthreads, and hybrid parallelism (and serial)
- Enhanced functionality (CUDA, OpenCL, highly scalable I/O)

Hands-on:
NPB-MZ-MPI / BT

Performance Analysis Steps

- 0.0 Reference preparation for validation

- 1.0 Program instrumentation
- 1.1 Summary measurement collection
- 1.2 Summary analysis report examination

- 2.0 Summary experiment scoring
- 2.1 Summary measurement collection with filtering
- 2.2 Filtered summary analysis report examination

- 3.0 Event trace collection
- 3.1 Event trace examination & analysis

NPB-MZ-MPI / BT Instrumentation – Make the tools available

- COSMA

```
% module switch \
  intel_comp intel_comp/c4/2015
% module load scalasca \
         scorep intel_mpi
% cd <…>/NPB3.3-MZ-MPI
```

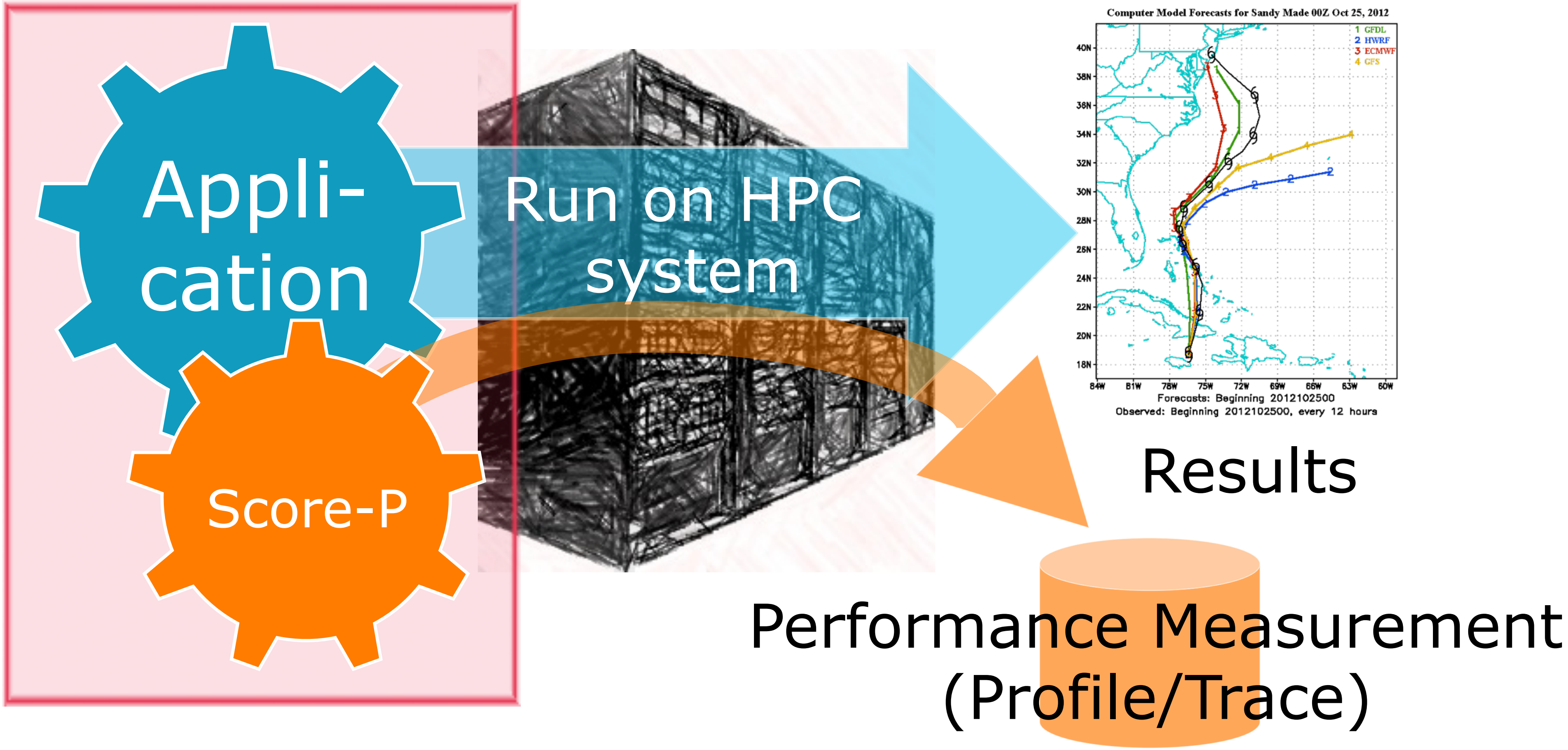
- Hamilton

```
% module load scalasca
% cd <…>/NPB3.3-MZ-MPI
```

- Archer

```
% module use \
 /home/y07/y07/scalasca/modules
% module switch \
         PrgEnv-cray PrgEnv-gnu
% module load scalasca
% cd <…>/NPB3.3-MZ-MPI
```

Overview – Next: Attach Score-P



NPB-MZ-MPI / BT Instrumentation – Link the tool to the application

- Edit config/make.def to adjust build configuration
  - Modify specification of compiler/linker: MPIF77 and COMPFLAGS

Uncomment and adapt Score-P compiler wrapper specification

- COSMA and Hamilton

```
#              SITE- AND/OR PLATFORM-SPECIFIC …
#---------------------------------------------
# Items in this file may need to be changed …
#---------------------------------------------
COMPFLAGS = -openmp
...
#---------------------------------------------
# The Fortran compiler used for MPI programs
#---------------------------------------------
#MPIF77 = mpiifort

# Alternative variants to perform instrum.
...
MPIF77 = scorep --user mpiifort
...
```

- Archer

```
#              SITE- AND/OR PLATF     PECIFIC …
#---------------------------------------------
# Items in this file may need     e changed …
#---------------------------------------------
COMPFLAGS = -fopenmp
...
#---------------------------------------------
# The Fortran compiler used f   MPI programs
#---------------------------------------------
#MPIF77 = ftn

# Alternative variants to perform instrum.
...
MPIF77 = scorep --user ftn
...
```

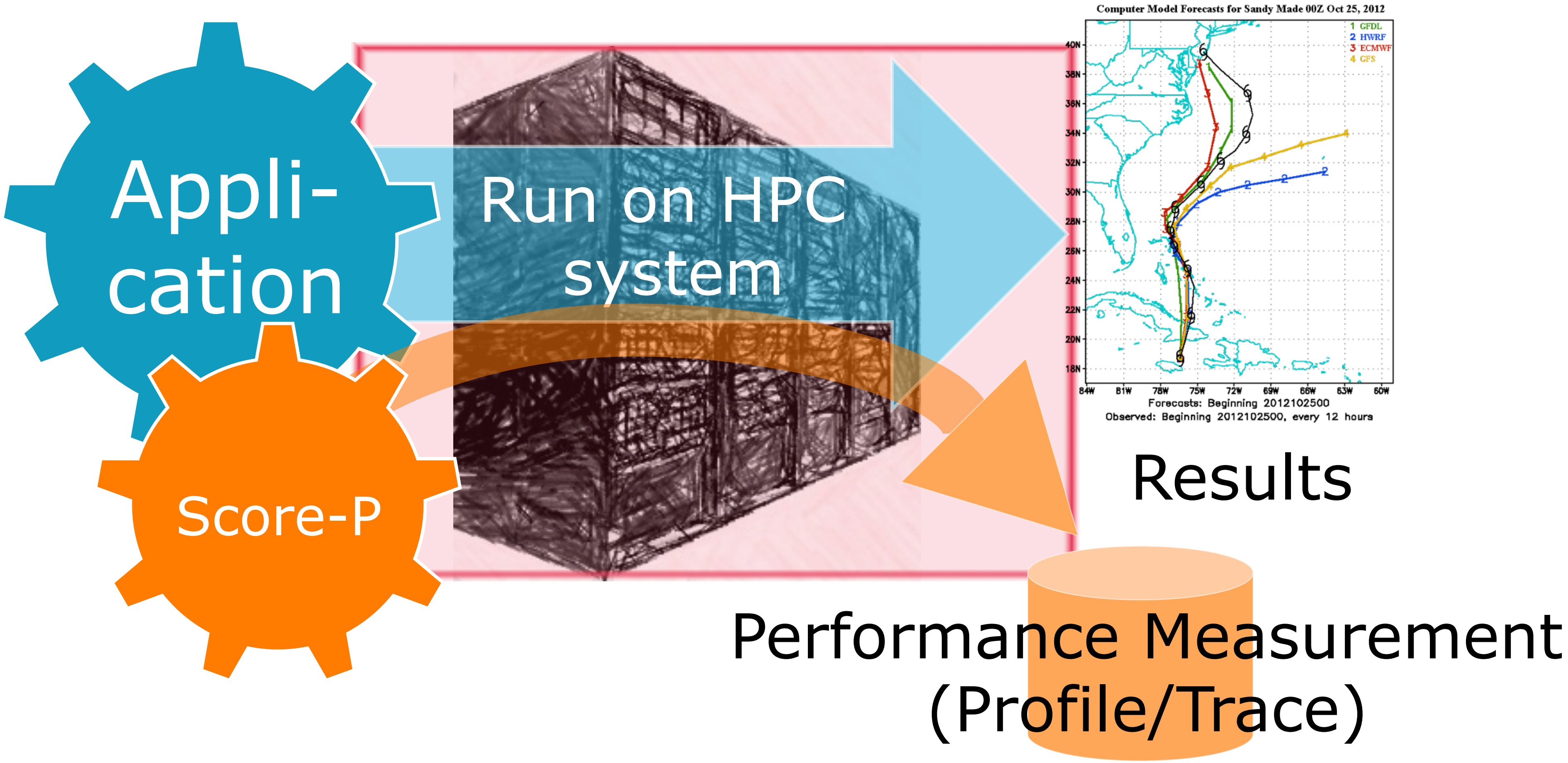
NPB-MZ-MPI / BT Instrumented – Build with presence of Score-P

```
% make clean

% make bt-mz CLASS=C NPROCS=8
cd BT-MZ; make CLASS=C NPROCS=8 VERSION=
make: Entering directory 'BT-MZ'
cd ../sys; cc  -o setparams setparams.c -lm
../sys/setparams bt-mz 8 C
scorep mpiifort -c  -O3 -openmp bt.f
 [...]
cd ../common;  scorep mpiifort -c  -O3 -openmp timers.f
scorep mpiifort -O3 -fopenmp -o ../bin.scorep/bt-mz_C.8 \
bt.o initialize.o exact_solution.o exact_rhs.o set_constants.o \
adi.o rhs.o zone_setup.o x_solve.o y_solve.o exch_qbc.o \
solve_subs.o z_solve.o add.o error.o verify.o mpi_setup.o \
../common/print_results.o ../common/timers.o
Built executable ../bin.scorep/bt-mz_C.8
make: Leaving directory 'BT-MZ'
```

If you run on the frontend of COSMA/ Hamilton, use “B” and 4 procs!

- Clean-up
- Re-build executable with NPB build system (this is unrelated to Score-P and simply part of the NPB benchmarks)

Overview – Next: Run with Score-P attached (Initial run)



Measurement Configuration: scorep-info

```
% scorep-info config-vars --full
SCOREP_ENABLE_PROFILING
  Description: Enable profiling
          [...]
SCOREP_ENABLE_TRACING
  Description: Enable tracing
          [...]
SCOREP_TOTAL_MEMORY
  Description: Total memory in bytes for the measurement system
          [...]
SCOREP_EXPERIMENT_DIRECTORY
  Description: Name of the experiment directory
          [...]
SCOREP_FILTERING_FILE
  Description: A file name which contain the filter rules
          [...]
SCOREP_METRIC_PAPI
  Description: PAPI metric names to measure
          [...]
SCOREP_METRIC_RUSAGE
  Description: Resource usage metric names to measure
          [... More configuration variables ...]
```

- Score-P measurements are configured via environmental variables:

Summary Measurement Collection – First execution with Score-P

- Change to the directory containing the new executable (bin.scorep)

- COSMA and Hamilton

```
% cd bin.scorep
% export OMP_NUM_THREADS=4
% export SCOREP_EXPERIMENT_DIRECTORY=\
              scorep_4x4_sum
% mpirun -np 4 ./bt-mz_B.4
```

Runs directly on frontend – Use a jobscript if you have access to quick to react queues
Example jobscripts available in:
../jobscripts/{cosma/hamilton}/

- Archer

```
% cd bin.scorep
% cp ../jobscript/archer/scorep.pbs ./
% nano scorep.pbs
...
#PBS -A y14
...
export OMP_NUM_THREADS=6
PROCS=8
CLASS=C
EXE=./bt-mz_$CLASS.$PROCS
export SCOREP_EXPERIMENT_DIRECTORY=\
scorep_${NPROCS}x${OMP_NUM_THREADS}_sum
#export SCOREP_FILTERING_FILE=../config/scorep.filt
#export SCOREP_METRIC_PAPI=PAPI_TOT_INS,PAPI_TOT_CYC
#export SCOREP_TOTAL_MEMORY=300M
...
% qsub -q short scorep.pbs
```

Adapt! (#PBS -A y14)

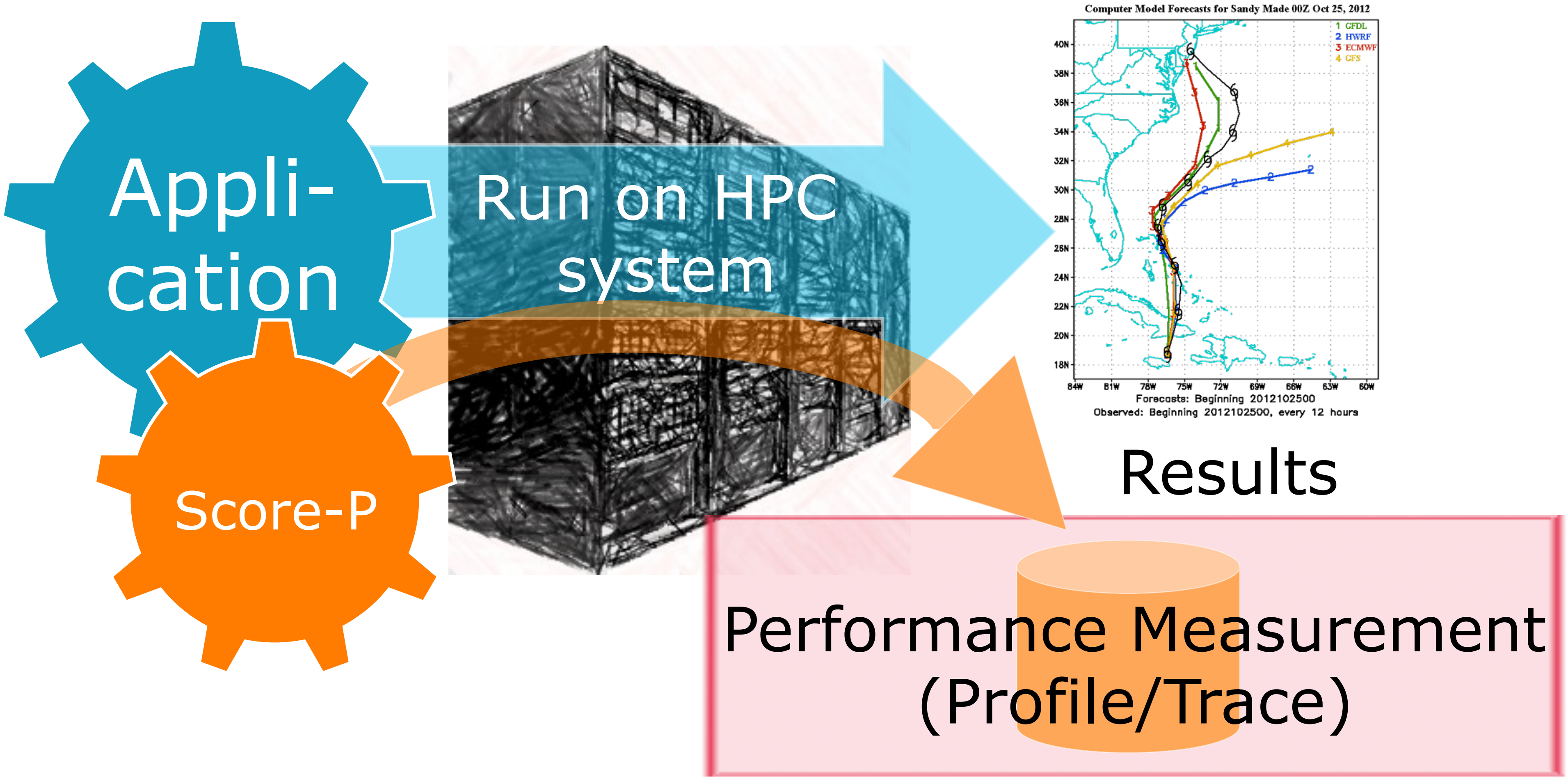
Keep them commented (#export lines)

Summary Measurement Collection – First execution with Score-P

```
% less <Jobscript/Shell-Output>

 NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP \
>Benchmark

 Number of zones:   8 x   8
 Iterations: 200    dt:   0.000300
 Number of active processes:     8

 Use the default load factors with threads
 Total number of threads:     32  (  4.0 threads/process)

 Calculated speedup =     31.99

 Time step    1

        [... More application output ...]
```

- Check the output of the application run

Overview – Next: Run with Score-P attached (Initial run)



BT-MZ Summary Analysis Report Examination

or 4x4

```
% ls
bt-mz_C.8  mzmpibt.o2969889 scorep_8x6_sum
% ls scorep_8x6_sum
profile.cubex  scorep.cfg

% cube scorep_8x6_sum/profile.cubex

       [CUBE GUI showing summary analysis report]
```

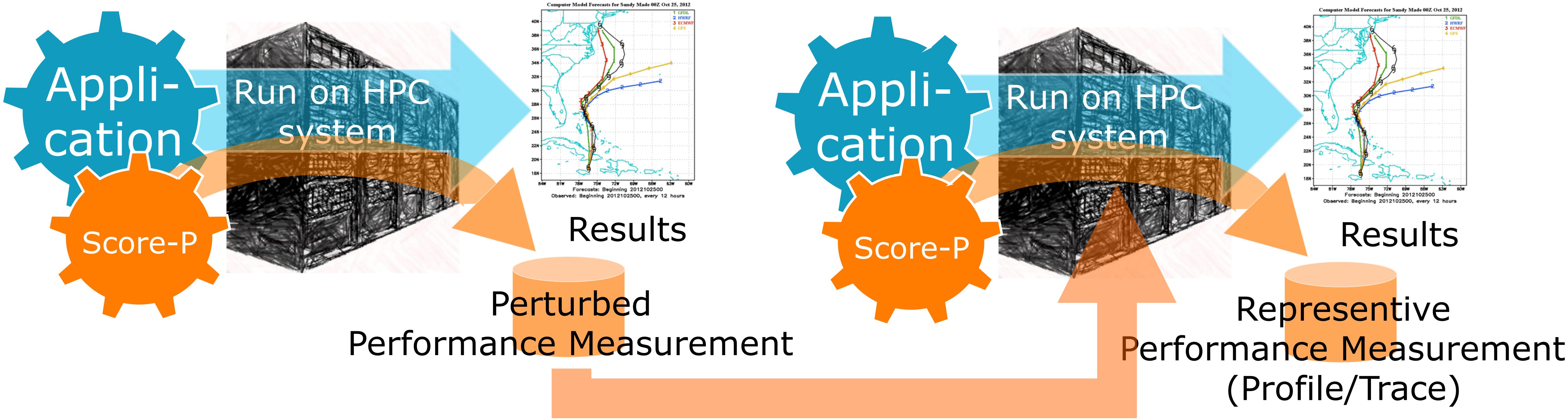
- Creates experiment directory
  - A record of the measurement configuration (scorep.cfg)
  - The analysis report that was collated after measurement (profile.cubex)
- Interactive exploration with CUBE

Congratulations!?

- If you made it this far, you successfully used Score-P to
  - instrument the application
  - analyze its execution with a summary measurement, and
  - examine it with one the interactive analysis report explorer GUIs
- ... revealing the call-path profile annotated with
  - the “Time” metric
  - Visit counts
  - MPI message statistics (bytes sent/received)
- ... but how ***good*** was the measurement?
  - The measured execution produced the desired valid result
  - however, the execution took rather longer than expected!
    - even when ignoring measurement start-up/completion, therefore
    - it was probably dilated by instrumentation/measurement overhead

Overview – Next: Filtering

- First profiling run
- Second filtered run (possibly tracing)



Filtering + performance counters + possibly tracing

Performance Analysis Steps

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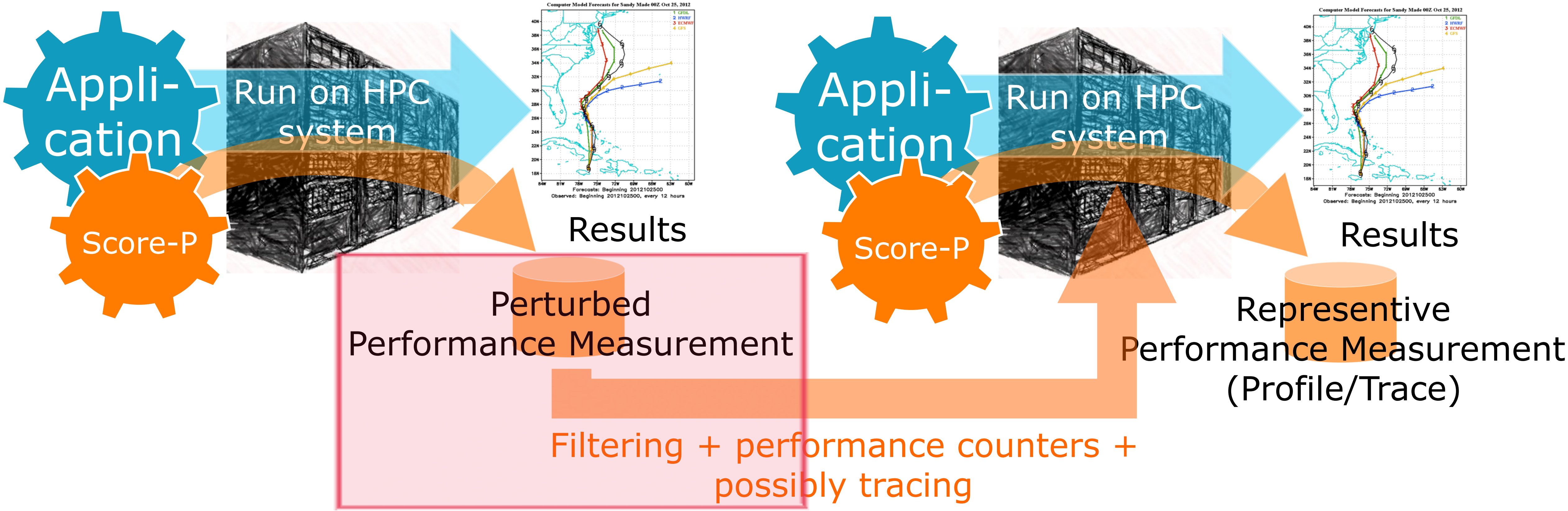
- 3.0 Event trace collection
- 3.1 Event trace examination & analysis

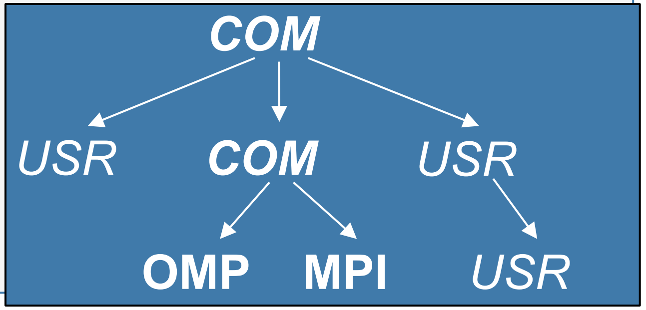
Overview – Next: Filtering

- First profiling run
- Second filtered run (possibly tracing)



BT-MZ Summary Analysis Result Scoring

```
% scorep-score scorep_8x6_sum/profile.cubex

Estimated aggregate size of event trace:                   159 GB
Estimated requirements for largest trace buffer (max_buf):  20 GB
Estimated memory requirements (SCOREP_TOTAL_MEMORY):        20 GB
(hint: When tracing set SCOREP_TOTAL_MEMORY=20GB to avoid intermediate flushes
 or reduce requirements using USR regions filters.)

flt     type     max_buf[B]        visits time[s] time[%] time/visit[us]  region
         ALL 21,377,442,117 6,554,106,201 4946.18   100.0           0.75  ALL
         USR 21,309,225,314 6,537,020,537 2326.51    47.0           0.36  USR
         OMP     65,624,896    16,327,168 2607.63    52.7         159.71  OMP
         COM      2,355,080       724,640    2.49     0.1           3.43  COM
         MPI        236,827        33,856    9.56     0.2         282.29  MPI
```



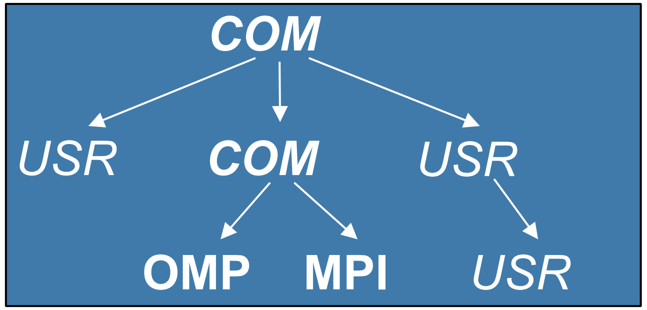
- Report scoring as textual output

159 GB total memory
20 GB per rank!

- Region/callpath classification
  - **MPI** pure MPI functions
  - **OMP** pure OpenMP regions
  - **USR** user-level computation
  - **COM** “combined” USR+OpenMP/MPI
  - **ANY/ALL** aggregate of all region types

BT-MZ Summary Analysis Report Breakdown

```
% scorep-score -r scorep_8x6_sum/profile.cubex
  [...]
  [...]
flt type      max_buf[B]        visits time[s] time[%] time/visit[us]region
     ALL 21,377,442,117 6,554,106,201 4946.18   100.0           0.75  ALL
     USR 21,309,225,314 6,537,020,537 2326.51    47.0           0.36  USR
     OMP     65,624,896    16,327,168 2607.63    52.7         159.71  OMP
     COM      2,355,080       724,640    2.49     0.1           3.43  COM
     MPI        236,827        33,856    9.56     0.2         282.29  MPI

     USR  6,883,222,086 2,110,313,472  651.44    13.2           0.31  matvec_sub_
     USR  6,883,222,086 2,110,313,472  720.38    14.6           0.34  matmul_sub_
     USR  6,883,222,086 2,110,313,472  881.32    17.8           0.42  binvcrhs_
     USR    293,617,584    87,475,200   29.93     0.6           0.34  binvrhs_
     USR    293,617,584    87,475,200   33.03     0.7           0.38  lhsinit_
     USR    101,320,128    31,129,600    7.78     0.2           0.25  exact_solution_
```



More than
18 GB just for these 6
regions

BT-MZ Summary Analysis Score

- Summary measurement analysis score reveals
  - Total size of event trace would be ~159 GB
  - Maximum trace buffer size would be ~20 GB per rank
    - smaller buffer would require flushes to disk during measurement resulting in substantial perturbation
  - 99.8% of the trace requirements are for USR regions
    - purely computational routines never found on COM call-paths common to communication routines or OpenMP parallel regions
  - These USR regions contribute around 32% of total time
    - however, much of that is very likely to be measurement overhead for frequently-executed small routines
- Advisable to tune measurement configuration
  - Specify an adequate trace buffer size
  - Specify a filter file listing (USR) regions not to be measured

BT-MZ Summary Analysis Report Filtering

```
% cat ../config/scorep.filt
SCOREP_REGION_NAMES_BEGIN EXCLUDE
binvcrhs*
matmul_sub*
matvec_sub*
exact_solution*
binvrhs*
lhs*init*
timer_*

% scorep-score -f ../config/scorep.filt -c 2 \
>scorep_8x6_sum/profile.cubex

Estimated aggregate size of event trace:                   521 MB
Estimated requirements for largest trace buffer (max_buf):  66 MB
Estimated memory requirements (SCOREP_TOTAL_MEMORY):        78 MB
(hint: When tracing set SCOREP_TOTAL_MEMORY=78MB to avoid \
>intermediate flushes
 or reduce requirements using USR regions filters.)
```

- Report scoring with prospective filter listing 6 USR regions

521 MB of memory in total, 66 MB per rank!

(Including 2 metric values)

BT-MZ Summary Analysis Report Filtering

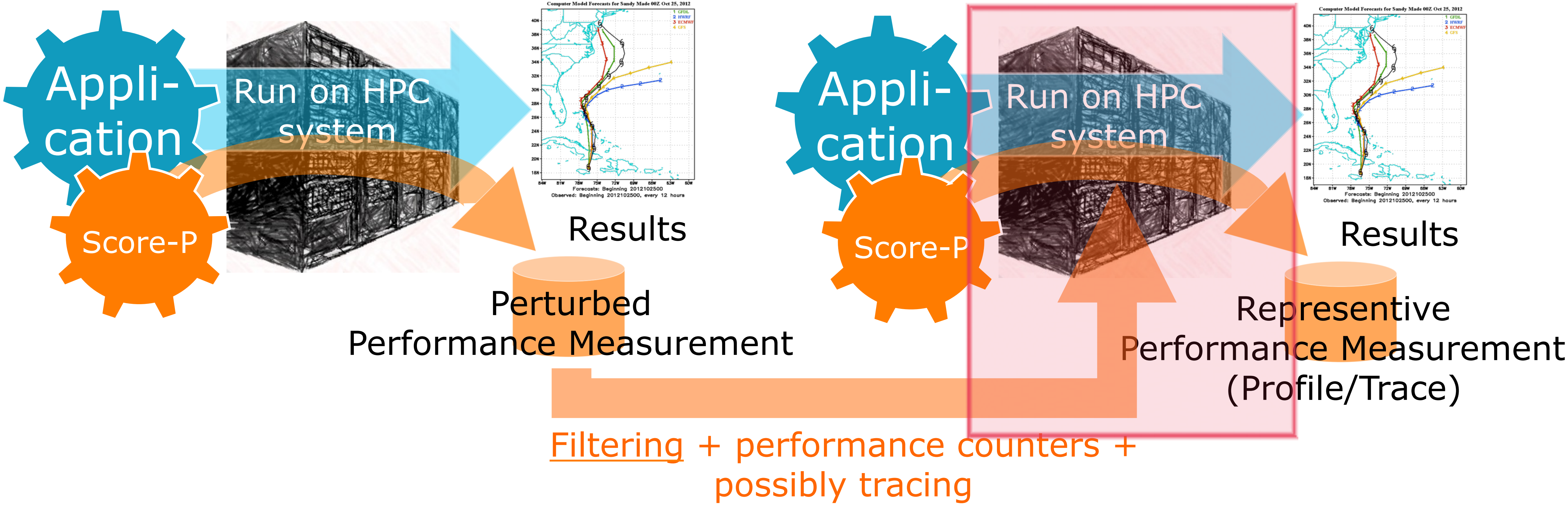
```
% scorep-score -r -f ../config/scorep.filt \
> scorep_8x6_sum/profile.cubex
flt type      max_buf[B]          visits time[s] time[%] time/visit[us] region
 -    ALL 21,377,442,117 6,554,106,201 4946.18   100.0           0.75 ALL
 -    USR 21,309,225,314 6,537,020,537 2326.51    47.0           0.36 USR
 -    OMP     65,624,896    16,327,168 2607.63    52.7         159.71 OMP
 -    COM      2,355,080       724,640    2.49     0.1           3.43 COM
 -    MPI        236,827        33,856    9.56     0.2         282.29 MPI

 *    ALL     68,216,855    17,085,673 2622.30    53.0         153.48 ALL-FLT
 +    FLT 21,309,225,262 6,537,020,528 2323.88    47.0           0.36 FLT
 -    OMP     65,624,896    16,327,168 2607.63    52.7         159.71 OMP-FLT
 *    COM      2,355,080       724,640    2.49     0.1           3.43 COM-FLT
 -    MPI        236,827        33,856    9.56     0.2         282.29 MPI-FLT
 *    USR             52             9    2.63     0.1      292158.12 USR-FLT

 +    USR  6,883,222,086 2,110,313,472  651.44    13.2           0.31 matvec_sub_
 +    USR  6,883,222,086 2,110,313,472  720.38    14.6           0.34 matmul_sub_
 +    USR  6,883,222,086 2,110,313,472  881.32    17.8           0.42 binvcrhs_
 +    USR    293,617,584    87,475,200   29.93     0.6           0.34 binvrhs_
 +    USR    293,617,584    87,475,200   33.03     0.7           0.38 lhsinit_
 +    USR    101,320,128    31,129,600    7.78     0.2           0.25 exact_solution_
```

Filtered routines marked with '+'

- Score report breakdown by region

Overview – Next: Filtering

- First profiling run
- Second filtered run (possibly tracing)



Summary Measurement Collection – Score-P w/ Filter

- Set new experiment directory and re-run measurement with new filter configuration

- COSMA and Hamilton

```
% cd bin.scorep
% export OMP_NUM_THREADS=4
% export SCOREP_EXPERIMENT_DIRECTORY=\
                scorep_4x4_sum_filter
% export SCOREP_FILTERING_FILE=\
                ../config/scorep.filt
% mpirun -np 4 ./bt-mz_B.4
```

Runs directly on frontend – Use a jobscript if you have access to quick to react queues
Example jobscripts available in:
../jobscripts/{cosma/hamilton}/

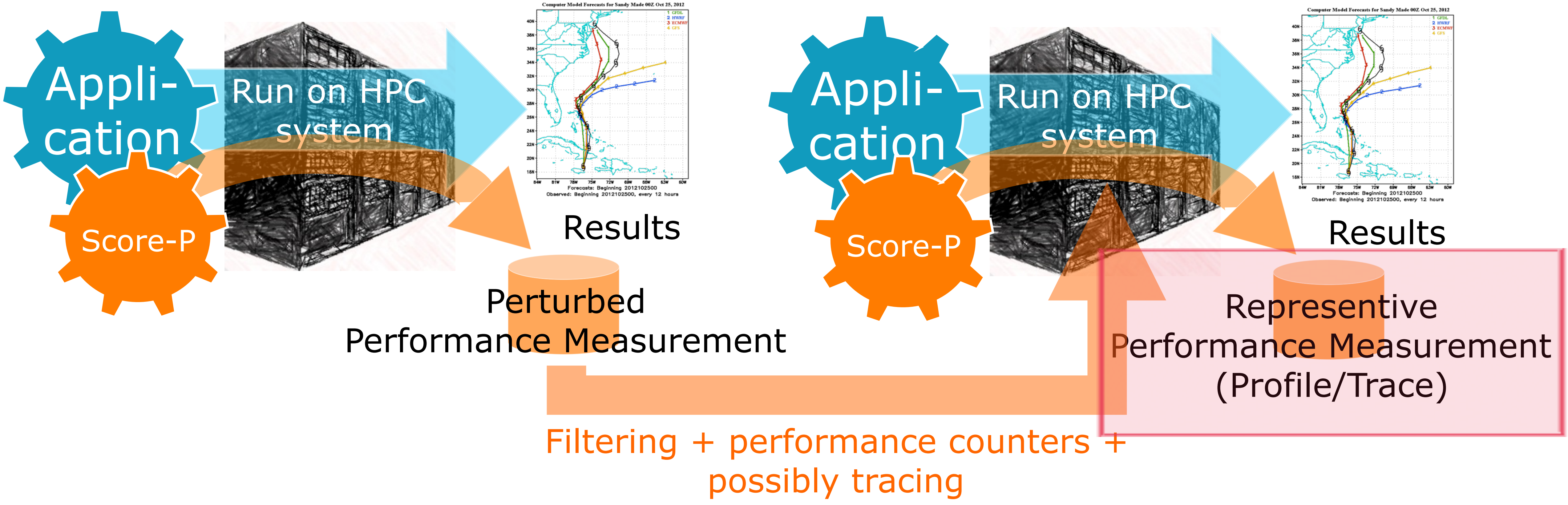
- Archer

```
% cd bin.scorep
% cp ../jobscript/archer/scorep.pbs ./
% nano scorep.pbs
...
#PBS -A y14
...
export OMP_NUM_THREADS=6
PROCS=8
CLASS=C
EXE=./bt-mz_$CLASS.$PROCS
export SCOREP_EXPERIMENT_DIRECTORY=\
scorep_${NPROCS}x${OMP_NUM_THREADS}_sum_filter
export SCOREP_FILTERING_FILE=../config/scorep.filt
#export SCOREP_METRIC_PAPI=PAPI_TOT_INS,PAPI_TOT_CYC
#export SCOREP_TOTAL_MEMORY=300M
...
% qsub -q short scorep.pbs
```

Adapt! (#PBS -A y14)

Overview – Next: Filtering

- First profiling run
- Second filtered run (possibly tracing)



BT-MZ Summary Analysis Report Examination – With Filter

or 4x4

```
% cube scorep_8x6_sum_filter/profile.cubex

      [CUBE GUI showing summary analysis report]
```

- Interactive exploration with CUBE
- This time reported times are representative of the actual application behavior

Score-P:
Advanced Measurement Configuration

Advanced Measurement Configuration: Metrics

- Available PAPI metrics
  - Preset events: common set of events deemed relevant and useful for application performance tuning
    - Abstraction from specific hardware performance counters, mapping onto available events done by PAPI internally

```
% papi_avail
```

  - Native events: set of all events that are available on the CPU (platform dependent)

```
% papi_native_avail
```

Note:
Due to hardware restrictions
- number of concurrently recorded events is limited
- there may be invalid combinations of concurrently recorded events

Advanced Measurement Configuration: Metrics

```
% man getrusage
struct rusage {
    struct timeval ru_utime; /* user CPU time used */
    struct timeval ru_stime; /* system CPU time used */
    long   ru_maxrss;        /* maximum resident set size */
    long   ru_ixrss;         /* integral shared memory size */
    long   ru_idrss;         /* integral unshared data size */
    long   ru_isrss;         /* integral unshared stack size */
    long   ru_minflt;        /* page reclaims (soft page faults) */
    long   ru_majflt;        /* page faults (hard page faults) */
    long   ru_nswap;         /* swaps */
    long   ru_inblock;       /* block input operations */
    long   ru_oublock;       /* block output operations */
    long   ru_msgsnd;        /* IPC messages sent */
    long   ru_msgrcv;        /* IPC messages received */
    long   ru_nsignals;      /* signals received */
    long   ru_nvcsw;         /* voluntary context switches */
    long   ru_nivcsw;        /* involuntary context switches */
};
```

- Available resource usage metrics
- Note:

(1) Not all fields are maintained on each platform.

(2) Check scope of metrics (per process vs. per thread)

Advanced Measurement Configuration: CUDA

- Record CUDA events with the CUPTI interface

```
% export SCOREP_CUDA_ENABLE=gpu,kernel,idle
```

- All possible recording types
  - runtime — CUDA runtime API
  - driver — CUDA driver API
  - gpu — GPU activities
  - kernel — CUDA kernels
  - idle — GPU compute idle time
  - memcpy — CUDA memory copies

Score-P User Instrumentation API

- Can be used to mark initialization, solver & other phases
  - Annotation macros ignored by default
  - Enabled with [--user] flag
- Appear as additional regions in analyses
  - Distinguishes performance of important phase from rest
- Can be of various type
  - E.g., function, loop, phase
  - See user manual for details
- Available for Fortran / C / C++

Score-P User Instrumentation API (Fortran)

```
#include "scorep/SCOREP_User.inc"

subroutine foo(…)
  ! Declarations
  SCOREP_USER_REGION_DEFINE( solve )

  ! Some code…
  SCOREP_USER_REGION_BEGIN( solve, “<solver>", \
                            SCOREP_USER_REGION_TYPE_LOOP )
  do i=1,100
    [...]
  end do
  SCOREP_USER_REGION_END( solve )
  ! Some more code…
end subroutine
```

- Requires processing by the C preprocessor

Score-P User Instrumentation API (C/C++)

```
#include "scorep/SCOREP_User.h"

void foo()
{
  /* Declarations */
  SCOREP_USER_REGION_DEFINE( solve )

  /* Some code… */
  SCOREP_USER_REGION_BEGIN( solve, “<solver>",
                            SCOREP_USER_REGION_TYPE_LOOP )
  for (i = 0; i < 100; i++)
  {
    [...]
  }
  SCOREP_USER_REGION_END( solve )
  /* Some more code… */
}
```

Score-P User Instrumentation API (C++)

```
#include "scorep/SCOREP_User.h"

void foo()
{
  // Declarations

  // Some code…
  {
    SCOREP_USER_REGION( “<solver>",
                        SCOREP_USER_REGION_TYPE_LOOP )
    for (i = 0; i < 100; i++)
    {
      [...]
    }
  }
  // Some more code…
}
```

Score-P Measurement Control API

- Can be used to temporarily disable measurement for certain intervals
  - Annotation macros ignored by default
  - Enabled with [--user] flag

```fortran
#include "scorep/SCOREP_User.inc"

subroutine foo(…)
  ! Some code…
  SCOREP_RECORDING_OFF()
  ! Loop will not be measured
  do i=1,100
    [...]
  end do
  SCOREP_RECORDING_ON()
  ! Some more code…
end subroutine
```

Fortran (requires Cpreprocessor)

```c
#include "scorep/SCOREP_User.h"

void foo(…) {
  /* Some code… */
  SCOREP_RECORDING_OFF()
  /* Loop will not be measured */
  for (i = 0; i < 100; i++) {
    [...]
  }
  SCOREP_RECORDING_ON()
  /* Some more code… */
}
```

C / C++

Further Information

- Community instrumentation & measurement infrastructure
  - Instrumentation (various methods)
  - Basic and advanced profile generation
  - Event trace recording
  - Online access to profiling data
- Available under New BSD open-source license
- Documentation & Sources:
  - http://www.score-p.org
- User guide also part of installation:
  - `<prefix>/share/doc/scorep/{pdf,html}/`
- Support and feedback: support@score-p.org
- Subscribe to news@score-p.org, to be up to date

Analysis report examination with CUBE

Brian Wylie
Jülich Supercomputing Centre

CUBE

Parallel program analysis report exploration tools

- Libraries for XML report reading & writing
- Algebra utilities for report processing
- GUI for interactive analysis exploration
  - requires Qt4/5

Originally developed as part of Scalasca toolset

Now available as a separate component

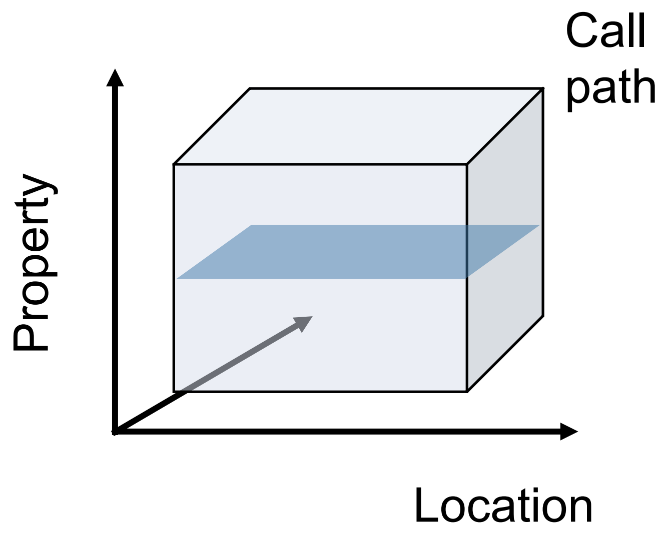
- Can be installed independently of Score-P, e.g., on laptop or desktop
- Latest release: CUBE 4.3.2 (June 2015)

Analysis presentation and exploration

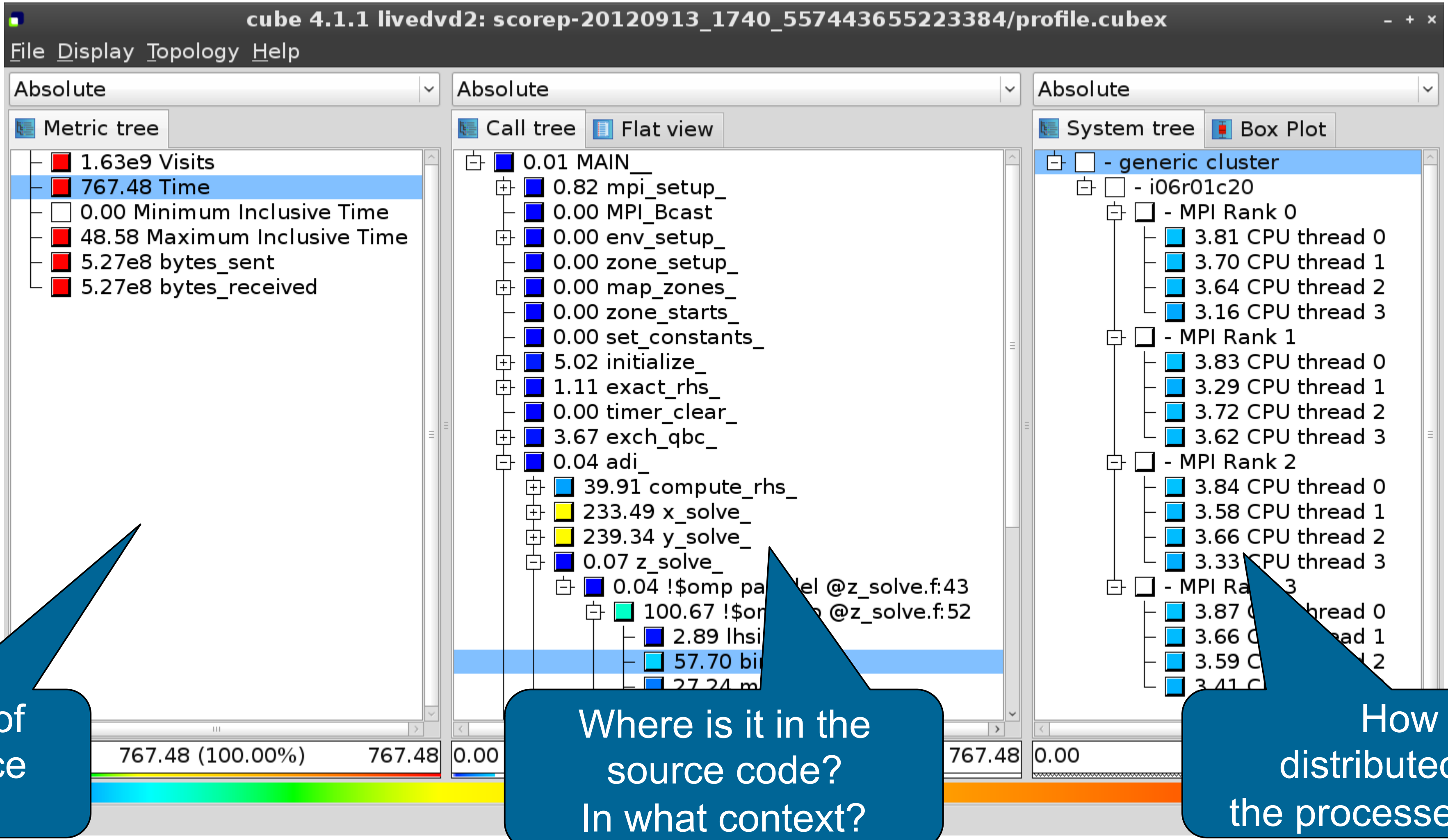
- Representation of values (severity matrix) on three hierarchical axes
  - Performance property (metric)
  - Call path (program location)
  - System location (process/thread)

- 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

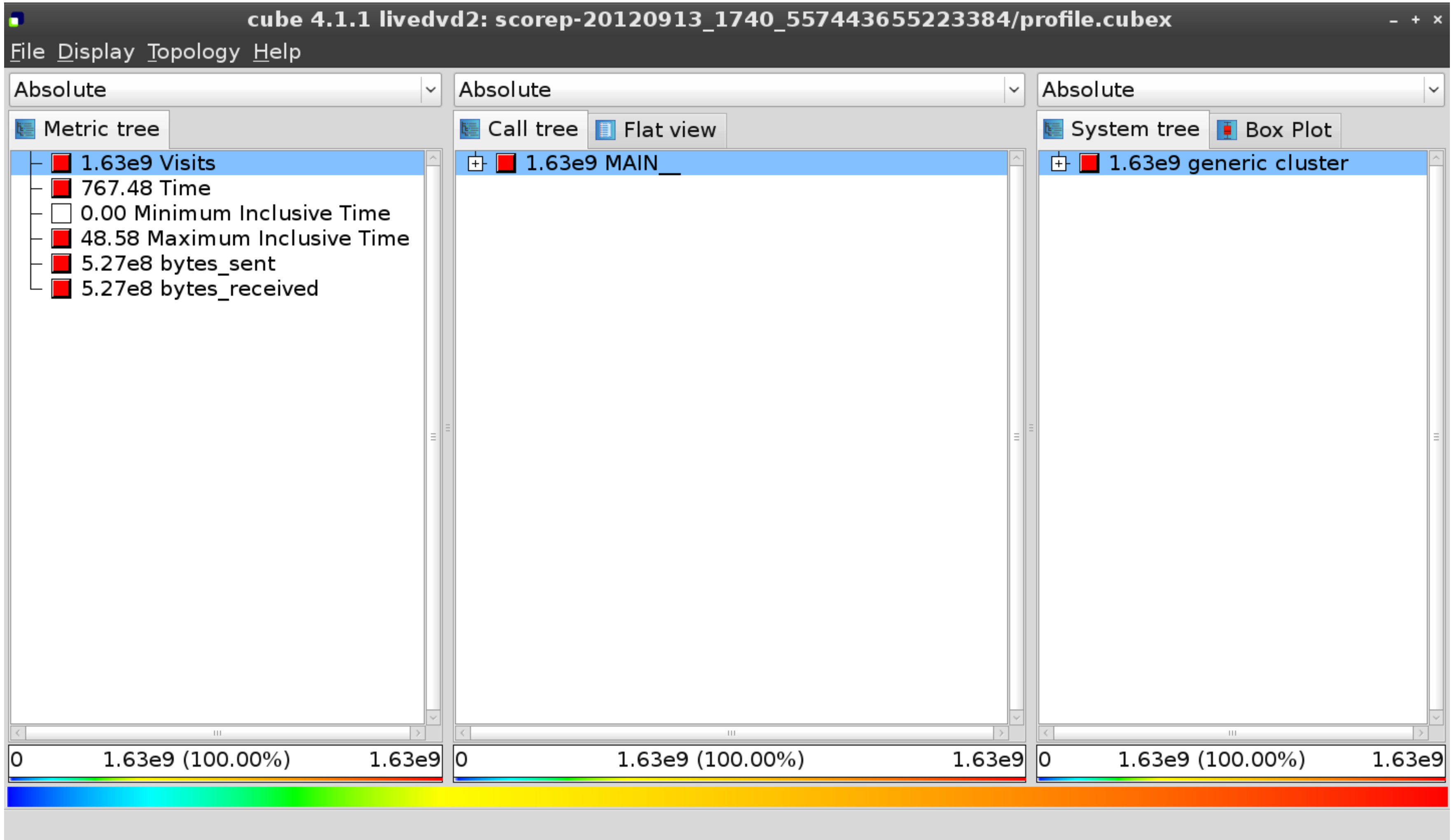


What kind of performance metric?

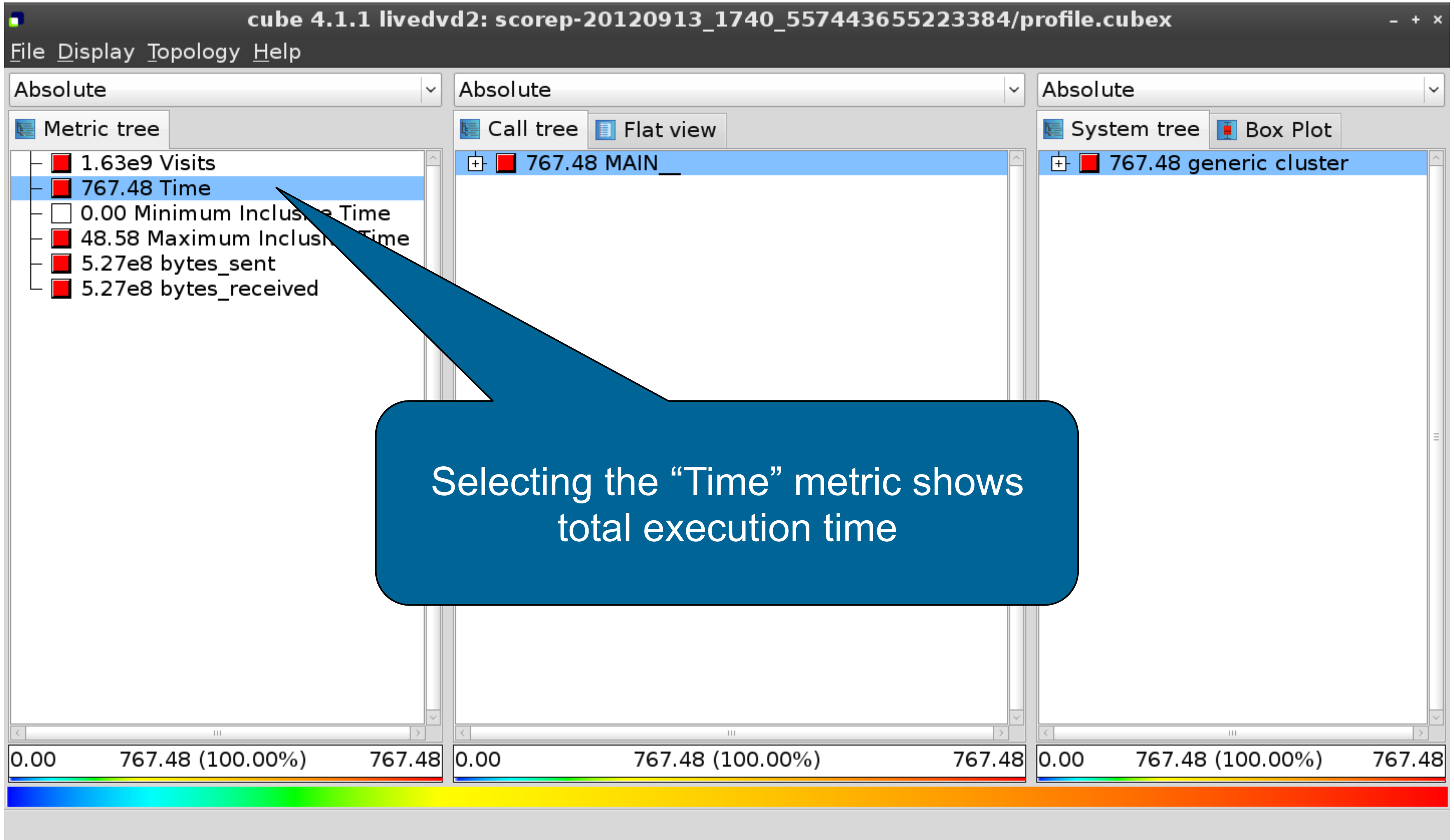
Where is it in the source code? In what context?

How is it distributed across the processes/threads?

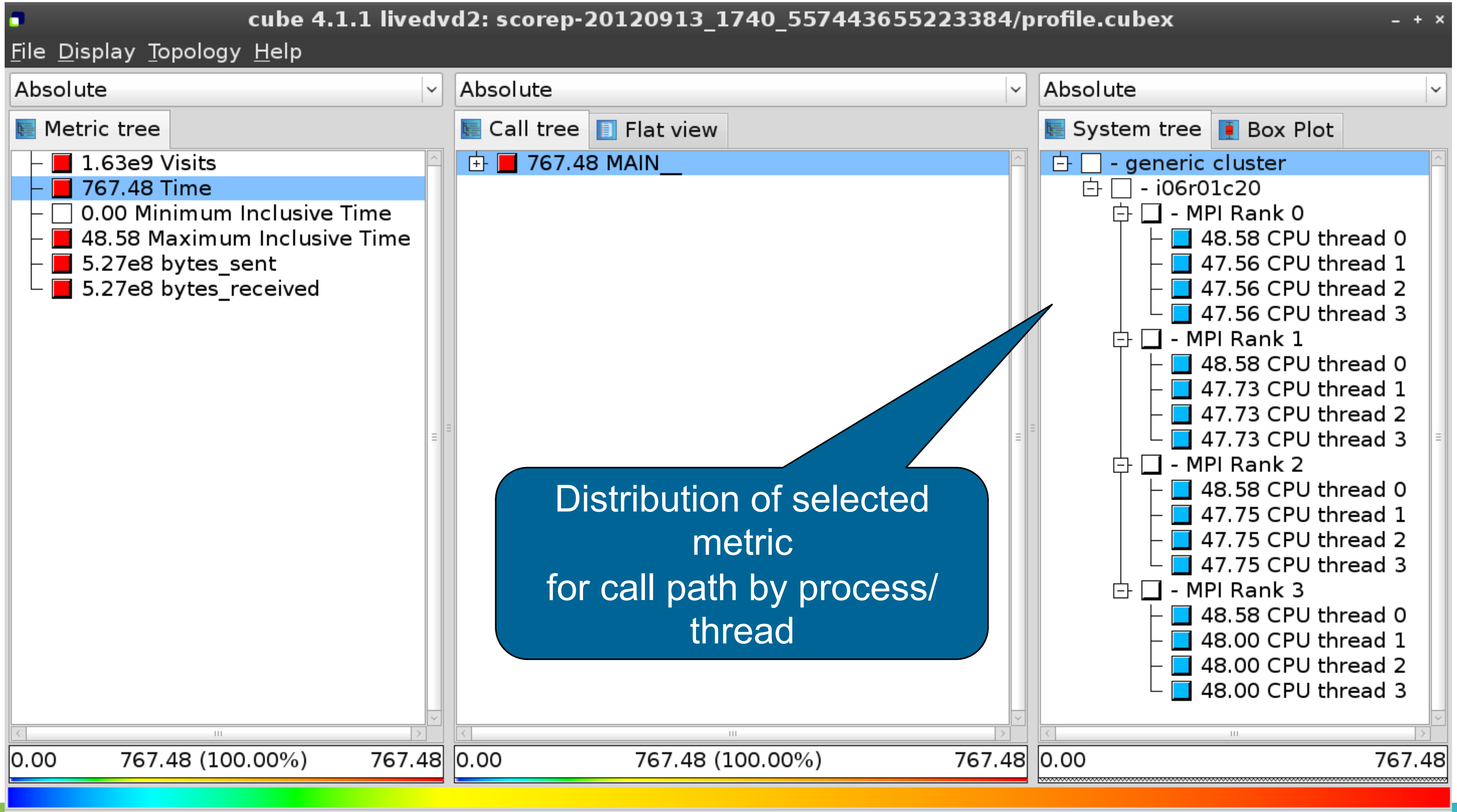
Analysis report exploration (opening view)



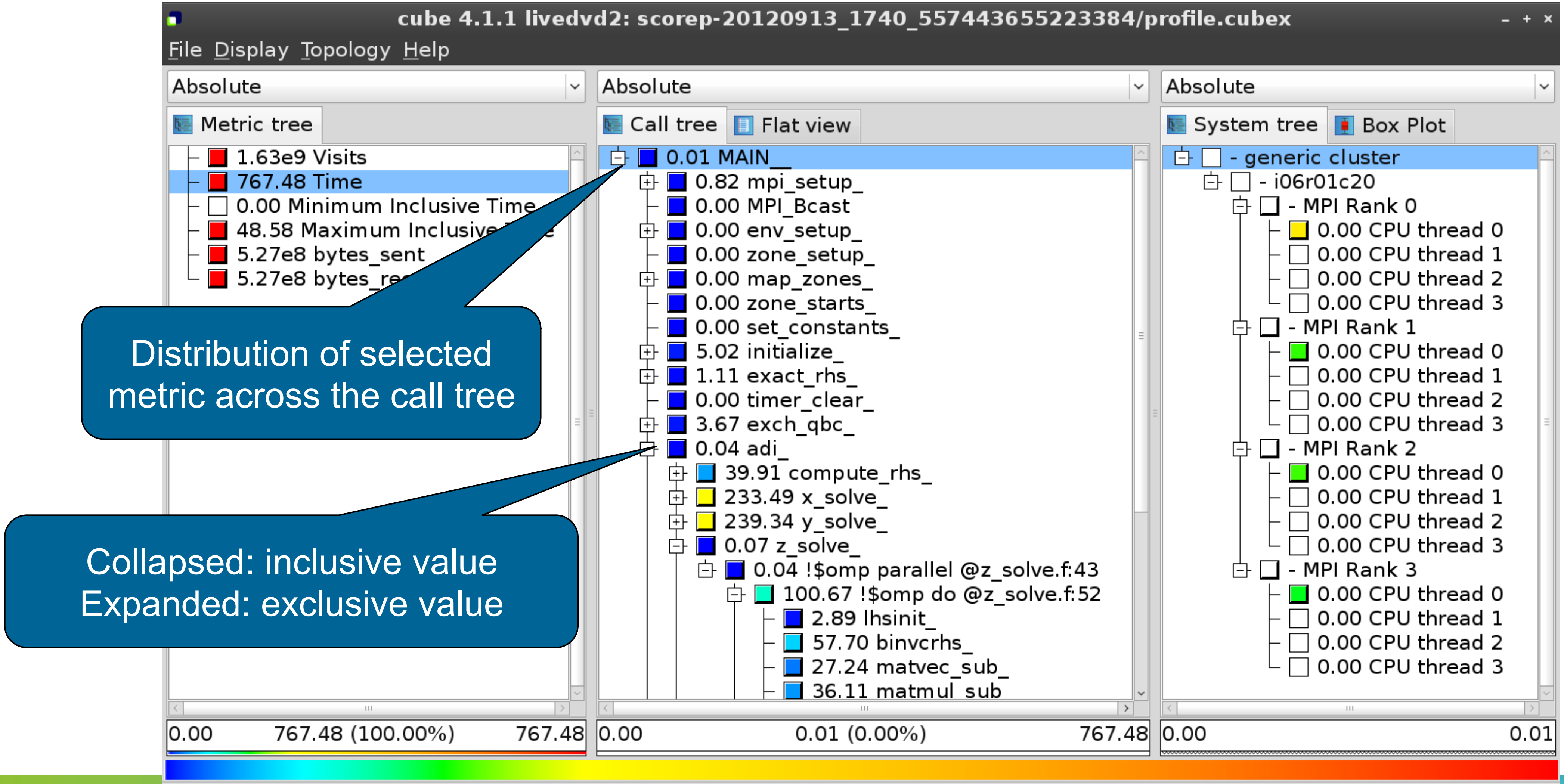
Metric selection



Expanding the system tree

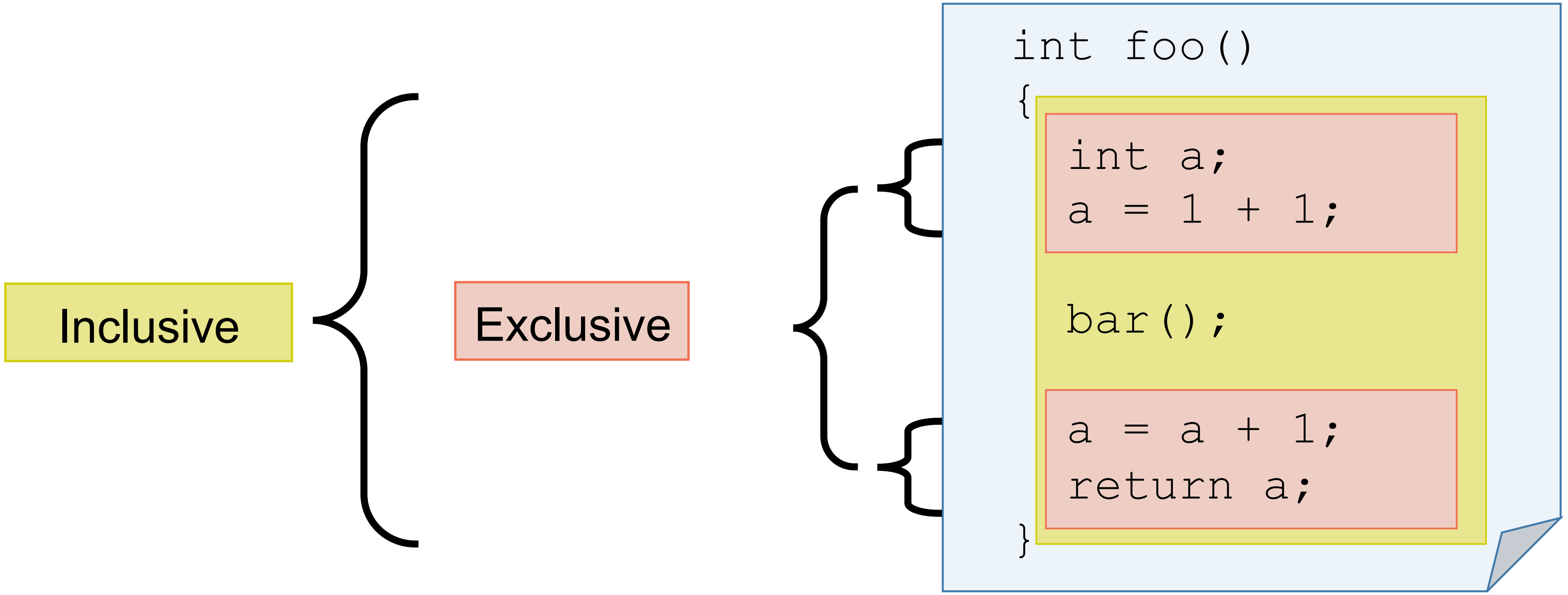


Expanding the call tree

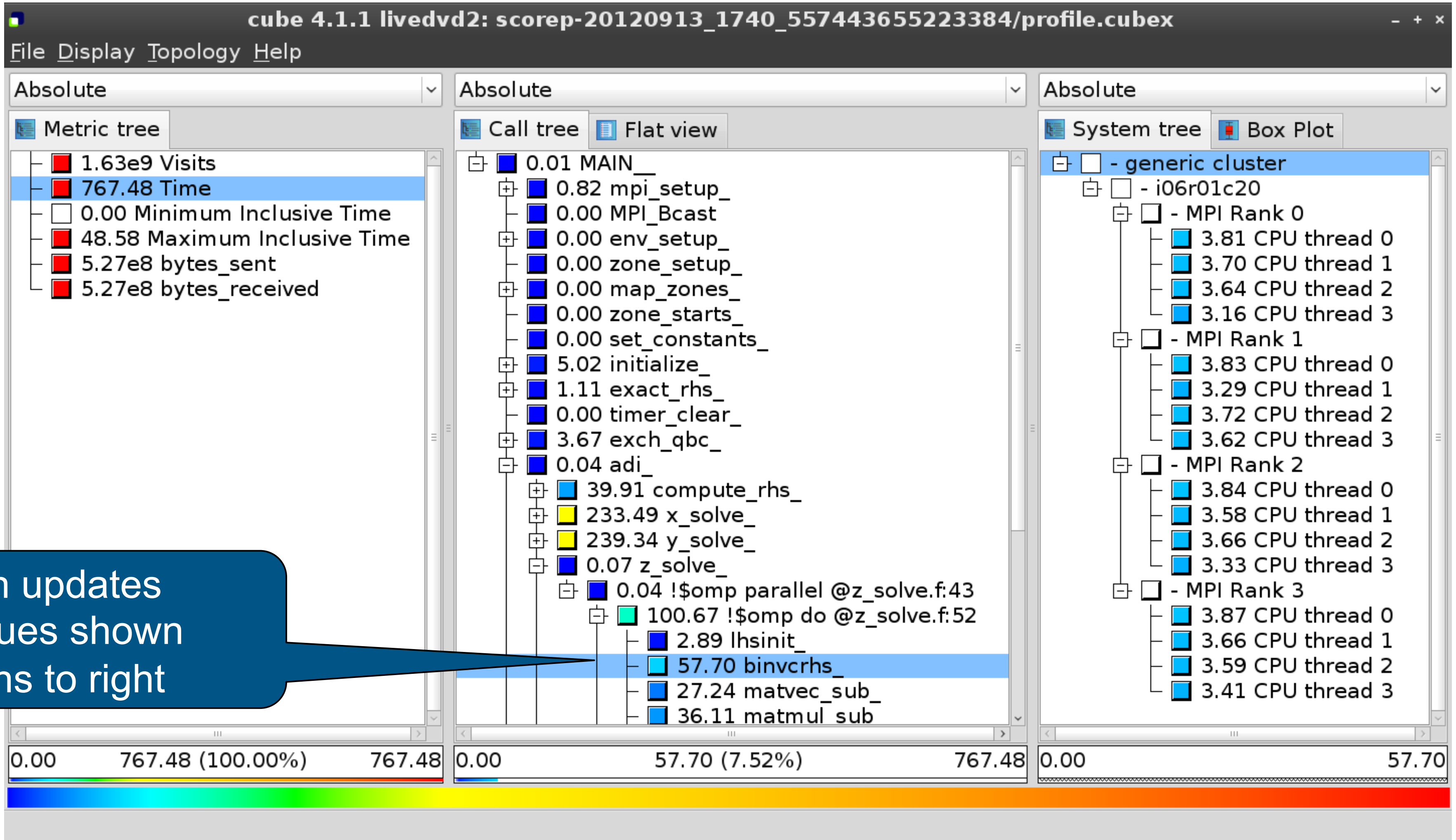


Inclusive vs. Exclusive values

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

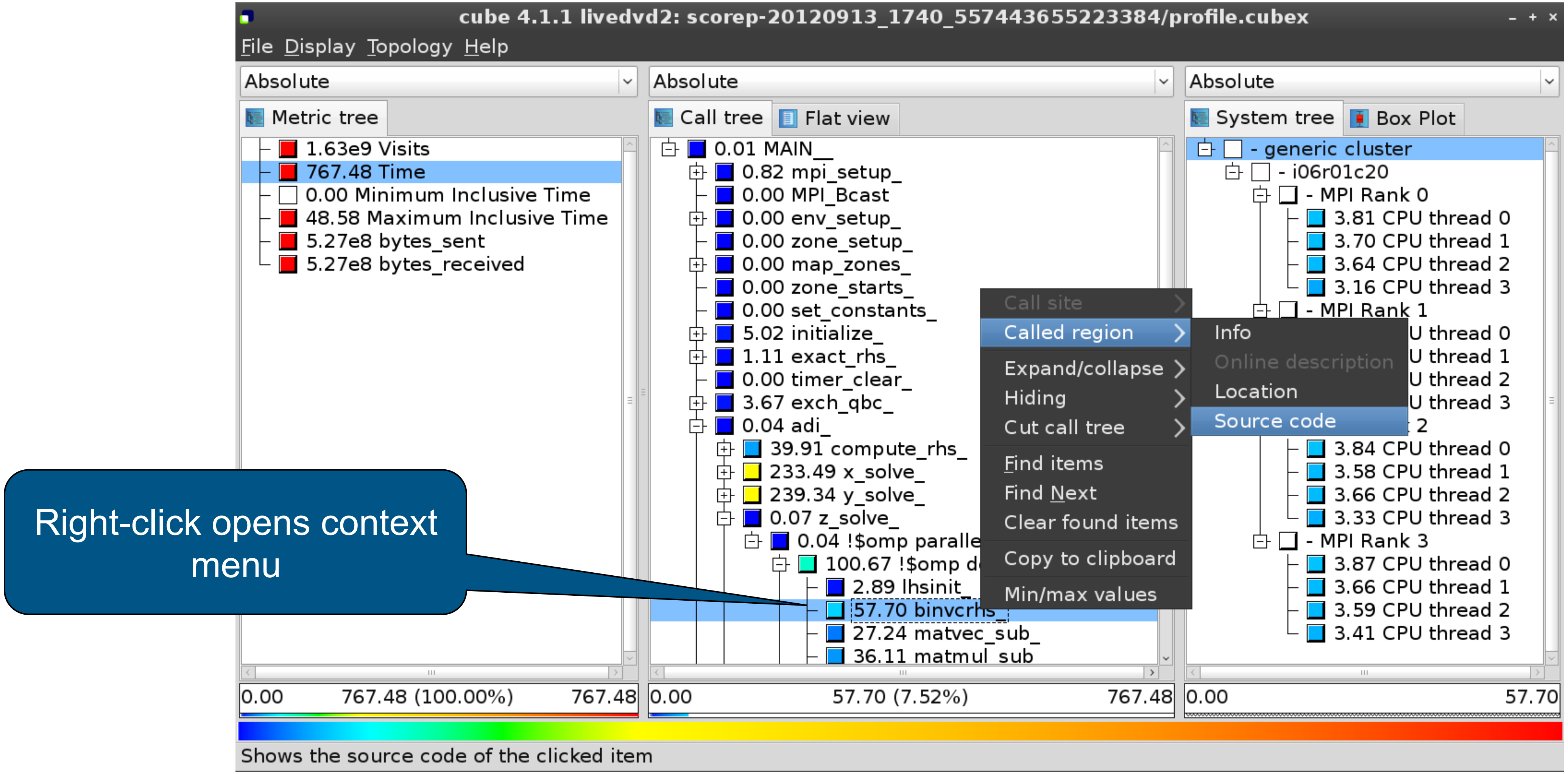


Selecting a call path



Selection updates metric values shown in columns to right

Source-code view via context menu



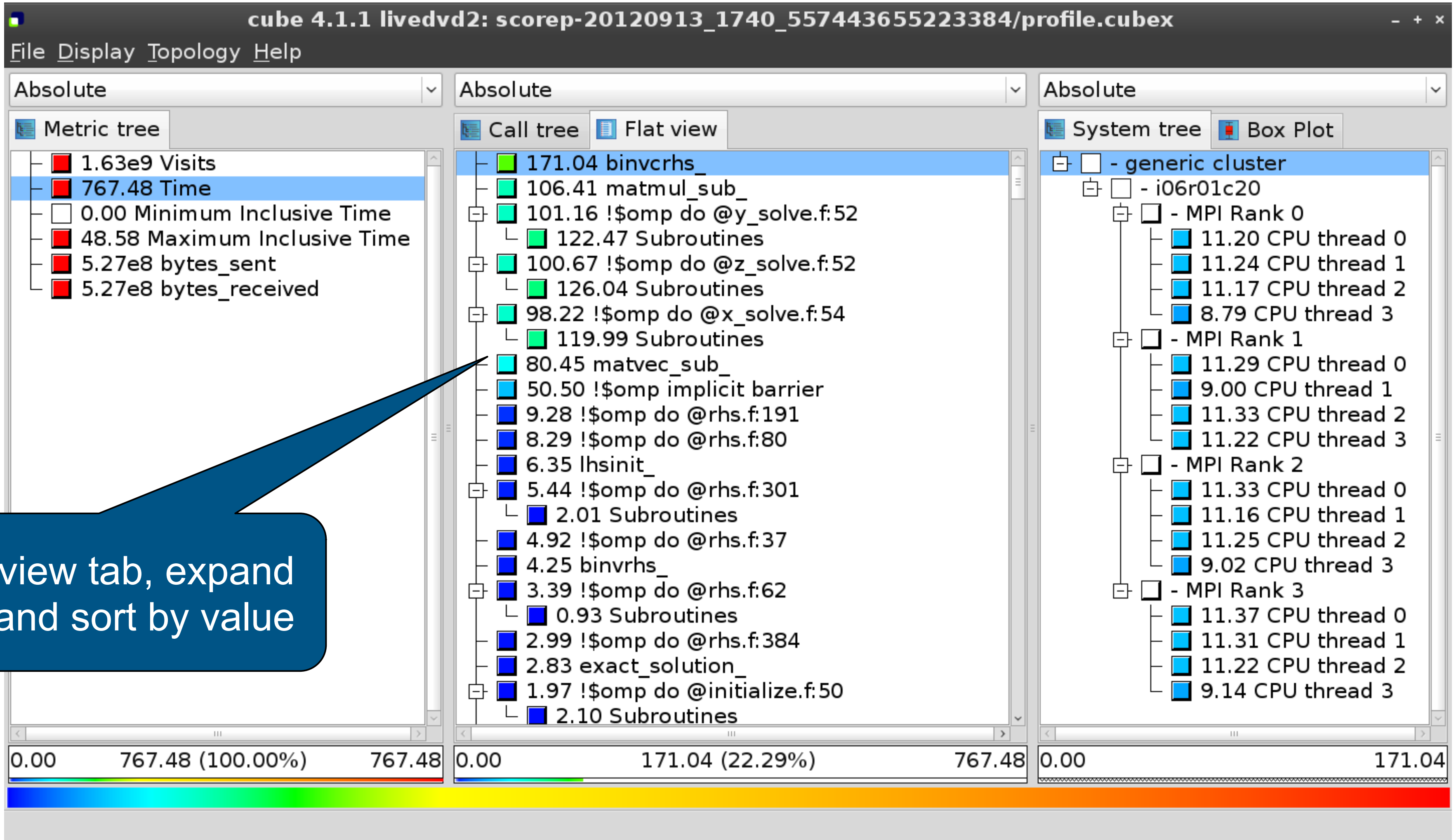
Source-code view

/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
```

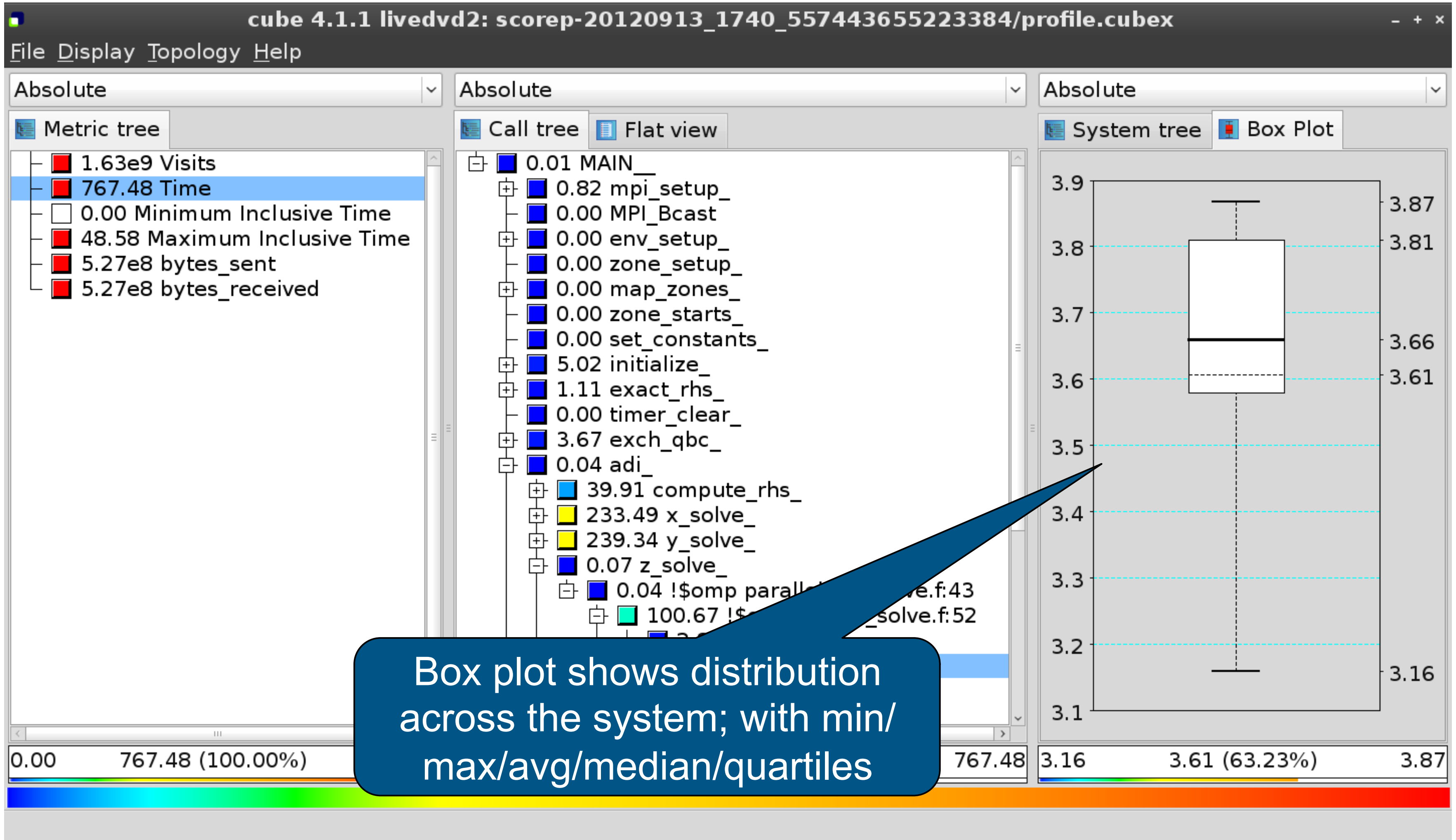
Read only | Save | Save as | Font... | Close

Flat profile view

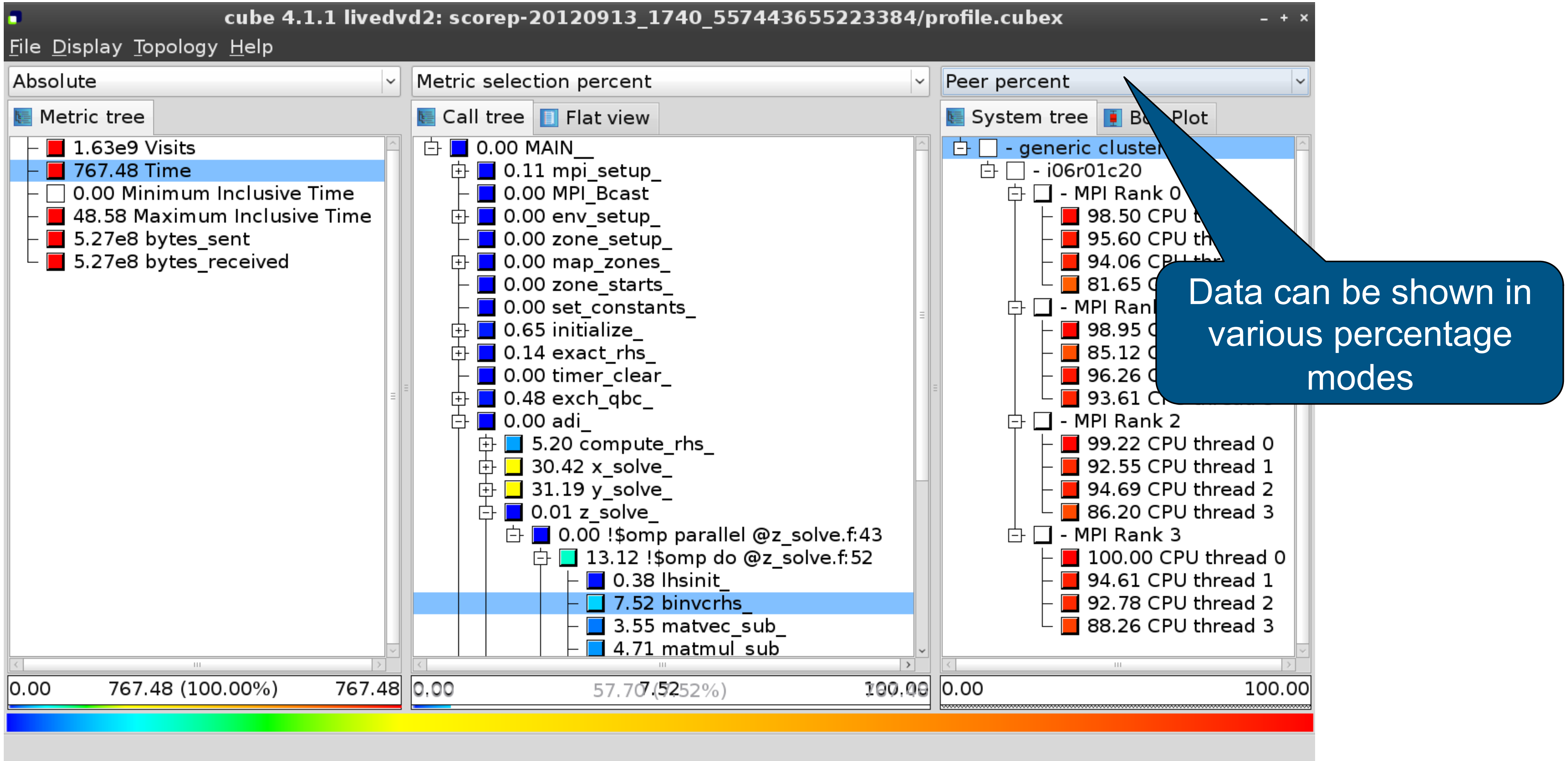


Select flat view tab, expand all nodes, and sort by value

Box plot view



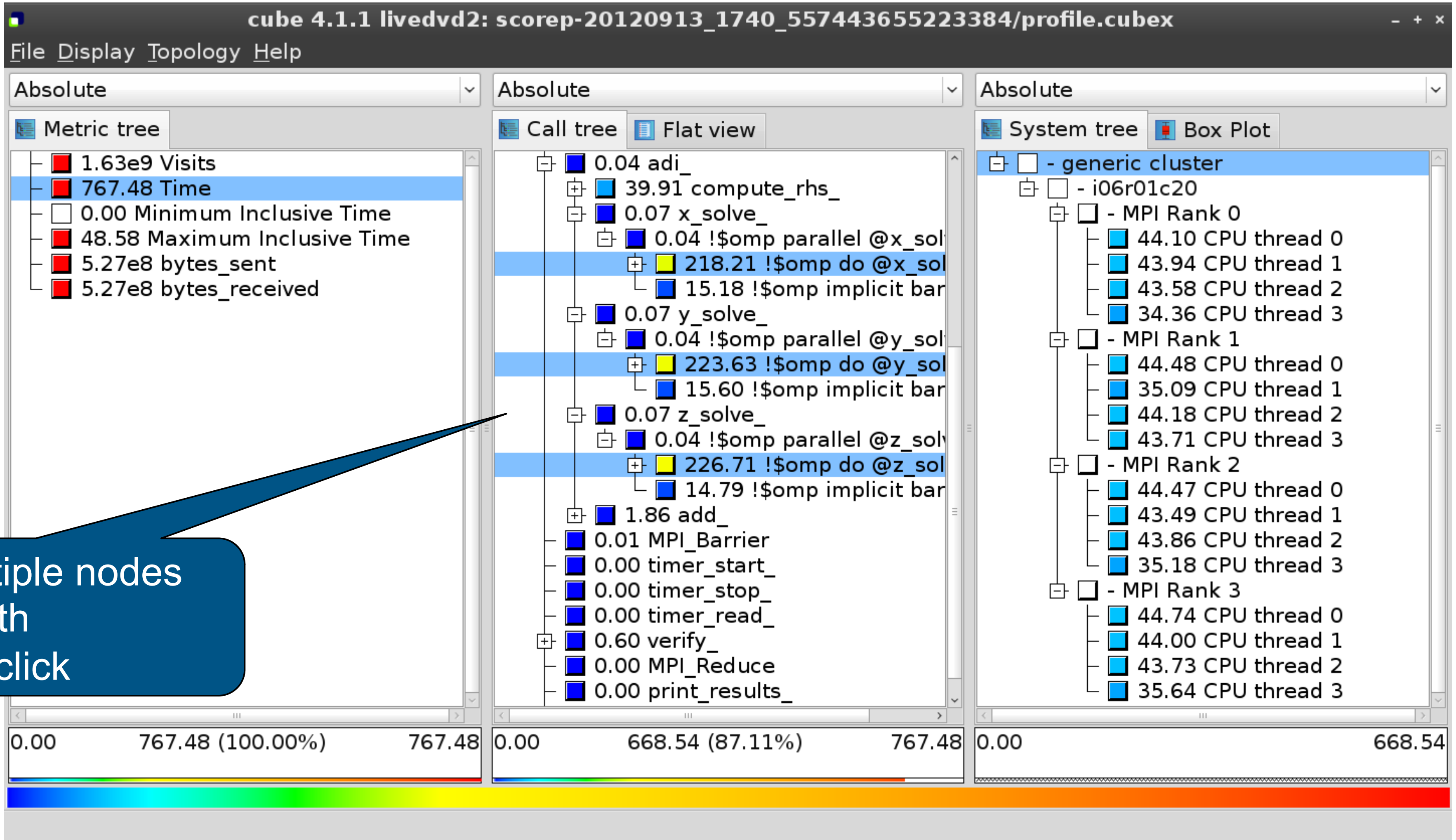
Alternative display modes



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



Select multiple nodes with Ctrl-click

Derived metrics in Cube

- Value of the derived metric is not stored, but **calculated** on-the-fly
- One defines an CubePL expression, e.g.:

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

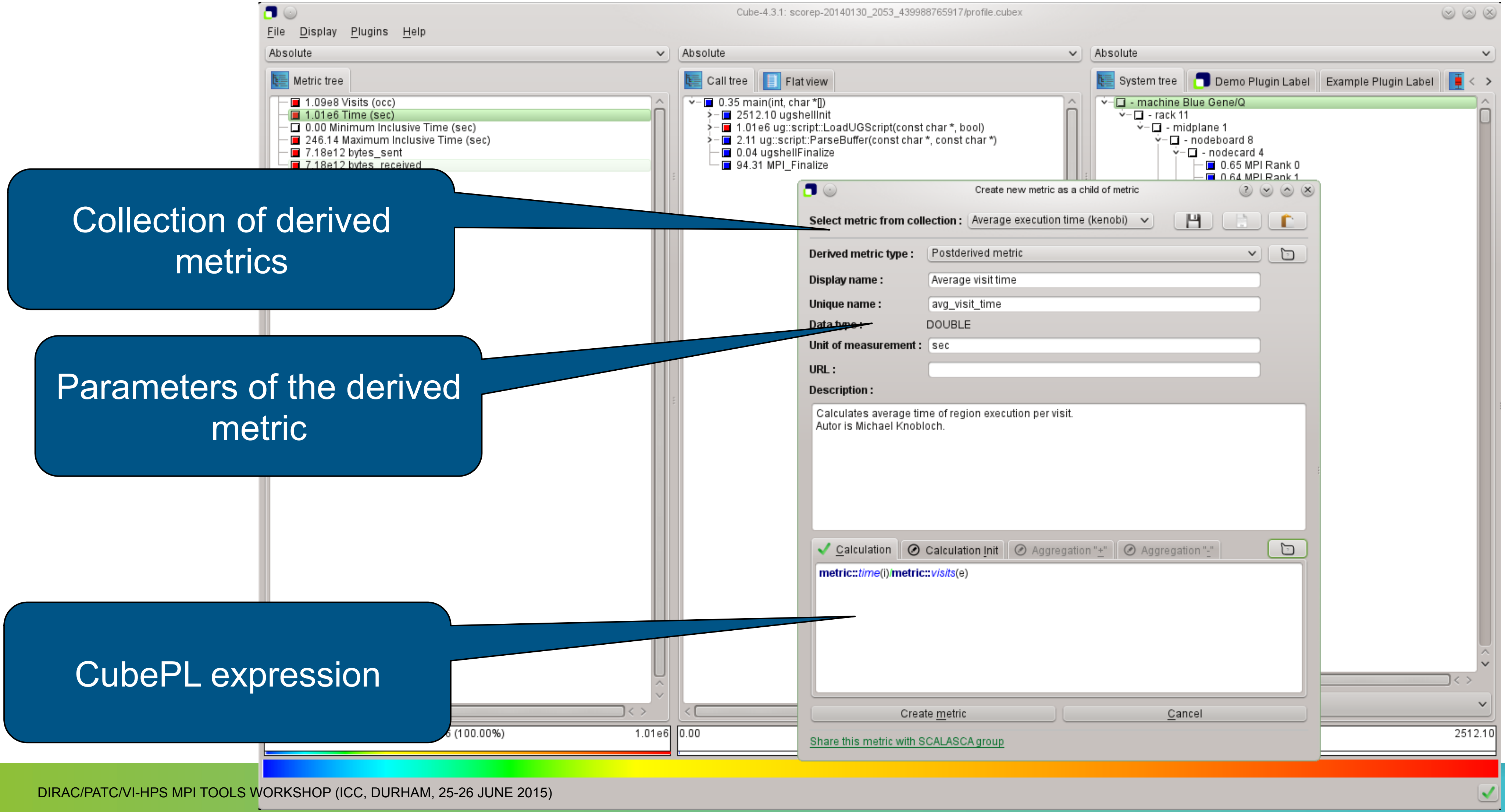
- Types of derived metrics:
  - **Prederived**: evaluation of the CubePL expression is done before the aggregation
  - **Postderived**: evaluation of the CubePL expression is performed after the aggregation

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

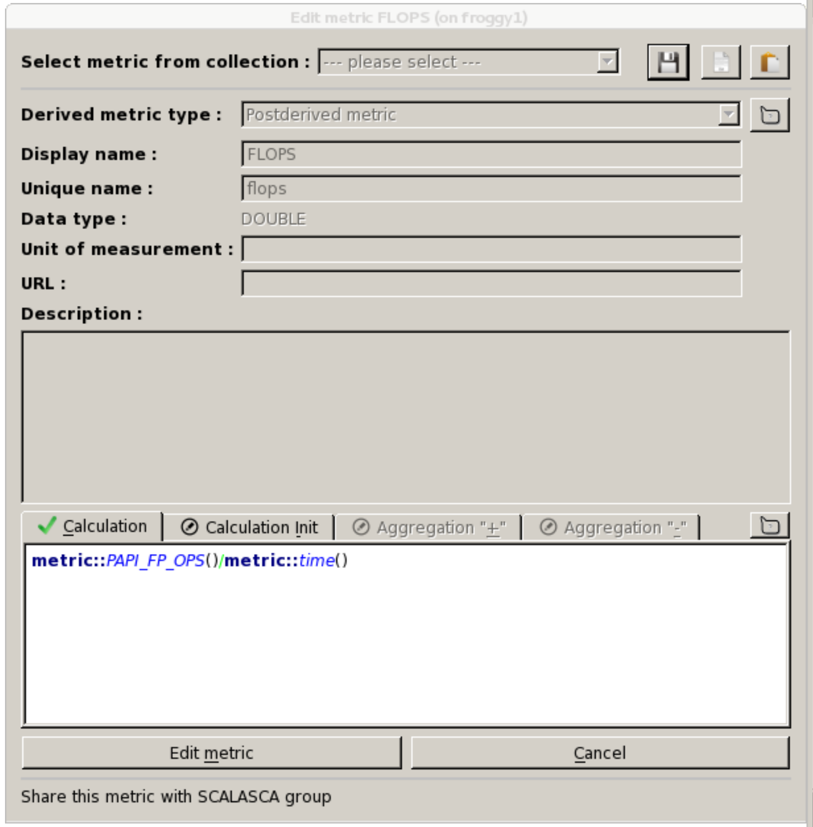
    metric::time(i)/metric::visits(e)
  - "Number of FLOP per second" Postderived metric with an expression:

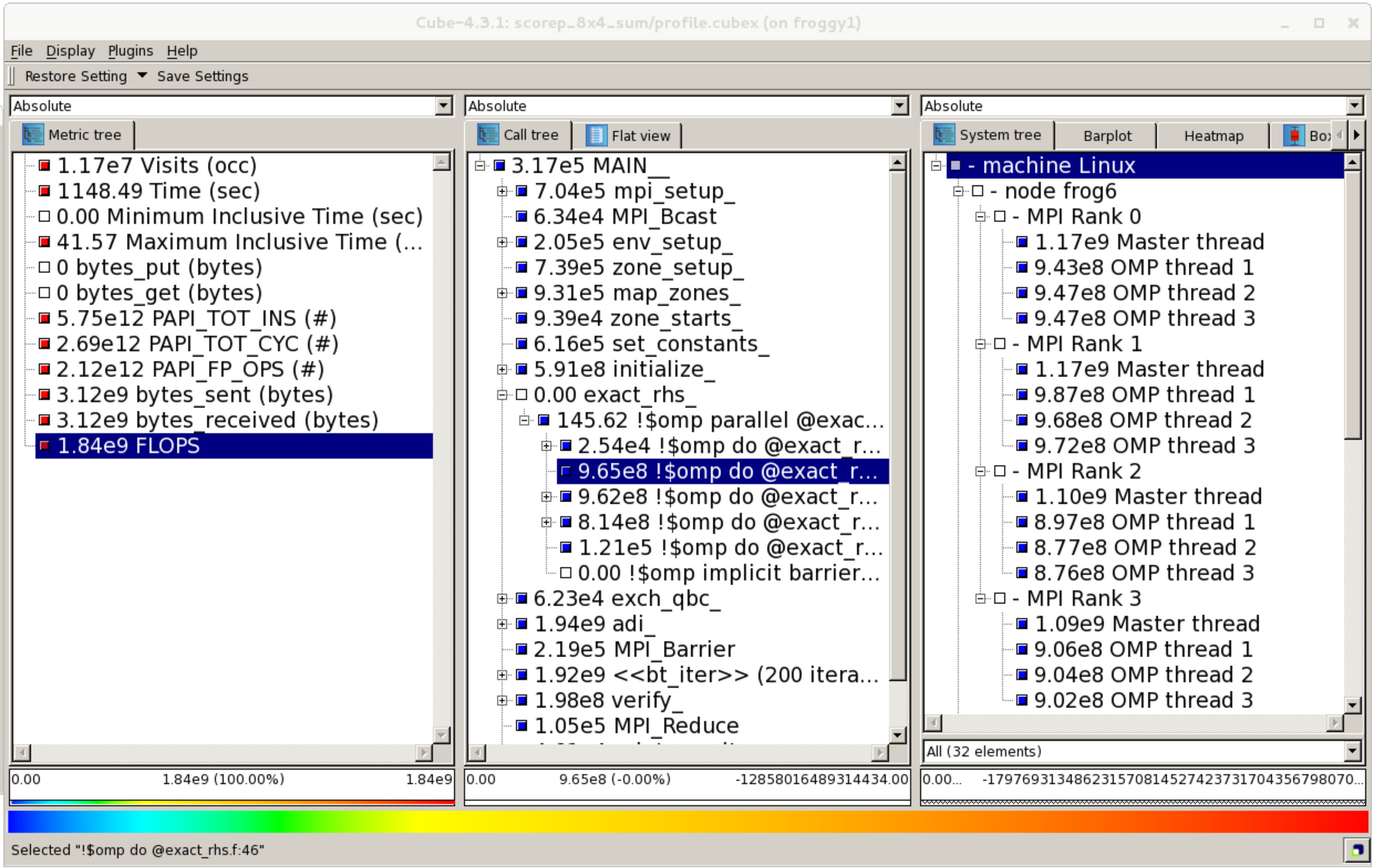
    metric::FLOP()/metric::time()

Derived metrics in Cube GUI

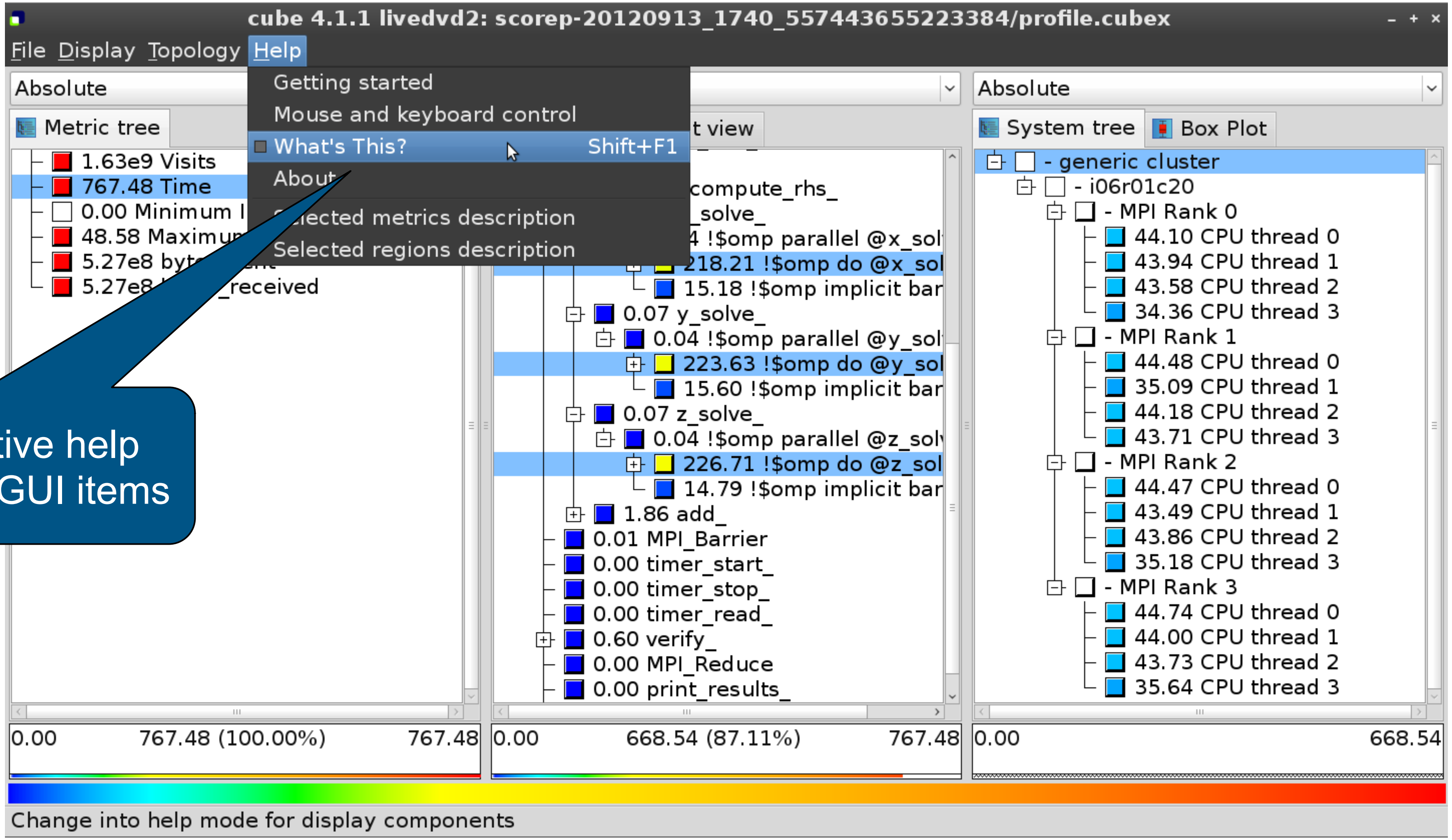


Example derived metric FLOPS based on PAPI_FP_OPS and time





Context-sensitive help



Context-sensitive help available for all GUI items

CUBE algebra utilities

- Extracting solver sub-tree from analysis report

```
% cube_cut  -r '<<ITERATION>>'  scorep_bt-mz_B_8x8_sum/profile.cubex
Writing cut.cubex... done.
```

- Calculating difference of two reports

```
% cube_diff  scorep_bt-mz_B_8x8_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

Loop Unrolling

- Show time dependent behavior by unrolling iterations

- Preparations:
  - Mark loops by using Score-P user instrumentation in your source code

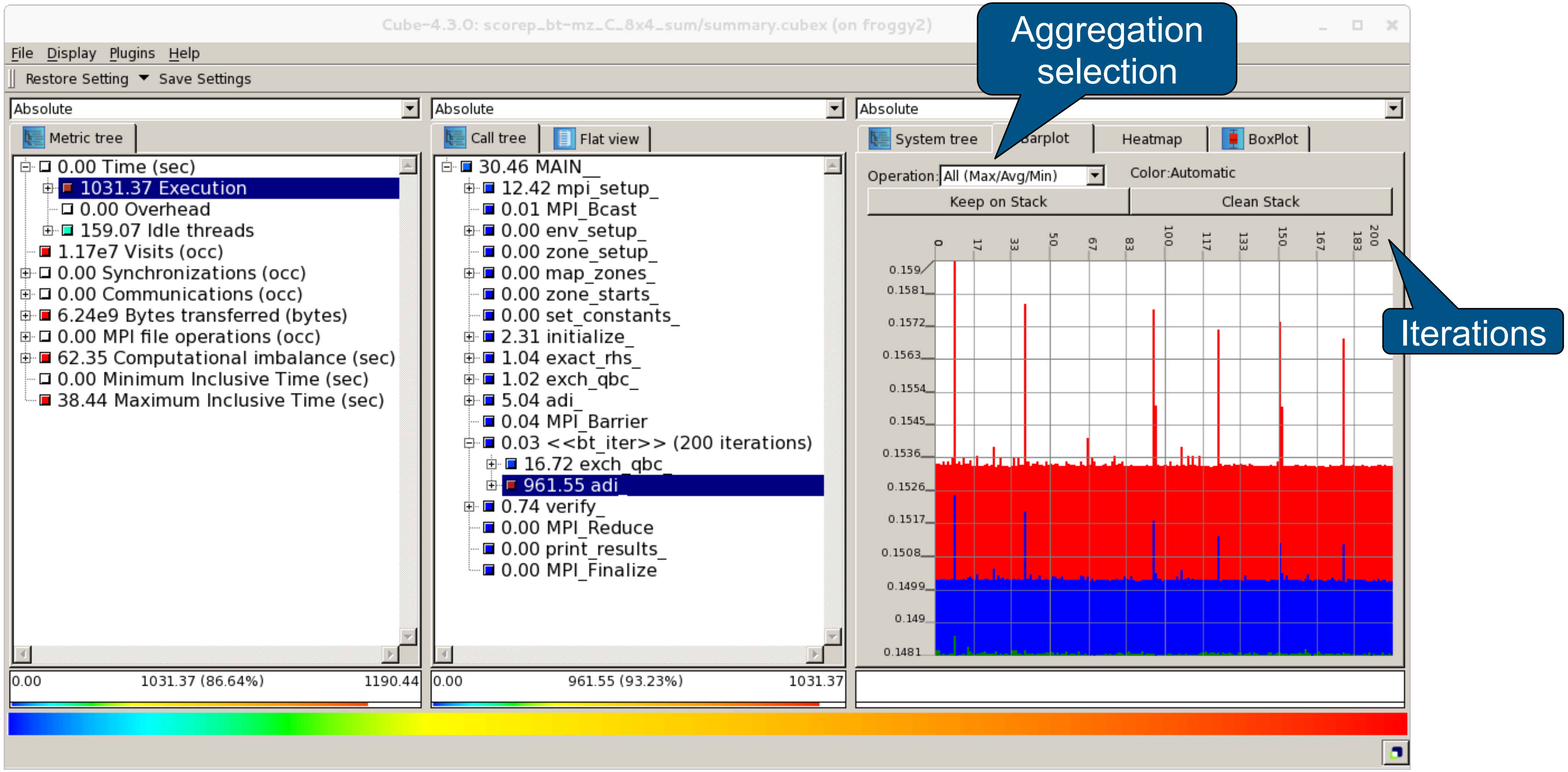
```
SCOREP_USER_REGION_BEGIN( scorep_bt_loop, "<<bt_iter>>", SCOREP_USER_REGION_TYPE_DYNAMIC )
```

- Result in the CUBE profile:
  - Iterations shown as separate call trees
  - ➢ Useful for checking results for specific iterations

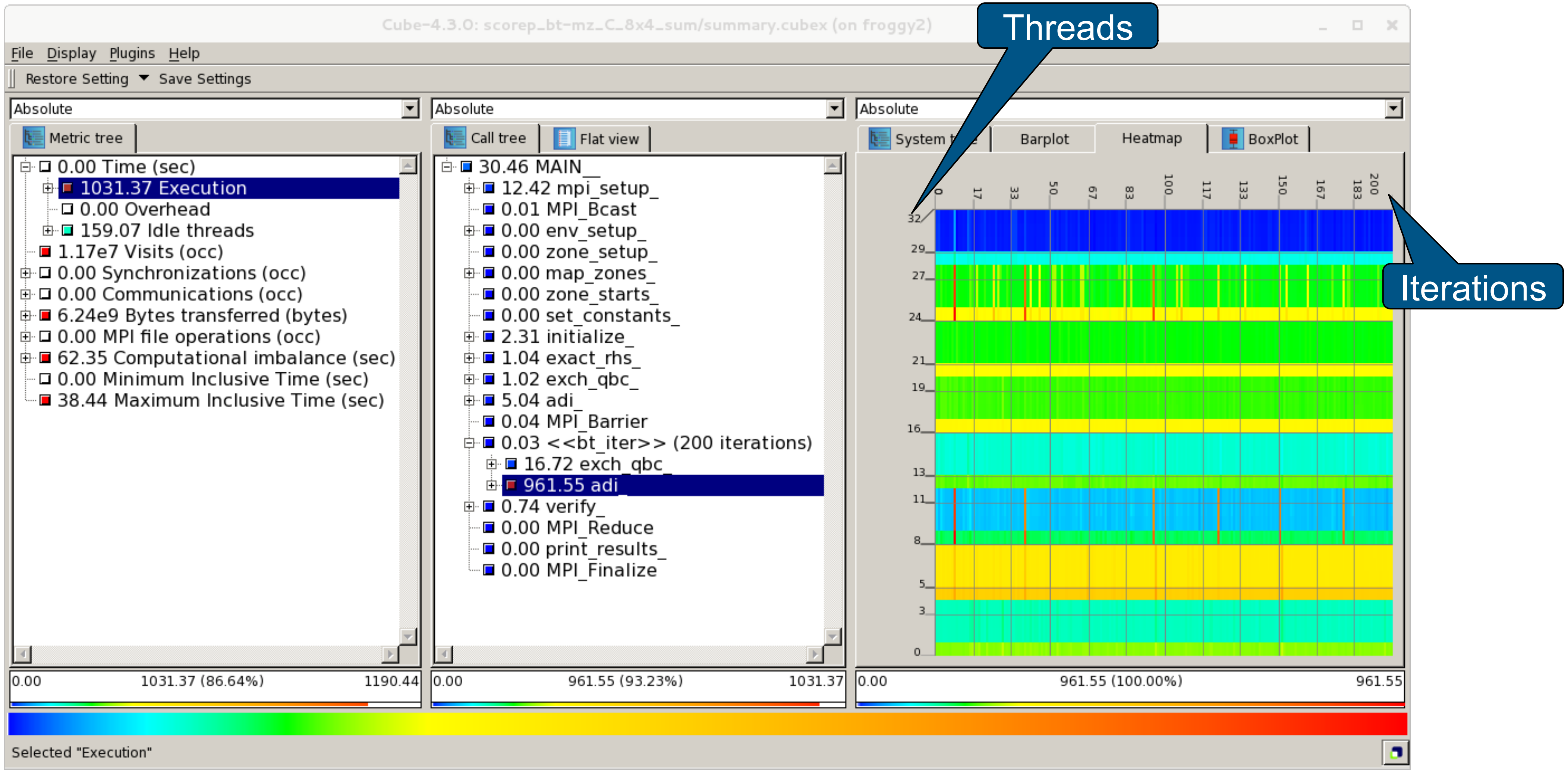
or

  - Select your user instrumented region and mark it as loop
  - Choose hide iterations
  - ➢ View the Barplot statistics or the (thread x iterations) Heatmap

Loop Unrolling - Barplot



Loop Unrolling – Heatmap



Further information

CUBE

- Parallel program analysis report exploration tools
  - Libraries for XML report reading & writing
  - Algebra utilities for report processing
  - GUI for interactive analysis exploration
- Available under New 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