

CubeLib 4.4 | Tools Guide

Description of Cube Command Line Tools

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Attention

The Cube Tool Developer Guide is currently being rewritten and still incomplete. However, it should already contain enough information to get you started and avoid the most common pitfalls.

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1 Cube Command Line Tools

1.1 Abstract

CUBE provides a set of various command line tools for different purposes.

1.2 Performance Algebra and Tools

As performance tuning of parallel applications usually involves multiple experiments to compare the effects of certain optimization strategies, CUBE offers a mechanism called *performance algebra* that can be used to merge, subtract, and average the data from different experiments and view the results in the form of a single “derived” experiment. Using the same representation for derived experiments and original experiments provides access to the derived behavior based on familiar metaphors and tools in addition to an arbitrary and easy composition of operations. The algebra is an ideal tool to verify and locate performance improvements and degradations likewise. The algebra includes three operators—*diff*, *merge*, and *mean*—provided as command-line utilities which take two or more CUBE files as input and generate another CUBE file as output. The operations are closed in the sense that the operators can be applied to the results of previous operations. Note that although all operators are defined for any valid CUBE data sets, not all possible operations make actually sense. For example, whereas it can be very helpful to compare two versions of the same code, computing the difference between entirely different programs is unlikely to yield any useful results.

1.2.1 Difference

Changing a program can alter its performance behavior. Altering the performance behavior means that different results are achieved for different metrics. Some might increase while others might decrease. Some might rise in certain parts of the program only, while they drop off in other parts. Finding the reason for a gain or loss in overall performance often requires considering the performance change as a multidimensional structure. With CUBE's difference operator, a user can view this structure by computing the difference between two experiments and rendering the derived result experiment like an original one. The difference operator takes two experiments and computes a derived experiment whose severity function reflects the difference between the minuend's severity and the subtrahend's severity.

The possible output is presented below.

```
user@host: cube_diff scout.cube remapped.cube -o result.cube
```

```
Reading scout.cube ... done.
Reading remapped.cube ... done.
+++++++ Diff operation begins ++++++
INFO::Merging metric dimension... done.
INFO::Merging program dimension... done.
INFO::Merging system dimension... done.
INFO::Mapping severities... done.
INFO::Adding topologies...
      Topology retained in experiment.
done.
INFO::Diff operation... done.
+++++++ Diff operation ends successfully ++++++
Writing result.cube ... done.
```

Usage: cube_diff [-o output] [-c] [-C] [-h] minuend subtrahend

- o** Name of the output file (default: diff.cube)
- c** Do not collapse system dimension, if experiments are incompatible
- C** Collapse system dimension
- h** Help; Output a brief help message.

1.2.2 Merge

The merge operator's purpose is the integration of performance data from different sources. Often a certain combination of performance metrics cannot be measured during a single run. For example, certain combinations of hardware events cannot be counted simultaneously due to hardware resource limits. Or the combination of performance metrics requires using different monitoring tools that cannot be deployed during the same run. The merge operator takes an arbitrary number of CUBE experiments with a different or overlapping set of metrics and yields a derived CUBE experiment with a joint set of metrics.

The possible output is presented below.

```
user@host: cube_merge scout.cube remapped.cube -o result.cube
+++++++ Merge operation begins ++++++
Reading scout.cube ... done.
Reading remapped.cube ... done.
INFO::Merging metric dimension... done.
INFO::Merging program dimension... done.
INFO::Merging system dimension... done.
INFO::Mapping severities... done.
INFO::Merge operation...
      Topology retained in experiment.

      Topology retained in experiment.
done.
+++++++ Merge operation ends successfully ++++++
Writing result.cube ... done.
```

Usage: cube_merge [-o output] [-c] [-C] [-h] cube ...

- o** Name of the output file (default: merge.cube)
- c** Do not collapse system dimension, if experiments are incompatible
- C** Collapse system dimension
- h** Help; Output a brief help message.

1.2.3 Mean

The mean operator is intended to smooth the effects of random errors introduced by unrelated system activity during an experiment or to summarize across a range of execution parameters. You can conduct several experiments and create a single average experiment from the whole series. The mean operator takes an arbitrary number of arguments.

The possible output is presented below.

```
user@host: cube_mean scout1.cube scout2.cube scout3.cube scout4.cube -o mean.cube
+++++++ Mean operation begins ++++++
Reading scout1.cube ... done.
INFO::Merging metric dimension... done.
INFO::Merging program dimension... done.
INFO::Merging system dimension... done.
INFO::Mapping severities... done.
INFO::Adding topologies... done.
INFO::Mean operation... done.
Reading scout2.cube ... done.
INFO::Merging metric dimension... done.
INFO::Merging program dimension... done.
INFO::Merging system dimension... done.
INFO::Mapping severities... done.
INFO::Adding topologies... done.
INFO::Mean operation... done.
Reading scout3.cube ... done.
INFO::Merging metric dimension... done.
INFO::Merging program dimension... done.
INFO::Merging system dimension... done.
INFO::Mapping severities... done.
INFO::Adding topologies... done.
INFO::Mean operation... done.
Reading scout4.cube ... done.
INFO::Merging metric dimension... done.
INFO::Merging program dimension... done.
INFO::Merging system dimension... done.
INFO::Mapping severities... done.
INFO::Adding topologies... done.
INFO::Mean operation... done.
+++++++ Mean operation ends successfully ++++++
Writing mean.cube ... done.
```

Usage: cube_mean [-o output] [-c] [-C] [-h] cube ...

- o Name of the output file (default: mean.cube)
- c Do not collapse system dimension, if experiments are incompatible
- C Collapse system dimension
- h Help; Output a brief help message.

1.2.4 Compare

Compares two experiments and prints out if they are equal or not. Two experiments are equal if they have same dimensions hierarchy and the equal values of the severities.

An example of the output is below.

```
user@host: cube_cmp remapped.cube scout1.cube
Reading remapped.cube ... done.
Reading scout1.cube ... done.
+++++ Compare operation begins +++++
Experiments are not equal.
+++++ Compare operation ends successfully +++++
```

Usage: cube_cmp [-h] cube1 cube2

- h Help; Output a brief help message.

1.3 Cube Remapping tool

CUBE provides an universal flexible tool, which allows to transform metric tree of an input .cubex into an arbitrary metric hierarchy according to user defined flexible rules. This can be used by performance analysis tools, such as Score-P or Scalasca. In particularly one classifies different call paths according to some user defined rules.

As well one can use this tool to convert derived metrics into the data (if possible) or to add an additional metric into the current .cubex file.

1.3.1 Tool Usage

Usage: ./cube_remap2 -r <remap specification file> [-o output] [-d] [-s] [-h] <cube experiment>

- r Name of the remapping specification file. By omitting this option the specification file from the cube experiment is taken if present.
- c Create output file with the same structure as an input file. It overrides option "-r"
- o Name of the output file (default: remap)
- d Convert all prederived metrics into usual metrics, calculate and store their values as a data.
- s Add hardcoded SCALASCA metrics "Idle threads" and "Limited parallelizm"

-h Help; Output a brief help message.

1.3.2 Remapping algorithm

The main idea behind the working way of the remapping tool is simple: user formulates the target hierarchy of the metrics in an external file (.spec) and defines rules how they are calculated using CubePL syntax. Remapping tool creates then an output cube with this metric hierarchy.

In particularly remapping tool performs following steps:

1. Is command-line option `-c` specified, remapping tool works in "Copy" mode: it creates output cube with identical metrics hierarchy. One combines it usual with the options `-d` and `-s`. Otherwise...
2. Is command-line option `-r` omit, remapping tool looks for the .spec file within the input .cubex file. Score-P starting with version v5 stores its .spec file within *profile.cubex*. Otherwise...
3. Is command-line option `-r` specified, remapping tool looks for .spec file and creates the new (working) cube object with the metric hierarchy as metric dimension specified in .spec file
4. Then it merges metric hierarchy of the input file into the current metric hierarchy. All metrics from the input file which present in .spec hierarchy gets mapped to them. All missing metrics will be added as additional metrics.
5. Is the command-line option `-s` specified, tool adds additional SCALASCA metrics "Idle threads" and "Limited parallelism"
6. Other dimensions and elements of the input .cubex file (topologies, mirrors and similar) get merged into the new cube object one-to-one (as the freshly created cube object doesn't have any)
7. If the command-line option `-d` is omit, remapping tool saves created cube on disk as it is. All derived metrics in .spec file will stay as derived metrics and will be executed only while working with the stored .cubex file in GUI or with command-line tools.
8. Did user specified command-line option `-d`, the second phase of the remapping is executed: calculation of derived metrics and converting them into the data. Note, that not all metrics are *convertible* (such as rates or similar) into data and should stay derived in the target file. To do so remapping tool creates an additional cube object with the identical structure (only convertible derived metrics are turned into the regular data metrics) of the intermediate working cube and copies metric-by-metric its data. As result, derived metrics are calculated and their value is stored as a data into the target cube.
9. Resulting cube object is saved on disk.

As one can see user can use remapping tool for different purposes:

1. Convert derived metrics of the current .cubex file into the data metrics. For that it is enough to execute remapping tool as:

```
./cube_remap2 -d <input>
```

2. Add an additional derived metric into the current .cubex cube
3. Create a new .cubex with the user specified metrics hierarchy. (standard usage)

1.3.3 Syntax of a .spec file

Examples for .spec files are shipped with the CUBE package and stored in the directory [prefix]/share/doc/cubelib/examples

Here we provide some commented examples of .spec files.

1. In first case we add an additional metric IPC into the cube file

```
1 <metrics>
2   <metric type="POSTDERIVED" convertible="false">
3     <disp_name>IPC, ipc</disp_name>
4     <uniq_name>ipc</uniq_name>
5     <dtype>FLOAT</dtype>
6     <uom></uom>
7     <descr>Value of IPC (instructions per cycle),
8           computed as PAPI_TOT_INS() / PAPI_TOT_CYC()
9     </descr>
10    <cubepl>
11      metric::PAPI_TOT_INS() / metric::PAPI_TOT_CYC()
12    </cubepl>
13  </metric>
14 </metrics>
```

Here the whole hierarchy consist of only one metric IPC, which is "non convertible" into data as it is a POSTDERIVED metric and usual aggregation rules are not applicable. This metric has a data type FLOAT and requires, that input file contains metrics PAPI_TOT_CYC and PAPI_TOT_INS. Otherwise this metric will be always evaluated to 0.

2. In second case we add two sub metrics to the metric "Time", in order to classify time spend in "MPI" regions and "Other"

```
1 <metrics>
2   <metric>
3     <!-- This metric is copied from the trace analysis -->
4     <disp_name>Time</disp_name>
5     <uniq_name>time</uniq_name>
6     <dtype>FLOAT</dtype>
7     <uom>sec</uom>
8     <url>@mirror@scalasca-patterns-2.1.html#time</url>
9     <descr>Total CPU allocation time
10           (includes time allocated for idle threads)
11   </descr>
12   <metric type="PREDERIVED_EXCLUSIVE">
13     <disp_name>MPI regions</disp_name>
14     <uniq_name>mpiregions</uniq_name>
15     <dtype>FLOAT</dtype>
16     <uom>sec</uom>
17     <url></url>
18     <descr>Time spend in MPI regions </descr>
19     <cubepl>
20       {
21         ${a}=0;
22         if (${cube::region::name}[${calculation::region::id}] =~ /^MPI_/)
23         {
24           ${a}=metric::time();
25         };
26         return ${a};
27       }
28     </cubepl>
29   </metric>
```

```

30     <metric type="PREDERIVED_EXCLUSIVE">
31       <disp_name>Other regions</disp_name>
32       <uniq_name>nonmpi</uniq_name>
33       <dtype>FLOAT</dtype>
34       <uom>sec</uom>
35       <url></url>
36       <descr>Time spend in non-MPI regions</descr>
37       <cubepl>
38         {
39           ${a}=0;
40           if (not(${cube::region::name}[${calculation::region::id}] =~ /^MPI_/))
41             {
42               ${a}=metric::time();
43             };
44           return ${a};
45         }
46       </cubepl>
47     </metric>
48   </metrics>
49 </metrics>

```

Here target hierarchy consist of the top metric "Time" and two sub metrics "MPI regions" and "Other regions". Clearly that they both will sum up to the total "Time" metric. Hence one expects that expanded metric "Time" will be always zero. Note that sub metrics are defined as PREDERIVED_EXCLUSIVE as their value is valid only for the one call path and not their children.

3. In third case we would like to split the time metric into two metrics and to hide the metric itself. For that we declare it as "GHOST" metric and declare sub metrics as root metrics.

```

1 <metrics>
2   <metric viztype="GHOST">
3     <!-- This metric is copied from the trace analysis -->
4     <disp_name>Time</disp_name>
5     <uniq_name>time</uniq_name>
6     <dtype>FLOAT</dtype>
7     <uom>sec</uom>
8     <url>@mirror@scalasca-patterns-2.1.html#time</url>
9     <descr>Total CPU allocation time
10      (includes time allocated for idle threads)
11   </descr>
12 </metric>
13   <metric type="PREDERIVED_EXCLUSIVE">
14     <disp_name>MPI regions</disp_name>
15     <uniq_name>mpiregions</uniq_name>
16     <dtype>FLOAT</dtype>
17     <uom>sec</uom>
18     <url></url>
19     <descr> Time spend in MPI regions </descr>
20     <cubepl>
21       {
22         ${a}=0;
23         if (${cube::region::name}[${calculation::region::id}] =~ /^MPI_/)
24           {
25             ${a}=metric::time();
26           };
27         return ${a};
28       }
29     </cubepl>
30   </metric>
31   <metric type="PREDERIVED_EXCLUSIVE">
32     <disp_name>Other regions</disp_name>
33     <uniq_name>nonmpi</uniq_name>
34     <dtype>FLOAT</dtype>
35     <uom>sec</uom>
36     <url></url>
37     <descr>Time spend in non-MPI regions</descr>
38     <cubepl>
39       {

```

```
40         ${a}=0;
41         if (not(${cube::region::name}[${calculation::region::id}] =~ /^MPI_/))
42         {
43             ${a}=metric::time();
44         };
45         return ${a};
46     }
47 </cubepl>
48 </metric>
49 </metrics>
```

As result, the target .cubex file will have only two new root metrics, "MPI regions" and "Other regions". Metric "Time" will be not visible in GUI and command line tools.

1.3.4 Optimization of the remapping.

As remapping process is defined in very general way, naive approach in .spec file formulation might take significant calculation time. Using advanced technics in CubePL one can optimize remapping process. For example one can:

- Using CubePL variables in order to avoid string comparison by every calculation step
- Using CubePL initialization step in order to perform some calculation only once
- Use bitmask multiplication for the evaluation of values along the system tree

Great example of usage of the optimization technics are the .spec files provided with Score-P or Scalasca.

1.4 Supplementary utilities and helping Cube command line tools

Besides of the remapping utility and the algebra tools CUBE provides various tool for different testing, checking, inspection tasks.

1.4.1 Sanity Check

This tool performs series of checks to confirm that stored data has a semantic sense, e.g. "non-negative time" and similar. It is being used as a correctness tool for the Score-P and Scalasca measurements.

```
user@host: cube_sanity profile.cubex
Name not empty or UNKNOWN ... 71 / 71 OK
  No ANONYMOUS functions ... 71 / 71 OK
  No TRUNCATED functions ... 71 / 71 OK
  File name not empty ... 71 / 71 OK
  Proper line numbers ... 0 / 71 OK
  No TRACING outside Init and Finalize ... 123 / 123 OK
No negative inclusive metrics ... 409344 / 440832 OK
No negative exclusive metrics ... 409344 / 440832 OK
```

Usage: cube_sanity [flags] cube experiment

- h** Help; Output a brief help message.
- n** Disables the (time consuming) check for negative inclusive metric values. <>
- x** Disables the (time consuming) check for negative exclusive metric values.
- l** Disables checks for line numbers.
- f file.filt** Checks whether a node's name is matched by a pattern in file.filt.
- o output_file** Path of the output file. If no output file is given, detailed output will be suppressed. A summary will always be printed out to stdout.
- v 0|1|2|3** Verbosity level of output

1.4.2 Addition of derived metric

One small tool, which does nothing but adding an additional user-defined derived metric into the input .cubex file. Functionality of this tool is provided by remapping tool [1.3](#) tool as well, but from historical reasons we still deliver this tool.

```
user@host: cube_derive -t postderived -r exclusive -e "metric::time()/metric::visits(e)" -p root kenobi

user@host: cube_dump -m kenobi -c 0 -t aggr -z incl result.cubex
===== DATA =====
Print out the data of the metric kenobi

All threads
-----
MAIN__ (id=0) 1389.06
```

Usage: cube_derive [-h] -t prederived|postderived -r exclusive|inclusive -e <cubepl expression>=""> -p <parent_metric> <targetmetric> <cube experiment>=""> [-o <output experiment>="">]

- h** Help; Output a brief help message.
- t prederived|postderived** Specifies, whether derived metric is PREDERIVED or POSTDERIVED
- r exclusive|inclusive** Specifies, whether derived metric is EXCLUSIVE or INCLUSIVE (has no effect for POSTDERIVED metrics)
- e** CubePL expression of the derived metric
- p** New metric will be added as a child of this metric. "root" is possible
Name of the created metric. It should not clash with the existing metric.
Name of the input file
- o** Name of the output file. Default "derived.cubex"

1.4.3 Inspection of a call tree

A small tool to inspect aggregated values in call tree of a specific metric. Functionality of this tool is reproduced in one of another way by [cube_dump 1.4.15](#) utility.

```
user@host:cube_calltree -m time -a -t 1 -i -p -c ~/Studies/Cube/Adviser/4n_256_/scorep_casino_1n_256_/profile.cubex...
Reading /home/zam/psaviank/Studies/Cube/Adviser/4n_256_/scorep_casino_1n_256x1_sum_br/profile.cubex...
355599 (100%)          MAIN__          USR:/MAIN__
353588 (99.435%)      + monte_carlo_          USR:/MAIN__/m
8941.95 (2.515%)      | + monte_carlo_IP_read_wave_function_          USR:/MAIN__/m
5980.68 (1.682%)      | | + MPI_Bcast          USR:/MAIN__/m
343175 (96.506%)      | + monte_carlo_IP_run_dmc_          USR:/MAIN__/m
4657.85 (1.31%)       | | + MPI_Ssend          USR:/MAIN__/m
303193 (85.263%)      | | + dmcdmc_main.move_config_          USR:/MAIN__/m
21668.4 (6.093%)      | | | + wfn_utils.wfn_loggrad_          USR:/MAIN__/m
19722.3 (5.546%)      | | | | + pjastrow.oneelec_jastrow_          USR:/MAIN__/m
28878.5 (8.121%)      | | | + wfn_utils.wfn_ratio_          USR:/MAIN__/m
6907.92 (1.943%)      | | | | + slater.wfn_ratio_slater_          USR:/MAIN__/m
19721.7 (5.546%)      | | | | + pjastrow.oneelec_jastrow_          USR:/MAIN__/m
241626 (67.949%)      | | | + energy_utils.eval_local_energy_          USR:/MAIN__/m
20785.6 (5.845%)      | | | | + wfn_utils.wfn_loggrad_          USR:/MAIN__/m
20298.1 (5.708%)      | | | | + pjastrow.oneelec_jastrow_          USR:/MAIN__/m
211484 (59.473%)      | | | | + non_local.calc_nl_projection_          USR:/MAIN__/m
208516 (58.638%)      | | | | | + wfn_utils.wfn_ratio_          USR:/MAIN__/m
8588.87 (2.415%)      | | | | | + slater.wfn_ratio_slater_          USR:/MAIN__/m
176779 (49.713%)      | | | | | + pjastrow.oneelec_jastrow_          USR:/MAIN__/m
14252.4 (4.008%)      | | | | | + scratch.get_eevecs1_ch_          USR:/MAIN__/m
34390.8 (9.671%)      | | + parallel.qmpi_reduce_d1_          USR:/MAIN__/m
34384.3 (9.669%)      | | + MPI_Reduce          USR:/MAIN__/m
```

Usage: cube_calltree -a -m metricname -t threshold -c -i -u -h [-f] filename

-m metricname print out values for the metric <metricname>;

-a annotate call path;

-t threshold print out only call path with a value, which is larger than <threshold>% of the total metric value. 0<=threshold<=100;

-i calculate inclusive values instead of exclusive.

-f open <filename>;

-p display percent value;

-c display callpath for every region;

-h display this help.

1.4.4 System tree partition

If one is interested in the performance profile of a PART of the system, e.g. only nodeplane 0, or ranks from 0 to N, one can set other locations to VOID and create a .cubex file, which has only data for the remaining part.

Partition some of system tree (processes) and void the remainder

```

user@host:cube_part -R 0-3,5 profile.cubex
Open the cube profile.cubex...done.
Copy the cube object...done.
+++++++ Part operation begins ++++++
Voiding 251 of 256 processes.
+++++++ Part operation ends successfully ++++++
Writing part ... done.

```

Usage: cube_part [-h] [-I] [-R ranks] [-o output] cubefile

- I** Invert sense of partition
- R** List of process ranks for partition (e.g., "0-3,7,13-")
- o** Name of the output file (default: part)
- h** Help; Show this brief help message and exit.

1.4.5 Region information

This tool displays a flat profile for the selected metrics and with the classification of regions. Similar functionality is provide by the tool [1.4.15](#)

Short call displays an overview across types of regions.

```

user@host:cube_regioninfo -m time,visits profile.cubex
done.

```

| bl | type | time | % | visits | % region |
|----|------|--------|--------|-----------|----------------------|
| | ANY | 355599 | 100.00 | 664724749 | 100.00 (summary) ALL |
| | MPI | 0 | 0.00 | 0 | 0.00 (summary) MPI |
| | USR | 355599 | 100.00 | 664724749 | 100.00 (summary) USR |
| | COM | 0 | 0.00 | 0 | 0.00 (summary) COM |

If one wants a detailed view of the flat profile, one uses -r command line option. Note that can provide list of regions for filtering (file filter.txt)

```

user@host:cube_regioninfo -l filter.txt -m time,visits -r profile.cubex
done.

```

| bl | type | time | % | visits | % region |
|----|------|------|------|--------|-------------------------|
| | USR | 0 | 0.00 | 0 | 0.00 MEASUREMENT OFF |
| | USR | 0 | 0.00 | 0 | 0.00 TRACE BUFFER FLUSH |
| | USR | 0 | 0.00 | 0 | 0.00 THREADS |
| | USR | 0 | 0.00 | 0 | 0.00 MPI_Accumulate |
| | USR | 68 | 0.02 | 6912 | 0.00 MPI_Allgather |
| | USR | 0 | 0.00 | 0 | 0.00 MPI_Allgatherv |
| | USR | 10 | 0.00 | 256 | 0.00 MPI_Allreduce |
| | USR | 0 | 0.00 | 0 | 0.00 MPI_Alltoall |
| | USR | 0 | 0.00 | 0 | 0.00 MPI_Alltoallv |
| | USR | 0 | 0.00 | 0 | 0.00 MPI_Alltoallw |

| | | | | | |
|-----|------|------|-------|------|--------------------------------|
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Attr_delete |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Attr_get |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Attr_put |
| USR | 2843 | 0.80 | 7168 | 0.00 | MPI_Barrier |
| USR | 6392 | 1.80 | 51072 | 0.01 | MPI_Bcast |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Bsend |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Bsend_init |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Buffer_attach |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Buffer_detach |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Cancel |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Cart_coords |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Cart_create |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Cart_get |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Cart_map |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Cart_rank |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Cart_shift |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Cart_sub |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Cartdim_get |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_call_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_compare |
| USR | 113 | 0.03 | 1792 | 0.00 | MPI_Comm_create |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_create_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_create_group |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_create_keyval |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_delete_attr |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_dup |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_dup_with_info |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_free |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_free_keyval |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_get_attr |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_get_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_get_info |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_get_name |
| USR | 0 | 0.00 | 1024 | 0.00 | MPI_Comm_group |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_idup |
| USR | 0 | 0.00 | 512 | 0.00 | MPI_Comm_rank |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_remote_group |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_remote_size |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_set_attr |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_set_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_set_info |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_set_name |
| USR | 0 | 0.00 | 512 | 0.00 | MPI_Comm_size |
| USR | 55 | 0.02 | 256 | 0.00 | MPI_Comm_split |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_split_type |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Comm_test_inter |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Compare_and_swap |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Dims_create |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Dist_graph_create |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Dist_graph_create_adjacent |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Dist_graph_neighbors |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Dist_graph_neighbors_count |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Exscan |

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|-----|---|------|---|------|------------------------------|
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Fetch_and_op |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_c2f |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_call_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_close |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_create_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_delete |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_f2c |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_amode |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_atomicsity |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_byte_offset |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_group |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_info |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_position |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_position_shared |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_size |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_type_extent |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_get_view |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iread |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iread_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iread_at |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iread_at_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iread_shared |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iwrite |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iwrite_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iwrite_at |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iwrite_at_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_iwrite_shared |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_open |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_preallocate |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_all_begin |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_all_end |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_at |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_at_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_at_all_begin |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_at_all_end |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_ordered |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_ordered_begin |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_ordered_end |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_read_shared |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_seek |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_seek_shared |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_set_atomicsity |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_set_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_set_info |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_set_size |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_set_view |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_sync |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_all_begin |

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|-----|-----|------|------|------|------------------------------|
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_all_end |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_at |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_at_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_at_all_begin |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_at_all_end |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_ordered |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_ordered_begin |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_ordered_end |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_File_write_shared |
| USR | 349 | 0.10 | 256 | 0.00 | MPI_Finalize |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Finalized |
| USR | 0 | 0.00 | 25 | 0.00 | MPI_Gather |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Gatherv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Get |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Get_accumulate |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Get_library_version |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Graph_create |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Graph_get |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Graph_map |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Graph_neighbors |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Graph_neighbors_count |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Graphdims_get |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_compare |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_difference |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_excl |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_free |
| USR | 0 | 0.00 | 1792 | 0.00 | MPI_Group_incl |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_intersection |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_range_excl |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_range_incl |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_rank |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_size |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_translate_ranks |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Group_union |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Iallgather |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Iallgatherv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Iallreduce |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ialltoall |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ialltoallv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ialltoallw |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ibarrier |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ibcast |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ibsend |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Iexscan |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Igather |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Igatherv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Iprobe |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Imrecv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ineighbor_allgather |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ineighbor_allgatherv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ineighbor_alltoall |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ineighbor_alltoallv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ineighbor_alltoallw |

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|-----|-------|------|-------|------|---------------------------|
| USR | 1411 | 0.40 | 256 | 0.00 | MPI_Init |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Init_thread |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Initialized |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Intercomm_create |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Intercomm_merge |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Iprobe |
| USR | 0 | 0.00 | 14337 | 0.00 | MPI_Irecv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ireduce |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ireduce_scatter |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ireduce_scatter_block |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Irsend |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Is_thread_main |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Iscan |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Iscatter |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Iscatterv |
| USR | 1 | 0.00 | 14337 | 0.00 | MPI_Isend |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Issend |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Keyval_create |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Keyval_free |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Mprobe |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Mrecv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Neighbor_allgather |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Neighbor_allgatherv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Neighbor_alltoall |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Neighbor_alltoallv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Neighbor_alltoallw |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Probe |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Put |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Query_thread |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Raccumulate |
| USR | 302 | 0.08 | 24728 | 0.00 | MPI_Recv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Recv_init |
| USR | 34384 | 9.67 | 6400 | 0.00 | MPI_Reduce |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Reduce_local |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Reduce_scatter |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Reduce_scatter_block |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Register_datarep |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Request_free |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Rget |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Rget_accumulate |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Rput |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Rsend |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Rsend_init |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Scan |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Scatter |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Scatterv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Send |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Send_init |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Sendrecv |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Sendrecv_replace |
| USR | 4695 | 1.32 | 24728 | 0.00 | MPI_Ssend |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Ssend_init |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Start |

| | | | | | |
|-------|-----|------|--------|------|---------------------------|
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Startall |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Test |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Test_cancelled |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Testall |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Testany |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Testsome |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Topo_test |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Wait |
| USR | 0 | 0.00 | 2982 | 0.00 | MPI_Waitall |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Waitany |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Waitsome |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_allocate |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_allocate_shared |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_attach |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_call_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_complete |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_create |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_create_dynamic |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_create_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_create_keyval |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_delete_attr |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_detach |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_fence |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_flush |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_flush_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_flush_local |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_flush_local_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_free |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_free_keyval |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_get_attr |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_get_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_get_group |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_get_info |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_get_name |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_lock |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_lock_all |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_post |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_set_attr |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_set_errhandler |
| USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_set_info |
| * USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_set_name |
| * USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_shared_query |
| * USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_start |
| * USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_sync |
| * USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_test |
| * USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_unlock |
| * USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_unlock_all |
| * USR | 0 | 0.00 | 0 | 0.00 | MPI_Win_wait |
| * USR | 0 | 0.00 | 0 | 0.00 | PARALLEL |
| * USR | 155 | 0.04 | 256 | 0.00 | MAIN__ |
| * USR | 0 | 0.00 | 256 | 0.00 | get_nnpsmp_ |
| * USR | 1 | 0.00 | 126669 | 0.02 | run_control.check_alloc_ |
| * USR | 8 | 0.00 | 256 | 0.00 | get_smp_list_ |

1.4 Supplementary utilities and helping Cube command line tools

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|---|-----|--------|--------|-----------|--------|-------------------------------------------|
| * | USR | 0 | 0.00 | 256 | 0.00 | set_shm_numablock |
| * | USR | 401 | 0.11 | 256 | 0.00 | monte_carlo_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_set_defaults_ |
| * | USR | 124 | 0.03 | 256 | 0.00 | monte_carlo_IP_set_input_parameters_ |
| * | USR | 10 | 0.00 | 256 | 0.00 | monte_carlo_IP_read_particles_ |
| * | USR | 3 | 0.00 | 256 | 0.00 | monte_carlo_IP_read_custom_spindep_ |
| * | USR | 6 | 0.00 | 256 | 0.00 | monte_carlo_IP_assign_spin_deps_ |
| * | USR | 2 | 0.00 | 256 | 0.00 | monte_carlo_IP_check_input_parameters_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_input_setup_ |
| * | USR | 0 | 0.00 | 1 | 0.00 | monte_carlo_IP_print_input_parameters_ |
| * | USR | 0 | 0.00 | 62 | 0.00 | monte_carlo_IP_wout_iparam_ |
| * | USR | 0 | 0.00 | 1 | 0.00 | monte_carlo_IP_print_particles_ |
| * | USR | 107 | 0.03 | 256 | 0.00 | monte_carlo_IP_read_wave_function_ |
| * | USR | 2 | 0.00 | 256 | 0.00 | alloc_shm_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | alloc_shm_sysv |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_flag_missing_dets_ |
| * | USR | 0 | 0.00 | 1 | 0.00 | monte_carlo_IP_check_wave_function_ |
| * | USR | 36 | 0.01 | 256 | 0.00 | monte_carlo_IP_calculate_geometry_ |
| * | USR | 27 | 0.01 | 256 | 0.00 | monte_carlo_IP_read_pseudopotentials_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_geometry_printout_ |
| * | USR | 1 | 0.00 | 256 | 0.00 | monte_carlo_IP_orbital_setup_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_check_orbital_derivatives_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_setup_expectation_values_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_setup_interactions_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_check_nn_ |
| * | USR | 98 | 0.03 | 256 | 0.00 | monte_carlo_IP_read_jastrow_function_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_read_backflow_ |
| * | USR | 8 | 0.00 | 256 | 0.00 | monte_carlo_IP_init_vcpp_ |
| * | USR | 0 | 0.00 | 256 | 0.00 | monte_carlo_IP_print_part_title_ |
| * | USR | 281 | 0.08 | 256 | 0.00 | monte_carlo_IP_run_dmc_ |
| * | USR | 11021 | 3.10 | 25041 | 0.00 | dmcdmc_main.move_config_ |
| | USR | 2434 | 0.68 | 45059225 | 6.78 | wfn_utils.wfn_loggrad_ |
| | USR | 236521 | 66.51 | 175964383 | 26.47 | pjastrow.oneelec_jastrow_ |
| | USR | 9886 | 2.78 | 144014658 | 21.67 | wfn_utils.wfn_ratio_ |
| | USR | 15497 | 4.36 | 144014658 | 21.67 | slater.wfn_ratio_slater_ |
| | USR | 15512 | 4.36 | 144014658 | 21.67 | scratch.get_eevecs1_ch_ |
| | USR | 9356 | 2.63 | 25041 | 0.00 | energy_utils.eval_local_energy_ |
| | USR | 2967 | 0.83 | 11268450 | 1.70 | non_local.calc_nl_projection_ |
| | USR | 7 | 0.00 | 6400 | 0.00 | parallel.qmpi_reduce_d1_ |
| | USR | 0 | 0.00 | 6400 | 0.00 | parallel.qmpi_bcast_d1_ |
| | USR | 0 | 0.00 | 12800 | 0.00 | parallel.qmpi_bcast_d_ |
| | USR | 16 | 0.00 | 9382 | 0.00 | dmc.branch_and_redist_ |
| | USR | 39 | 0.01 | 6144 | 0.00 | dmc.branch_and_redist_send_ |
| | USR | 1 | 0.00 | 2982 | 0.00 | dmc.branch_and_redist_recv_ |
| | USR | 4 | 0.00 | 256 | 0.00 | dmc.branch_and_redist_sendrecv_ |
| | USR | 0 | 0.00 | 256 | 0.00 | dealloc_shm_ |
| | USR | 445 | 0.13 | 256 | 0.00 | dealloc_shm_sysv |
| | USR | 0 | 0.00 | 256 | 0.00 | clean_shm_ |
| | ANY | 355599 | 100.00 | 664724749 | 100.00 | (summary) ALL |
| | MPI | 0 | 0.00 | 0 | 0.00 | (summary) MPI |
| | USR | 355599 | 100.00 | 664724749 | 100.00 | (summary) USR |
| | COM | 0 | 0.00 | 0 | 0.00 | (summary) COM |

| | | | | | |
|-----|--------|-------|-----------|-----------------|--------|
| BL | 12291 | 3.46 | 159199 | 0.02 (summary) | BL |
| ANY | 343308 | 96.54 | 664565550 | 99.98 (summary) | ALL-BL |
| MPI | 0 | 0.00 | 0 | 0.00 (summary) | MPI-BL |
| USR | 343308 | 96.54 | 664565550 | 99.98 (summary) | USR-BL |
| COM | 0 | 0.00 | 0 | 0.00 (summary) | COM-BL |

Usage: cube_regioninfo [-l filename] [-m filename] [-h] [-s] cubefile

-h Help; Output this help message

-r be verbose, print info about any region

-l Specify a list of regions for the blacklist

-m Specify a list of metrics, the list has to be comma-seperated, no spaces allowed

1.4.6 Cube Information

Another tool which allows to examine performance data along the call tree with ability to filter accordingly to user defined criteria. Partially same functionality is implemented by [1.4.15](#) and call tree.

```
user@host: cube_info -t -m bytes_sent profile.cubex
|          Time |      bytes_sent | Diff-Calltree
|          355598 |    14204637004 | * MAIN__
|           1411 |           0 | | * MPI_Init
|            0 |           0 | | * MPI_Comm_size
|            0 |           0 | | * MPI_Comm_rank
|            0 |           0 | | * get_nnpssp_
|            0 |           0 | | * run_control.check_alloc_
|            69 |     917504 | | * get_smp_list_
|            0 |           0 | | | * MPI_Comm_rank
|            0 |           0 | | | * MPI_Comm_size
|            9 |    262144 | | | * MPI_Allreduce
|            0 |           0 | | | * set_shm_numablock
|           27 |    655360 | | | * MPI_Allgather
|            0 |           0 | | | * MPI_Comm_group
|            0 |           0 | | | * MPI_Group_incl
|           25 |           0 | | | * MPI_Comm_create
|            0 |           0 | | | * MPI_Comm_group
|            0 |           0 | | | * MPI_Group_incl
|           24 |           0 | | | * MPI_Comm_create
|          353588 |    14203719500 | | * monte_carlo_
|            0 |           0 | | | * monte_carlo_IP_set_defaults_
|           142 |           0 | | | * monte_carlo_IP_set_input_parameters_
|            0 |           0 | | | * run_control.check_alloc_
|           10 |           0 | | | * monte_carlo_IP_read_particles_
|            0 |           0 | | | | * run_control.check_alloc_
|            3 |           0 | | | | * monte_carlo_IP_read_custom_spindep_
|            5 |           0 | | | | * monte_carlo_IP_assign_spin_deps_
|            0 |           0 | | | | * run_control.check_alloc_
|           174 |         1024 | | | * monte_carlo_IP_check_input_parameters_
```

| | | | | | |
|--------|-------------|--|--|--|---------------------------------------------|
| 172 | 1024 | | | | * MPI_Bcast |
| 0 | 0 | | | | * monte_carlo_IP_input_setup_ |
| 0 | 0 | | | | * monte_carlo_IP_print_input_parameters_ |
| 0 | 0 | | | | * monte_carlo_IP_wout_iparam_ |
| 0 | 0 | | | | * monte_carlo_IP_print_particles_ |
| 68 | 12288 | | | | * MPI_Bcast |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 0 | 0 | | | | * MPI_Comm_group |
| 0 | 0 | | | | * MPI_Group_incl |
| 23 | 0 | | | | * MPI_Comm_create |
| 8941 | 12811606784 | | | | * monte_carlo_IP_read_wave_function_ |
| 2792 | 0 | | | | * MPI_Barrier |
| 55 | 0 | | | | * MPI_Comm_split |
| 5980 | 12811605760 | | | | * MPI_Bcast |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 5 | 1024 | | | | * alloc_shm_ |
| 4 | 1024 | | | | * alloc_shm_sysv |
| 3 | 1024 | | | | * MPI_Bcast |
| 0 | 0 | | | | * MPI_Barrier |
| 0 | 0 | | | | * monte_carlo_IP_flag_missing_dets_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 0 | 0 | | | | * monte_carlo_IP_check_wave_function_ |
| 36 | 0 | | | | * monte_carlo_IP_calculate_geometry_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 27 | 0 | | | | * monte_carlo_IP_read_pseudopotentials_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 0 | 0 | | | | * monte_carlo_IP_geometry_printout_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 0 | 0 | | | | * monte_carlo_IP_orbital_setup_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 0 | 0 | | | | * monte_carlo_IP_check_orbital_derivatives_ |
| 0 | 0 | | | | * monte_carlo_IP_setup_expectation_values_ |
| 0 | 0 | | | | * monte_carlo_IP_setup_interactions_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 46 | 2048 | | | | * monte_carlo_IP_check_nn_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 46 | 2048 | | | | * MPI_Bcast |
| 97 | 0 | | | | * monte_carlo_IP_read_jastrow_function_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 0 | 0 | | | | * monte_carlo_IP_read_backflow_ |
| 7 | 0 | | | | * monte_carlo_IP_init_vcpp_ |
| 0 | 0 | | | | * monte_carlo_IP_print_part_title_ |
| 343175 | 1392097356 | | | | * monte_carlo_IP_run_dmc_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 0 | 0 | | | | * MPI_Comm_group |
| 0 | 0 | | | | * MPI_Group_incl |
| 38 | 0 | | | | * MPI_Comm_create |
| 64 | 747520 | | | | * MPI_Bcast |
| 4657 | 11140276 | | | | * MPI_Ssend |
| 303193 | 0 | | | | * dmcdmc_main.move_config_ |
| 0 | 0 | | | | * run_control.check_alloc_ |
| 21668 | 0 | | | | * wfn_utils.wfn_loggrad_ |
| 19722 | 0 | | | | * pjastrow.oneelec_jastrow_ |

- l** Lists all available metrics.
- b** Shows some basic information about the cube file.
- a met,thrh** Checks whether a node's value for a certain metric is below a given threshold with respect to the node's absolute value. Affected nodes are aggregated to a single node and output of their children is suppressed.
- r met,thrh** Like **-absolute**, but based on a percentage of the root's value.
- x met,thrh** Like **-absolute**, but based on selecting most relevant children of a node at each level.

met must have the following form: *unique_metric_name:[incl|excl]:process_number.thread_number*
It is allowed to omit anything except for the metric's unique name, so "time" would compute the inclusive time aggregated over all threads or "time:excl:2" would compute the exclusive time aggregated over all threads that belong to the process with the id 2.

1.4.7 Tester

With the tool `cube_test` one can perform various test on `.cubex` file such as range test on metric values and similar. This is used usually in the correctness tests of Score-P and SCALASCA.

Usage: `cube_test [flags] cube1 cube2`

- ?** Help; Output a brief help message.
- h** Help; Output a long help message.
- o** Set the output file. If omitted, STDOUT is used.
- c tree1[,tree2]** Create a new copy of the tree "tree2" that is called "tree1". If "tree2" is omitted, "tree1" will be a copy of the "ALL"
- e metric[,tree]** Checks whether the metric described by the string "metric" is equal for all provided CUBE files and for all nodes of the tree "tree". If tree is omitted, all nodes are checked.
- s metric,type,tol[,tree]** Checks whether the metric described by the string "metric" is sufficiently similar for all CUBE files, according to the qualifiers type and "tol". "tol" specifies the tolerance which is given as a real number. The meaning of the tolerance value depends on the "type". "type" is either ABS or REL. If "type" is ABS than the nodes are similar if the difference between all values for that metric is below "tol". If "type" is REL than the nodes are similar if the difference between all values for that metric is below: $\sum_{i=1}^n tol * v_i^m$, where n is the number of CUBE files, i-th file and V is value of metric If "tree" is omitted, all nodes are checked.
- a metric,thrh[,tree]** Removes all nodes from the tree "tree" whose values are below "thrh" for the metric "metric". If tree is omitted, nodes are removed from the default tree ALL.
- r metric,thrh[,tree]** Removes all nodes from the tree "tree" whose values are below "thrh" percent of the sum of all roots values. "thrh" is supposed to be a value between 0 and 1. If "tree" is omitted, nodes are removed from the default tree ALL.

-x metric,thr[tree] For each node of the tree tree we consider all children N of that node. Let v_i be the value for the given metric and the node i in N. Then we select a maximal subset M (smaller than N) with the property $\sum_{i \in M} v_i \leq thr \times \sum_{i \in N} v_i$ and remove all nodes from M. If tree is omitted, nodes are removed from the default tree ALL.

-v [0,1,2,3] Verbosity level: 0 - silent, 1 - report only summary, 2 - report only errors, 3 - report status of all tests

WARNING: The order of the options matters.

1.4.8 Canonizer

With this tool user can convert all regions into canonical form, names into lower case, removing lines and filenames, in order to be able to compare measurements results.

Here is an example of execution

```
cube_canonize -p -m 10 -c -f -l profile.cubex canonized.cubex
```

```
cube_dump -w profile.cubex
```

```
....
```

```
----- LIST OF REGIONS -----
```

```
MEASUREMENT OFF:MEASUREMENT OFF ( id=0, -1, -1, paradigm=user, role=artificial, url=, descr=, mod=)
TRACE BUFFER FLUSH:TRACE BUFFER FLUSH ( id=1, -1, -1, paradigm=measurement, role=artificial, url=, descr=, mod=)
THREADS:THREADS ( id=2, -1, -1, paradigm=measurement, role=artificial, url=, descr=, mod=)
MPI_Accumulate:MPI_Accumulate ( id=3, -1, -1, paradigm=mpi, role=atomic, url=, descr=, mod=)
...
PARALLEL:PARALLEL ( id=270, -1, -1, paradigm=mpi, role=artificial, url=, descr=, mod=)
MAIN__:MAIN__ ( id=271, -1, -1, paradigm=compiler, role=function, url=, descr=, mod=/marc
get_nnpsmp:get_nnpsmp_ ( id=272, -1, -1, paradigm=compiler, role=function, url=, descr=, m
run_control.check_alloc_:run_control.check_alloc_ ( id=273, -1, -1, paradigm=compiler
get_smp_list_:get_smp_list_ ( id=274, -1, -1, paradigm=compiler, role=function, url=, d
set_shm_numablock:set_shm_numablock ( id=275, -1, -1, paradigm=compiler, role=function,
monte_carlo_:monte_carlo_ ( id=276, -1, -1, paradigm=compiler, role=function, url=, d
```

```
...
```

```
cube_dump -w canonized.cubex
```

```
----- LIST OF REGIONS -----
```

```
off:MEASUREMENT OFF ( id=0, 0, 0, paradigm=user, role=artificial, url=, descr=, mod=)
flush:TRACE BUFFER FLUSH ( id=1, 0, 0, paradigm=measurement, role=artificial, url=, descr=, mod=)
threads:THREADS ( id=2, 0, 0, paradigm=measurement, role=artificial, url=, descr=, mod=)
mpi_accumu:MPI_Accumulate ( id=3, 0, 0, paradigm=mpi, role=atomic, url=, descr=, mod=)
...
parallel:PARALLEL ( id=270, 0, 0, paradigm=mpi, role=artificial, url=, descr=, mod=)
main:MAIN__ ( id=271, 0, 0, paradigm=compiler, role=function, url=, descr=, mod=)
get_nnpsmp:get_nnpsmp_ ( id=272, 0, 0, paradigm=compiler, role=function, url=, descr=, mod=)
run_contro:run_control.check_alloc_ ( id=273, 0, 0, paradigm=compiler, role=function, u
get_smp_li:get_smp_list_ ( id=274, 0, 0, paradigm=compiler, role=function, url=, des
set_shm_nu:set_shm_numablock ( id=275, 0, 0, paradigm=compiler, role=function, url=, des
monte_carl:monte_carlo_ ( id=276, 0, 0, paradigm=compiler, role=function, url=, descr=, mod=)
```

```
...
```

Usage: cube_canonize [flags] input output

- h** Print this help
- p** Use PDT format
- m num** Maximum length
- c** Lower case
- f** Remove file names
- l** Remove line numbers

1.4.9 Clean

CUBE files may contain more data in the definition part than absolutely necessary. The cube_clean utility creates a new CUBE file with an identical structure as the input experiment, but with the definition part cleaned up.

An example of the output is presented below.

```
user@host: cube_clean remapped.cube -o cleaned.cube
+++++++ Clean operation begins ++++++
Reading remapped.cube ... done.

      Topology retained in experiment.
+++++++ Clean operation ends successfully ++++++
Writing cleaned.cube ... done.
```

Usage: cube_clean [-o output] [-h cube

- o** Name of the output file (default: clean.cube|.gz)
- h** Help; Output a brief help message.

1.4.10 Reroot, Prune

For the detailed study of some part of the execution, the CUBE file can be modified based on a given call-tree node. Two different operations are possible:

- The call tree may be re-rooted, i.e., only sub-trees with the given call-tree node as root are retained in the experiment.
- An entire sub-tree may be pruned, i.e., removed from the experiment. In this case, all metric values for that sub-tree will be attributed to it's parent call-tree node (= "inlined").

An example of the output is presented below.

```
user@host: cube_cut -r inner_auto_ -p flux_err_ -o cutted.cube remapped.cube
Reading remapped.cube ... done.
+++++++ Cut operation begins ++++++
```

```

Topology retained in experiment.
+++++++ Cut operation ends successfully ++++++
Writing cutted.cube ... done.

```

Usage: cube_cut [-h] [-r nodename] [-p nodename] [-o output cube]

- o** Name of the output file (default: cut.cube|.gz)
- r** Re-root call tree at named node
- p** Prune call tree from named node (= "inline")
- h** Help; Output a brief help message.

1.4.11 Statistics

Extracts statistical information from the CUBE files.

```

user@host: ./cube_stat -m time,mpi -p remapped.cube -%
MetricRoutine      Count      Sum      Mean      Variance  Minimum      ...      Maximum
time INCL(MAIN_)    4    143.199101  35.799775  0.001783  35.759769    ...    35.839160
time EXCL(MAIN_)    4     0.078037  0.019509  0.000441   0.001156    ...     0.037711
time task_init_     4     0.568882  0.142221  0.001802   0.102174    ...     0.181852
time read_input_    4     0.101781  0.025445  0.000622   0.000703    ...     0.051980
time decomp_        4     0.000005  0.000001  0.000000   0.000001    ...     0.000002
time inner_auto_    4    142.361593  35.590398  0.000609  35.566589    ...    35.612125
time task_end_      4     0.088803  0.022201  0.000473   0.000468    ...     0.043699

mpi  INCL(MAIN_)    4     62.530811  15.632703  2.190396  13.607989    ...    17.162466
mpi  EXCL(MAIN_)    4     0.000000  0.000000  0.000000   0.000000    ...     0.000000
mpi  task_init_     4     0.304931  0.076233  0.001438   0.040472    ...     0.113223
mpi  read_input_    4     0.101017  0.025254  0.000633   0.000034    ...     0.051952
mpi  decomp_        4     0.000000  0.000000  0.000000   0.000000    ...     0.000000
pi   inner_auto_    4     62.037503  15.509376  2.194255  13.478049    ...    17.031288
mpi  task_end_      4     0.087360  0.021840  0.000473   0.000108    ...     0.043333

```

```

user@host: ./cube_stat -t33 remapped.cube -p -m time,mpi,visits
Region      NumberOfCalls ExclusiveTime InclusiveTime      time      mpi      visits
sweep_      48      76.438435    130.972847    76.438435  0.000000      48
MPI_Recv    39936    36.632249    36.632249    36.632249  36.632249  39936
MPI_Send    39936    17.684986    17.684986    17.684986  17.684986  39936
MPI_Allreduce 128      7.383530     7.383530     7.383530   7.383530   128
source_     48      3.059890     3.059890     3.059890   0.000000    48
MPI_Barrier 12      0.382902     0.382902     0.382902   0.382902    12
flux_err_   48      0.380047     1.754759     0.380047   0.000000    48
TRACING      8      0.251017     0.251017     0.251017   0.000000     8
MPI_Bcast   16      0.189381     0.189381     0.189381   0.189381    16
MPI_Init     4      0.170402     0.419989     0.170402   0.170402     4
snd_real_   39936    0.139266    17.824251     0.139266   0.000000  39936
MPI_Finalize  4      0.087360     0.088790     0.087360   0.087360     4
initialize_  4      0.084858     0.168192     0.084858   0.000000     4

```

| | | | | | | |
|------------------|-------|----------|------------|----------|----------|-------|
| initxs_ | 4 | 0.083242 | 0.083242 | 0.083242 | 0.000000 | 4 |
| MAIN_ | 4 | 0.078037 | 143.199101 | 0.078037 | 0.000000 | 4 |
| rcv_real_ | 39936 | 0.077341 | 36.709590 | 0.077341 | 0.000000 | 39936 |
| inner_ | 4 | 0.034985 | 142.337220 | 0.034985 | 0.000000 | 4 |
| inner_auto_ | 4 | 0.024373 | 142.361593 | 0.024373 | 0.000000 | 4 |
| task_init_ | 4 | 0.014327 | 0.568882 | 0.014327 | 0.000000 | 4 |
| read_input_ | 4 | 0.000716 | 0.101781 | 0.000716 | 0.000000 | 4 |
| octant_ | 416 | 0.000581 | 0.000581 | 0.000581 | 0.000000 | 416 |
| global_real_max_ | 48 | 0.000441 | 1.374712 | 0.000441 | 0.000000 | 48 |
| global_int_sum_ | 48 | 0.000298 | 5.978850 | 0.000298 | 0.000000 | 48 |
| global_real_sum_ | 32 | 0.000108 | 0.030815 | 0.000108 | 0.000000 | 32 |
| barrier_sync_ | 12 | 0.000105 | 0.383007 | 0.000105 | 0.000000 | 12 |
| bcast_int_ | 12 | 0.000068 | 0.189395 | 0.000068 | 0.000000 | 12 |
| timers | 2 | 0.000044 | 0.000044 | 0.000044 | 0.000000 | 2 |
| initgeom_ | 4 | 0.000042 | 0.000042 | 0.000042 | 0.000000 | 4 |
| initsnc_ | 4 | 0.000038 | 0.000050 | 0.000038 | 0.000000 | 4 |
| task_end_ | 4 | 0.000013 | 0.088803 | 0.000013 | 0.000000 | 4 |
| bcast_real_ | 4 | 0.000010 | 0.000065 | 0.000010 | 0.000000 | 4 |
| decomp_ | 4 | 0.000005 | 0.000005 | 0.000005 | 0.000000 | 4 |
| timers_ | 2 | 0.000004 | 0.000048 | 0.000004 | 0.000000 | 2 |

Usage: cube_stat [-h] [-p] [-m metric[,metric...] -%] [-r routine[,routine...]] cubefile

OR

cube_stat -h] [-p] [-m metric[,metric...] -t topN cubefile

- h** Display this help message
- p** Pretty-print statistics (instead of CSV output)
- %** Provide statistics about process/thread metric values
- m** List of metrics (default: time)
- r** List of routines (default: main)
- t** Number for topN regions flat profile

1.4.12 from TAU to CUBE

Converts a profile generated by the TAU Performance System into the CUBE format. Currently, only 1-level, 2-level and full call-path profiles are supported.

An example of the output is presented below.

```

user@host: ./tau2cube3 tau2 -o b.cube
  Parsing TAU profile...
tau2/profile.0.0.2
tau2/profile.1.0.0
  Parsing TAU profile...      done.
  Creating CUBE profile...
Number of call paths : 5
Childmain int (int, char **)
Number of call paths : 5

```

```
ChildsomeA void (void)
Number of call paths : 5
ChildsomeB void (void)
Number of call paths : 5
ChildsomeC void (void)
Number of call paths : 5
ChildsomeD void (void)
Path to Parents : 5
Path to Child : 1
Number of roots : 5
Call-tree node created
Call-tree node created
Call-tree node created
Call-tree node created
Call-tree node created
value time :: 8.0151
value ncalls :: 1
value time :: 11.0138
value ncalls :: 1
value time :: 8.01506
value ncalls :: 1
value time :: 11.0138
value ncalls :: 1
value time :: 5.00815
value ncalls :: 1
value time :: 11.0138
value ncalls :: 1
value time :: 0.000287
value ncalls :: 1
value time :: 11.0138
value ncalls :: 1
value time :: 0
value ncalls :: 0
value time :: 9.00879
value ncalls :: 1
done.
```

Usage: tau2cube [tau-profile-dir][-o cube]

1.4.13 Common Calltree

Common Calltree is a tool to reduce call trees of a set of cube files to the common part.

Usage: cube_commoncalltree cubefile1 cubefile2 ... cubefileN

The tool *cube_commoncalltree* takes set of input cubefiles

(*cubefile1 cubefile2 ... cubefileN*)

and creates corresponding set of cube files

(*cubefile1_commoncalltree cubefile2_commoncalltree ... cubefileN_commoncalltree*).

Output cube files *cubeX_commoncalltree* do have the equal system and metric dimensions like corresponding *cubeX* file.

Call trees among *cubeX_commoncalltree* files are reduced to the maximal (up to a special case in region naming scheme) common part. Inclusive value of the "missing" part is added as a exclusive value to its parent (which is a part of common part of call tree)

This tool is particularly useful for comparison of experiments with the different recursion depth or with the additional sub call trees depending on some loop iteration index.

1.4.14 Topology Assistant

Topology assistant is a tool to handle topologies in cube files. It is able to add or edit a topology.

Usage: `cube_topoassist {OPTION} cubefile`

The current available options are:

- To create a new topology in an existing cube file,
- To [re]name an existing virtual topology, and
- To [re]name the dimensions of a virtual topology.

The command-line switches for this utility are:

- c:** creates a new topology in a given cube file.
- n:** displays a numbered list of the existing topologies in the given cube file, and lets the user choose one to be named or renamed.
- d:** displays the existing topologies, and lets the user name the dimensions of one of them.

The resulting CUBE file is named `topo.cube.gz`, in the current directory.

As mentioned above, when using the **-d** or **-n** command-line options, a numbered list of the current topologies will appear, showing the topology names, its dimension names (when existing), and the number of coordinates in each dimension, as well as the total number of threads. This is an example of the usage:

```
$ cube_topoassist topo.cube.gz -n
Reading topo.cube.gz . Please wait... Done.
Processes are ordered by rank. For more information about this file,
use cube_info -S <cube experiment>

This CUBE has 3 topologie(s).
0. <Unnamed topology>, 3 dimensions: x: 3, y: 1, z: 4. Total = 12 threads.
1. Test topology, 1 dimensions: dim_x: 12. Total = 12 threads.
2. <Unnamed topology>, 3 dimensions: 3, 1, 4. Total = 12 threads. <Dimensions are not named>

Topology to [re]name?
1
New name:
Hardware topology
```

Topology successfully [re]named.

Writing topo.cube.gz ... done.

The process is similar for [re]naming dimensions within a topology. One characteristic is that either all dimensions are named, or none.

One could easily create a script to generate the coordinates according to some algorithm/equation, and feed this to the assistant as an input. The only requirement is to answer the questions in the order they appear, and after that, feed the coordinates. Coordinates are asked for in rank order, and inside every rank, in thread order.

The sequence of questions made by the assistant when creating a new topology (the `-c` switch) is:

- New topology's name
- Number of dimensions
- Will the above dimensions be named? (Y/N)
- If yes, asks the name. Empty is not valid.
- Number of coordinates in that dimension
- Asks if this dimension is either periodic or not (Y/N)
- Repeat the previous three steps for every dimension
- After that, it expects the coordinates for each thread in this topology, separated by spaces, in the order described above.

This is a sample session of the assistant:

```
$ cube_topoassist -c experiment.cube.gz
Reading experiment.cube.gz. Please wait... Done.
Processes are ordered by rank. For more information about this file, use cube_info -S <cube experiment
```

So far, only cartesian topologies are accepted.

Name for new topology?

Test topology

Number of Dimensions?

3

Do you want to name the dimensions (axis) of this topology? (Y/N)

y

Name for dimension 0

torque

Number of elements for dimension 0

2000

Is dimension 0 periodic?

y

Name for dimension 1

rotation

Number of elements for dimension 1

1500

Is dimension 1 periodic?

n

Name for dimension 2

period

```
Number of elements for dimension 2
50
Is dimension 2 periodic?
n
Alert: The number of possible coordinates (1500000000) is bigger than the number of threads
on the specified cube file (12). Some positions will stay empty.
Topology on THREAD level.
Thread 0's (rank 0) coordinates in 3 dimensions, separated by spaces
0 0 0
0 0 1
0 0 2
...
...
...
Writing topo.cube.gz ... done.
$
```

So, a possible input file for this cube experiment could be:

```
Test topology
3
y
torque
2000
y
rotation
1500
n
period
50
n
0 0 0
0 0 1
0 0 2
... (the remaining coordinates)
```

And then call the assistant: `cube_topoassist -c cubefile.cube < input.txt`

1.4.15 Dump

To export values from the cube report into another tool or to examine internal structure of the cube report CUBE framework provides a tool `cube_dump` tool, which prints out different values. It calculates inclusive and exclusive values along metric tree and call tree, aggregates over system tree or displays values for every thread separately. In addition it provides user to define new metrics(see file `CubeDerivedMetrics.pdf`). Results are calculated and shown. For convenience user can invoke defined metrics along with new once in any order. For doing so one lists unique names of metrics separated by commas. For access to more than one callpaths, user can specify the ids or a range of them like "2-9". This also can be done for threads. Additionally provides a calculation of the flat profile values.

-m **<metrics>|<new metrics>|all|<filename>** Select one or more of metrics (unique names) for data dump.

By giving a CubePL expression one can define one or more new metrics by giving correspond formula. If the expression prefixed with "**< name \>:**", **< name >** is used as a unique name for the new metric.

<filename> - takes a CubePL expression from file **<filename>** and defines a derived metric with it

all - all metrics will be printed.

Combination of these three is possible.

-c **<cnode ids>|all|leafs|roots|level>X|level=X|level<X|name=/regexp/|<filename>**

Select one or more call paths to be printed out .

<cnode ids> - list or range of call path ids: 0,3,5-10,25

all - all call paths are printed

leafs - only call paths without children are printed

roots - only root cnodes are printed

level<X, level=X or level>X - only cnodes of the level more, equal or less than N are printed

name=/regexp/- only cnodes with the region name matching to the regular expression *regexp*

<filename> - takes a CubePL expression from file **<filename>** and evaluates it for every callpath.

If the result is non-zero - call path is included into the output.

-x incl|excl Selects, if the data along the metric tree should be calculated as an inclusive or an exclusive value.

(Default value: incl).

-z incl|excl|stored Selects, if the data along the call tree should be calculated as an inclusive or an exclusive value.

(Default value: excl).

-t <thread id>|aggr Show data for one or more selected threads or aggregated over system tree.

-r Prints aggregated values for every region (flat profile), sorted by id.

-f < name > Selects a stored data with the name **< name >** to display

-d Shows the coordinates for every topology as well.

-y Disables expansion of clusters and shows bare stored meta structure.

-w Prints out the information about structure of the cube.

-o <filename>|- Uses a device or STDOUT for the output. If omit, STDOUT is used.

-s human|gnuplot|gnuplot2|csv|csv2|R Uses either human readable form, GNUPLOT or CSV (two different layouts) format or binary R matrix for data export.

-h|-? Help; Output a brief help message.

This is examples of the usage.

Example 1:

```
$cube_dump -m time,"metric::visits(e)","metric::time(i)/metric::visits(e)" -c 0 \  
-z incl -s gnuplot profile.cubex
```

```
# ===== DATA =====
```

```
# Print out the data of the metric time
```

```
#main(id=0)
```

```
0 0 80.549003343  
0 1 44.115097986  
0 2 43.486614165  
0 3 43.940738098  
0 4 80.539393011  
0 5 42.723353088  
0 6 42.61159706  
0 7 43.108220977  
0 8 80.635220741  
0 9 43.788284208  
0 10 43.831524441  
0 11 43.652044759  
0 12 80.629776666  
0 13 42.692885677  
0 14 42.719330066  
0 15 42.732487708
```

```
# Print out the data of the metric New Metric1
```

```
#main(id=0)
```

```
0 0 80.549003343  
0 1 1.79769313486e+308  
0 2 1.79769313486e+308  
0 3 1.79769313486e+308  
0 4 80.539393011  
0 5 1.79769313486e+308  
0 6 1.79769313486e+308  
0 7 1.79769313486e+308  
0 8 80.635220741  
0 9 1.79769313486e+308  
0 10 1.79769313486e+308  
0 11 1.79769313486e+308  
0 12 80.629776666  
0 13 1.79769313486e+308  
0 14 1.79769313486e+308  
0 15 1.79769313486e+308
```

```
# Print out the data of the metric New Metric2
```

```
#main(id=0)
```

```
0 0 1
```

```
0  1  0
0  2  0
0  3  0
0  4  1
0  5  0
0  6  0
0  7  0
0  8  1
0  9  0
0 10  0
0 11  0
0 12  1
0 13  0
0 14  0
0 15  0
```

Example 2:

```
$cube_dump -m time -s gnuplot2 profile.cubex

# ===== CONFIGURE GNUPLOT =====
set logscal x ; set logscal y ; set grid ; set xrange [16:300000]
; set terminal png size "600,400"

# ===== DATA =====
# Print out the data of the metric time

;set output "0.png"
; plot 6.4e-18*x**(5.0/2.0) + 5.2e-05 t "setPrecision(int, PrecisionFormat)(id=18)" ,
1.2e-17*x**(7.0/3.0) + 3.6e-05 t "setRoundNr(int, PrecisionFormat)(id=19)" ,
2.1e-17*x**(9.0/4.0) + 3.1e-05 t "setUpperExpNr(int, PrecisionFormat)(id=20)" ,
7.1e-19*x**(5.0/2.0) + 8.8e-06 t "getInstance()(id=21)" ,
2.8e-18*x**(2.0/1.0)*log(x) + 3.3e-06 t "getCubePluginCount()(id=24)"

;set output "1.png"
; plot 1.3e-20*x**(5.0/2.0)*log(x) + 4.2e-06 t "PluginList()(id=25)" ,
9.7e-18*x**(7.0/3.0) + 1.1e-05 t "loadContextFreePlugin(PluginData&)(id=28)" ,
1e-17*x**(9.0/4.0) + 8.8e-06 t "loadCubePlugin(PluginData&)(id=29)" ,
1e-18*x**(9.0/4.0) + 1.1e-06 t "name() const(id=35)" ,
2.6e-18*x**(2.0/1.0)*log(x) + 3.7e-06 t "getCubePlugin(int)(id=44)"
```

Example 3:

```
$cube_dump -m time,"metric::visits(e)","metric::time(i)/metric::visits(e)" -c 0 \
-t aggr -z incl -s human profile.cubex
```

```
===== DATA =====
Print out the data of the metric time
```

All threads

```
main(id=0) 841.755571994
Print out the data of the metric New Metric1
```

All threads

```
-----
main(id=0) 210.438892999
Print out the data of the metric New Metric2
```

All threads

```
-----
main(id=0) 4
-----
```

Example 4:

```
$cube_dump -m time,"metric::visits(e)","metric::time(i)/metric::visits(e)" -c 20 \
-z incl -s csv profile.cubex
```

```
20,0,8.9812e-05
20,1,0
20,2,0
20,3,0
20,4,9.7463e-05
20,5,0
20,6,0
20,7,0
20,8,0.000132327
20,9,0
20,10,0
20,11,0
20,12,7.2788e-05
20,13,0
20,14,0
20,15,0
```

```
20,0,8.9812e-05
20,1,-1.79769313486e+308
20,2,-1.79769313486e+308
20,3,-1.79769313486e+308
20,4,9.7463e-05
20,5,-1.79769313486e+308
20,6,-1.79769313486e+308
20,7,-1.79769313486e+308
20,8,0.000132327
20,9,-1.79769313486e+308
20,10,-1.79769313486e+308
20,11,-1.79769313486e+308
20,12,7.2788e-05
20,13,-1.79769313486e+308
20,14,-1.79769313486e+308
20,15,-1.79769313486e+308
```

```
20,0,1
20,1,0
```

```
20,2,0
20,3,0
20,4,1
20,5,0
20,6,0
20,7,0
20,8,1
20,9,0
20,10,0
20,11,0
20,12,1
20,13,0
20,14,0
20,15,0
```

Example 5:

```
$cube_dump -m time,"metric::visits(e)","metric::time(i)/metric::visits(e)" -c 1 \
  -z incl -s csv2 profile.cubex
```

```
Cnode ID, Thread ID,time,New Metric1,New Metric2
1,0,80.548967177,80.548967177,1
1,1,44.115097986,1.79769313486e+308,0
1,2,43.486614165,1.79769313486e+308,0
1,3,43.940738098,1.79769313486e+308,0
1,4,80.539359524,80.539359524,1
1,5,42.723353088,1.79769313486e+308,0
1,6,42.61159706,1.79769313486e+308,0
1,7,43.108220977,1.79769313486e+308,0
1,8,80.635176341,80.635176341,1
1,9,43.788284208,1.79769313486e+308,0
1,10,43.831524441,1.79769313486e+308,0
1,11,43.652044759,1.79769313486e+308,0
1,12,80.629742485,80.629742485,1
1,13,42.692885677,1.79769313486e+308,0
1,14,42.719330066,1.79769313486e+308,0
1,15,42.732487708,1.79769313486e+308,0
```

Example 6:

```
$cube_dump -m time,"metric::visits(e)","metric::time(i)/metric::visits(e)" -c 1 \
  -z incl -s R profile.cubex -o output_file
```

This will generate binary file "output_file" which can be loaded in R. It consists of three matrices, each one corresponding to one metric. Each matrix is named after the metric and it contains values for all threads and nodes.

Example 7: We select only call path names, starting with "main" using the CubePL expression (stored in file name "selection.cubep1") :


```
{
  ${a}=0;
  if (${cube::region::name}[${calculation::region::id}] =~ /^main/ )
  { ${a}=1; }; return ${a};
}
```

Then:

```
cube_dump -m time,"metric::visits(e)","metric::time(i)/metric::visits(e)" -c selection.cubep1 \
-z incl -t aggr profile.cubex
```

```
===== DATA =====
```

Print out the data of the metric time

All threads

```
-----
main(id=0)          841.755571994
main_loop(id=12)    840.73706946
```

Print out the data of the metric New Metric1

All threads

```
-----
main(id=0)          210.438892999
main_loop(id=12)    0.210184267365
```

Print out the data of the metric New Metric2

All threads

```
-----
main(id=0)          4
main_loop(id=12)    4000
```

Options "leafs", "roots", "level=", "level<", "level>" and "name=/regexp/" are shortcuts for a build-in CubePL expression, which is used to select a call path.

- **"leafs"** : stands for:

```
{
  ${a}=0;
  if (${cube::callpath::#children}[${calculation::callpath::id}] == 0 )
  { ${a}=1; }; return ${a};
}
```

- **"roots"** : stands for:

```
{
  ${a}=0;
  if (${cube::callpath::parent::id}[${calculation::callpath::id}] == -1 )
  { ${a}=1; }; return ${a};
}
```

- **"level=N"** : stands for:

```
{
  ${level}=N;
  ${index}=0;
```

```
{i}=${calculation::callpath::id};
while ( ${cube::callpath::parent::id}[{i}] != -1 )
{ {i}= ${cube::callpath::parent::id}[{i}]; {index}=${index}+1; };
{a}=0;
if ( {index} ==  ${level} )
{ {a}=1; };
return {a};
}
```

- **"name=/regexp/"** : stands for:

```
{
  {a}=0;
  if ( ${cube::region::name}[ ${calculation::region::id} ] =~ /regexp/ )
  { {a}=1; }; return {a};
};
```

"level<N" and "level>N" differ from "level=N" in the boolean operation in the line 8. For detailed documentation of the syntax of CubePL please see.

