JÜLICH
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Scalasca 1.2 – User Guide

Scalable Automatic Performance Analysis

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Contents

1 Introduction

Supercomputing is a key technology of modern science and engineering, indispensable to solve critical problems of high complexity. As a prerequisite for the productive use of today's large-scale computing systems, the HPC community needs powerful and robust performance analysis tools that make the optimization of parallel applications both more effective and more efficient.

Developed at the Jülich Supercomputing Centre, Scalasca is a performance analysis toolset that has been specifically designed for use on large-scale systems including IBM Blue Gene and Cray XT, but also suitable for smaller HPC platforms using MPI and/or OpenMP. Scalasca supports an incremental performance analysis process that integrates runtime summaries with in-depth studies of concurrent behavior via event tracing, adopting a strategy of successively refined measurement configurations. A distinctive feature of Scalasca is the ability to identify wait states that occur, for example, as a result of unevenly distributed workloads. Especially when trying to scale communication intensive applications to large processor counts, such wait states can present severe challenges to achieving good performance. Compared to its predecessor KOJAK [9], Scalasca can detect such wait states even in very large configurations of processes using a novel parallel trace-analysis scheme [4].

1.1 How to read this document

This user guide is structured into three parts:

- This introductory chapter gives a short introduction into performance analysis in general and the components of the Scalasca toolset in particular. If you are already familiar with performance analysis of parallel scientific applications you might skip the following section and continue reading directly with Section 1.3.
- The next part in Chapter 2 introduces the basic steps and commands required for initial performance analyses of parallel applications. It also includes a full example describing the Scalasca performance analysis workflow.
- The remainder of this user guide in Chapters 3 to 5 provide a more in-depth discussion of the individual steps in evaluating the performance of a parallel application.

1.2 Performance optimization cycle

Regardless of whether an application should be optimized for single-core performance or for scalability, the basic approach is very similar. First, the behavior of the application needs to be monitored, and afterwards the recorded behavior can be evaluated to draw conclusions for further improvement. This is an iterative process that can be described by a cycle, the so-called performance optimization cycle. When broken down into phases, it is comprised of:

- Instrumentation
- Measurement
- Analysis
- Presentation
- Evaluation
- Optimization of the code

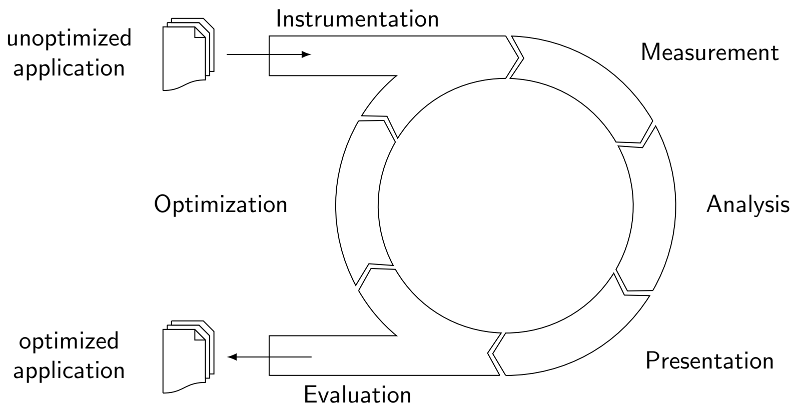


Figure 1.1: Performance optimization cycle

As shown in Figure 1.1, the user starts with the original (i.e., unoptimized) application, which enters the optimization cycle in the instrumentation phase. Instrumentation describes the process of modifying the application code to enable measurement of performance relevant data during the application run. In the context of Scalasca, this can be achieved by different mechanisms, such as source-code instrumentation, automatic compiler-based instrumentation or linking with pre-instrumented libraries. Instrumentation on the source-code level can be done by introducing additional instructions into the source code prior to compilation. On most systems, this process can be automated by using special features of the compiler. However, this approach typically does not allow a fine-grained control of the instrumention. The third method is to use pre-instrumented libraries, which contain instrumented versions of the relevant library functions. The Message-Passing Interface standard MPI [7] provides a special interface for this kind of instrumentation, the so-called PMPI interface. As this interface is defined in the MPI standard, its API is portable and creates an opportunity for tool developers to provide a single portable measurement library for multiple different MPI implementations.

When the instrumented code is executed during the measurement phase, performance data is collected. This can be stored as a profile or an event trace, depending on the desired level of information needed. The additional instructions inserted during instrumentation and associated measurement storage require resources (memory as well as CPU time). Therefore the application execution is affected to a certain degree. Perturbation by the additional measurement instructions may be small enough to get a fairly accurate view of the application behavior. However, certain application properties like frequently executed regions with extremely small temporal extent, will always lead to a high perturbation. Thus the measurement of those regions must be avoided.

The measurement data can then be analyzed after application execution. If a detailed event trace has been collected, more sophisticated dependencies between events occuring on different provesses can be investigated, resulting in a more detailed analysis report. Especially inter-process event correlations can usually only be analyzed by a post-mortem analysis. The information which is needed to analyze these correlations are usually distributed over the processes. Transferring the data during normal application runtime would lead to a significant perturbation during measurement, as it would require application resources on the network for this.

After analyzing the collected data, the result needs to be presented in an analysis report. This leads to the next phase in the performance optimization cycle, namely the presentation phase. At this stage, it is important to reduce the complexity of the collected performance data to ease evaluation by the user. If the presented data is too abstract, performance critical event patterns might not be recognized by the user. If it is too detailed, the user might drown in too much data. User guidance is therefore the key to productive application optimization.

In the evaluation phase, conclusions are drawn from the presented information, leading to optimization hypotheses. The user proposes optimization strategies for the application, which are then implemented in the following optimization phase. Afterwards, the effectiveness of the optimization has to be verified by another pass through the performance optimization cycle. When the user is satisfied with the application performance during evaluation, and no further optimization is needed, the instrumentation can be disabled, and the performance of the uninstrumented application execution can be assessed.

1.3 Scalasca overview

Scalasca supports measurement and analysis of the MPI, OpenMP and hybrid MPI/OpenMP programming constructs most widely used in highly scalable HPC applications written in C, C++ and Fortran on a wide range of current HPC platforms. Usage is primarily via the `scalasca` command with appropriate action flags. Figure 1.2 shows the basic analysis workflow supported by Scalasca. Before any performance data can be collected, the target application needs to be instrumented. Instrumentation means, that the code must be modified to record performance-relevant events whenever they occur. On most systems, this can be done completely automatically using compiler support. On other systems, a mix of manual and automatic instrumentation mechanisms is offered. When executing the instrumented code on a parallel machine, the user can generate a summary report (also known as *profile*) with aggregate performance metrics for individual function call paths. Furthermore, event traces can be generated by recording individual runtime events from which a profile or a time-line visualization can later be produced. The runtime summarization capability is useful to obtain an overview of the performance behaviour and also to optimize the instrumentation for later trace generation. Since traces tend to become very large, and inappropriate instrumentation and measurement configuration will compromise the resulting analysis, this step is highly recommended.

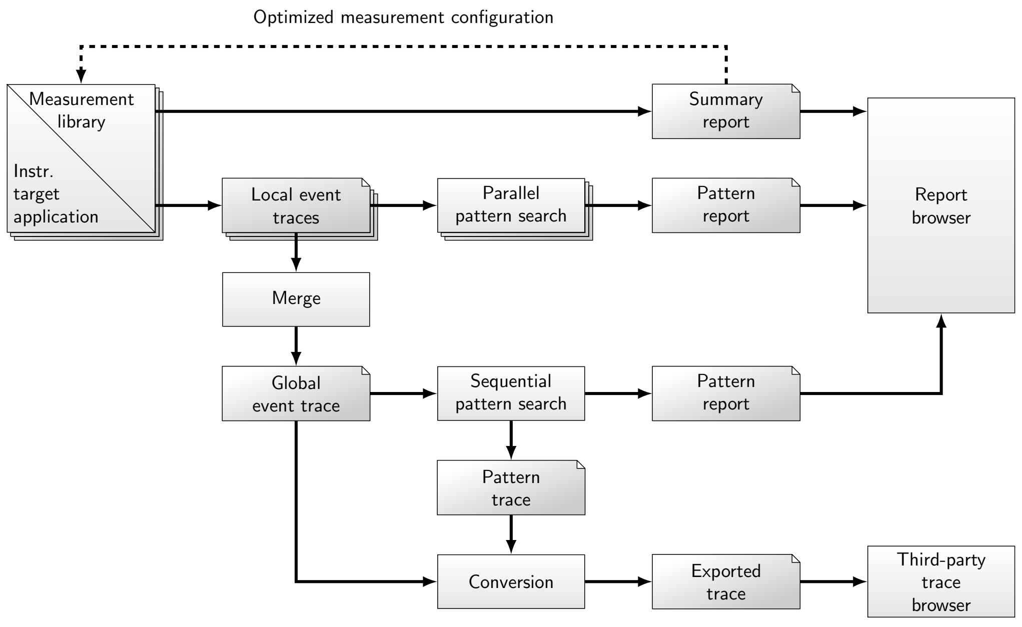


Figure 1.2: Scalasca's performance analysis workflow

When tracing is enabled, each process generates a trace file containing records for all its process-local events. After program termination, Scalasca reloads the trace files back into main memory and analyzes them in parallel using as many CPUs as have been used for the target application itself. During the analysis, Scalasca searches for characteristic patterns indicating wait states and related performance properties, classifies detected instances by category and quantifies their significance. The result is a pattern-analysis report similar in structure to the summary report but enriched with higher-level communication and synchronization inefficiency metrics. Both summary and pattern reports contain performance metrics for every function call path and system resource which can be interactively explored in a graphical report explorer (see Figure 2.1 for an example). As an alternative to the automatic analysis, the event traces can be converted and investigated using third-party trace browsers such as Paraver [6, 3] or Vampir [8, 5], taking advantage of their powerful time-line visualizations and rich statistical functionality.

2 Getting Started

This chapter will provide a hands-on introduction to the use of the Scalasca toolset on the basis of the analysis of an example application. The most prominent features will be addressed, and at times a reference to later chapters with more in-depth information on the corresponding topic will be given.

Use of Scalasca involves three phases: program instrumentation, execution measurement and analysis, and analysis report examination. The `scalasca` command provides action options that invoke the corresponding commands `skin`, `scan` and `square`.

These actions are:

1. `scalasca -instrument`

   used to insert calls to the Scalasca measurement system into the application's code, either automatically, semi-automatically or by linking with pre-instrumented libraries.

2. `scalasca -analyze`

   used to control the measurement environment during the application execution, and to automatically perform trace analysis after measurement completion if tracing was enabled.

   The Scalasca measurement system supports runtime summarization and/or event trace collection and analyses, optionally including hardware-counter information.

3. `scalasca -examine`

   used to postprocess the analysis report generated by the measurement runtime summarization and/or post-mortem trace analysis, and to start Scalasca's analysis report examination browser CUBE3.

To get a brief usage summary, call the `scalasca` command with no arguments, or use `scalasca -h` to open the Scalasca Quick Reference (only works if a suitable PDF viewer can be found).

The following three sections provide a quick overview of each of these actions and how to use them during the corresponding step of the performance analysis, before a full workflow example is presented in Section 2.4.

2.1 Instrumentation

To make measurements with the Scalasca measurement system, user application programs need to be instrumented, i.e., at specific important points (events) during the application run, special measurement calls have to be inserted. In addition to an almost automatic approach using compiler-inserted instrumentation (Section 3.1), semi-automatic "POMP" (Section 3.3) and manual instrumentation (Section 3.2) approaches are also supported.

For pure OpenMP or hybrid MPI/OpenMP applications, or when using the semi-automatic "POMP" directive-based approach, the OPARI source code instrumenter is used internally. Read the OPARI section in the OPEN_ISSUES file provided as part of the Scalasca documentation to be aware of its current limitations and how to work around some of them, including:

- parallel builds (e.g., using `gmake -j`)
- multiple applications built within a single directory
- applications with sources spread over multiple directories

All the necessary instrumentation of user and MPI functions is handled by the Scalasca instrumenter, which is accessed through the `scalasca -instrument` command. Therefore, the compile and link commands to build the application that is to be analyzed should be prefixed with `scalasca -instrument` (e.g., in a Makefile).

For example, to instrument the application executable `myprog` generated from the two source files `myprog1.f90` and `myprog2.f90`, replace the combined compile and link command

```
mpif90 myprog1.f90 myprog2.f90 -o myprog
```

by the following command using the Scalasca instrumenter:

```
scalasca -instrument mpif90 myprog1.f90 myprog2.f90 -o myprog
```

Note:

The instrumenter must be used with the link command. However, not all object files need to be instrumented, and it is often sufficient to only instrument source modules containing MPI code.

When using Makefiles, it is often convenient to define a "preparation" placeholder variable (e.g., `PREP`) which can be prefixed to (selected) compile and link commands:

```
MPICC  = $(PREP) mpicc
MPICXX = $(PREP) mpicxx
MPIF90 = $(PREP) mpif90
```

These can make it easier to prepare an instrumented version of the program by building with

```
make PREP="scalasca -instrument"
```

while default builds (without specifying `PREP` on the command line) remain fully optimized and without instrumentation.

Although generally most convenient, automatic function instrumentation may result in too many and/or too disruptive measurements, which can be addressed with selective instrumentation and measurement filtering (see Section 3.4).

2.2 Runtime Measurement Collection & Analysis

The Scalasca measurement collection & analysis nexus accessed through the `scalasca -analyze` command integrates the following steps:

- Measurement configuration
- Application execution
- Collection of measured data
- Automatic post-mortem trace analysis (if configured)

To make a performance measurement using an instrumented executable, the target application execution command is prefixed with the `scalasca -analyze` command:

```
scalasca -analyze [options] \
         $MPIEXEC $MPI_FLAGS [target [target args]]
```

For non-MPI (i.e., serial and pure OpenMP) applications, the MPI launch command and associated flags should be omitted.

A unique directory is used for each measurement experiment, which must not already exist when measurement starts. Measurement is aborted if the specified directory exists. A default name for each EPIK measurement archive directory is created from the name of the target application, the run configuration (e.g., number of processes and `OMP_NUM_THREADS` specified), and the measurement configuration. This archive name has an `epik_` prefix and its location can be explicitly specified to Scalasca with the `-e <path>` option or changed via configuration variables.

When the measurement has completed, the measurement archive directory contains various log files and one or more analysis reports. By default, runtime summarization is used to provide a summary report of the number of visits and time spent on each callpath by each process. For MPI measurements, MPI time and message and file I/O statistics are included. For OpenMP measurements, OpenMP-specific metrics are calculated. Hybrid OpenMP/MPI measurements contain both sets of metrics. If hardware counter metrics were requested, these are also included in the summary report.

Event trace data can also be collected as a part of the measurement, producing an EPILOG trace file for each process. To collect event trace data as part of the measurement, use the `scalasca -analyze -t` command or set the configuration variable `EPK_TRACE=1`. In this case, experiment trace analysis is automatically initiated by `scalasca -analyze` after measurement is complete.

The `scalasca -analyze -n` preview mode can be used to show (but not actually execute) the measurement and analysis launch commands, along with various checks to determine the possible success. Additional comments (via `-v`) may also be revealing, especially if measurement or analysis was unsuccessful.

In case of problems which are not obvious from reported errors or warnings, set the configuration variable `EPK_VERBOSE=1` before executing the instrumented application to see control messages of the Scalasca measurement system. This might help to track down the problem or allow a detailed problem report to be given to the Scalasca developers.

When using environment variables in a cluster environment, make sure that they have the same value for all application processes on *all* nodes of the cluster. Some cluster environments do not automatically transfer the environment when executing parts of the job on remote nodes of the cluster, and may need to be explicitly set and exported in batch job submission scripts.

2.3 Analysis Report Examination

The results of the automatic analysis are stored in one or more reports in the experiment archive. These reports can be processed and examined using the `scalasca -examine` command on the experiment archive:

```
scalasca -examine epik_<title>
```

Post-processing is done the first time that an archive is examined, before launching the CUBE3 report viewer. If the `scalasca -examine` command is executed on an already processed experiment archive, or with a CUBE file specified as argument, the viewer is launched immediately.

A short textual score report can be obtained without launching the viewer:

```
scalasca -examine -s epik_<title>
```

This score report comes from the `cube3_score` utility and provides a breakdown of the different types of region included in the measurement and their estimated associated trace buffer costs, aggregate trace size (total_tbc) and largest process trace size (max_-tbc), which can be used to specify an appropriate `ELG_BUFFER_SIZE` for a subsequent trace measurement.

The CUBE3 viewer can also be used on an experiment archive or CUBE file:

```
cube3 epik_<title>
cube3 <file>.cube
```

However, keep in mind that no post-processing is performed in this case, so that only a subset of Scalasca analyses and metrics may be shown.

2.3.1 Using CUBE3

The following paragraphs provide a very brief introduction of the CUBE3 usage. To effectively use the GUI, you should also read the CUBE3 manual provided with the Scalasca distribution.

CUBE3 is a generic user interface for presenting and browsing performance and debugging information from parallel applications. The underlying data model is independent from particular performance properties to be displayed. The CUBE3 main window consists of three panels containing tree displays or alternate graphical views of analysis reports. The left panel shows performance properties of the execution, the middle pane shows the call-tree or a flat profile of the application, and the right tree either shows the system hierarchy consisting of machines, compute nodes, processes, and threads or a topological view of the application's processes and threads. All tree nodes are labeled with a metric value and a coloured box which can help identify hotspots. The metric value colour is determined from the proportion of the total (root) value or some other specified reference value.

A click on a performance property or a call path selects the corresponding node. This has the effect that the metric value held by this node (such as execution time) will be further broken down into its constituents. That is, after selecting a performance property, the middle panel shows its distribution across the call tree. After selecting a call path (i.e., a node in the call tree), the system tree shows the distribution of the performance property in that call path across the system locations. A click on the icon left to a node in each tree expands or collapses that node. By expanding or collapsing nodes in each of the three trees, the analysis results can be viewed on different levels of granularity.

To obtain the exact definition of a performance property, select "Online Description" in the context menu associated with each performance property, which is accessible using the right mouse button. A brief description can be obtained from the menu option "Info". Further information is also available at the Scalasca website

http://www.scalasca.org/

CUBE3 also provides a number of algebra utilities which are command-line tools that operate on analysis reports. (The utililties currently only work on the CUBE files within experiment archive directories, not on the archives themselves.) Multiple analysis reports can be averaged with `cube3_mean` or merged with `cube3_merge`. The difference between two analysis reports can be calculated using `cube3_diff`. Finally, a new analysis report can be generated after pruning specified call trees and/or specifying a call-tree node as a new root with `cube3_cut`. The latter can be particularly useful for eliminating uninteresting phases (e.g., initialization) and focussing the analysis on a selected part of the execution. Each of these utilities generates a new CUBE-formated report as output.

The `cube3_score` utility can be used to estimate trace buffer requirements from summary or trace analysis reports. If sufficient memory is physically available, this can be specified in the ELG_BUFFER_SIZE configuration variable for a subsequent trace collection. Detailed region output (`cube3_score -r`) can also be examined to identify frequently executed regions that may adversely impact measurement and not be considered valuable as part of the analysis. Such regions without OpenMP and MPI operations may be appropriate for exclusion from subsequent experiments via selective instrumentation and measurement (see Section 3.4). Trace buffer capacity can be saved by eliminating certain functions from the measurement. This could be done by providing a filter file, which lists the function names of the functions to be excluded. A potential filter file can be evaluated with the option `-f <filter_file>`.

2.4 A Full Workflow Example

The previous sections introduced the general usage of Scalasca. This section will guide through an example analysis of a solver kernel called SOR, solving the Poisson equation using a red-black successive over-relaxation method. The environment used in the following examples is the IBM Blue Gene/P, present at the Jülich Supercomputing Centre of Forschungszentrum Jülich. The commands and outputs presented in this section might differ from the commands and outputs of your system.

By default, Scalasca uses the automatic compiler-based instrumentation feature. This is usually the best first approach, when you don't have detailed knowledge about the application and need to identify the hotspots in your code. SOR consists of only a single source file, which can be compiled and linked using the following two commands:

```
scalasca -instrument mpixlc -c sor.c
scalasca -instrument mpixlc sor.o -o sor.x
```

Now the instrumented binary must be executed on the system. On supercomputing systems, users usually have to submit their jobs to a batch system and are not allowed to start parallel jobs directly. Therefore, the call to the `scalasca` command has to be provided within a batch script, which will be scheduled for execution when the required resources are available.

The syntax of the batch script differs between the different scheduling systems. However, common to every batch script format is a passage where all shell commands can be placed that will be executed. Here, the call to the Scalasca analyzer has to be placed in front of the application execution command:

```
scalasca -analyze mpirun -mode vn -np 128 ./sor.x
```

Ensure that the `scalasca` command is accessible when the batch script is executed, e.g., by updating the PATH if necessary. The parameters `-mode` and `-np` are options of the `mpirun` command on the Blue Gene system and other launchers will have different flags and syntax.

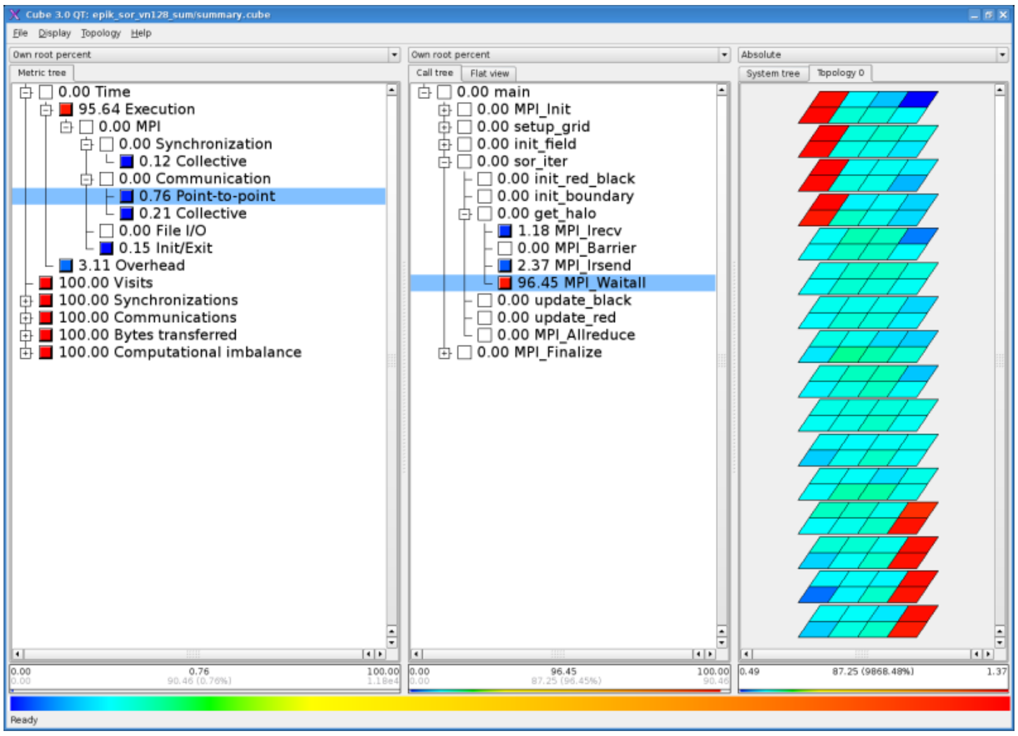
The Scalasca analyzer will take care of certain control variables, which assist in the measurement of your application. The default behaviour of the Scalasca analyzer is to create a summary file, and not to create a detailed event trace, as indicated by the initial messages from the EPIK measurement system.

```
S=C=A=N: Scalasca 1.2 runtime summarization
S=C=A=N: ./epik_sor_vn128_sum experiment archive
S=C=A=N: Collect start
mpirun -mode vn -np 128 ./sor.x
[00000]EPIK: Created new measurement archive ./epik_sor_vn128_sum
[00000]EPIK: Activated ./epik_sor_vn128_sum [NO TRACE]

            [... Application output ...]

[00000]EPIK: Closing experiment ./epik_sor_vn128_sum
...
[00000]EPIK: Closed experiment ./epik_sor_vn128_sum
S=C=A=N: Collect done
S=C=A=N: ./epik_sor_vn128_sum complete.
```

After successful execution of the job, a summary report file is created within a new measurement directory. In this example, the automatically generated name of the measurement directory is `epik_sor_vn128_sum`, indicating that the job was executed in Blue Gene's virtual node mode (`-mode vn`) with 128 processes (`-np 128`). The suffix `_sum` refers to a runtime summarization experiment. The summary analysis report can then be postprocessed and examined with the Scalasca report browser:

```
scalasca -examine epik_sor_vn128_sum
INFO: Post-processing runtime summarization report ...
INFO: Displaying ./epik_sor_vn128_sum/summary.cube ...
```

Figure 2.1 shows a screenshot of the Scalasca report browser CUBE3 with the summary analysis report of SOR opened. The examination of the application performance summary may indicate several influences of the measurement on your application behaviour. For example, frequently executed, short functions may lead to significant pertubation and would be prohibitive to trace: these need to be eliminated before further investigations using trace analysis are taken into account.



```
0.00 Time
  95.64 Execution
    0.00 MPI
      0.00 Synchronization
        0.12 Collective
      0.00 Communication
        0.76 Point-to-point
        0.21 Collective
      0.00 File I/O
      0.15 Init/Exit
  3.11 Overhead
100.00 Visits
100.00 Synchronizations
100.00 Communications
100.00 Bytes transferred
100.00 Computational imbalance
```

```
0.00 main
  0.00 MPI_Init
  0.00 setup_grid
  0.00 init_field
  0.00 sor_iter
    0.00 init_red_black
    0.00 init_boundary
    0.00 get_halo
      1.18 MPI_Irecv
      0.00 MPI_Barrier
      2.37 MPI_Irsend
      96.45 MPI_Waitall
    0.00 update_black
    0.00 update_red
    0.00 MPI_Allreduce
  0.00 MPI_Finalize
```

```
0.00          0.76             100.00   0.00          96.45             100.00   0.49     87.25 (9868.48%)     1.37
0.00    90.46 (0.76%)          1.18e4   0.00    87.25 (96.45%)           90.46
```

Figure 2.1: Viewing a runtime summary in CUBE

During trace collection, information about the application's execution behaviour is recorded in so-called event streams. The number of events in the streams determines the size of the buffer required to hold the stream in memory. To minimize the amount of memory required, and to reduce the time to flush the event buffers to disk, only the most relevant function calls should be instrumented.

When the complete event stream is larger than the memory buffer, it has to be flushed to disk during application runtime. This flush impacts application performance, as flushing is not coordinated between processes, and runtime imbalances are induced into the measurement. The Scalasca measurement system uses a default value of 10 MB per process or thread for the event trace: when this is not adequate it can be adjusted to minimize or eliminate flushing of the internal buffers. However, if too large a value is specified for the buffers, the application may be left with insufficient memory to run, or run adversely with paging to disk. Larger traces also require more disk space (at least temporarily, until analysis is complete), and are correspondingly slower to write to and read back from disk. Often it is more appropriate to reduce the size of the trace (e.g., by specifying a shorter execution, or more selective instrumentation and measurement), than to increase the buffer size.

To estimate the buffer requirements for a trace measurement, `scalasca -examine -s` will generate a brief overview of the estimated maximal number of bytes required.

```
scalasca -examine -s epik_sor_vn128_sum

[cube3_score epik_sor_vn128_sum/summary.cube]
Reading ./epik_sor_vn128_sum/summary.cube... done.
Estimated aggregate size of event trace (total_tbc): 25698304 bytes
Estimated size of largest process trace (max_tbc):   215168 bytes
(When tracing set ELG_BUFFER_SIZE > max_tbc to avoid intermediate flushes
 or reduce requirements using a file listing USR regions to be filtered.)

flt  type       max_tbc          time       % region
      ANY        215168      11849.04  100.00 (summary) ALL
      MPI        195728        147.47    1.24 (summary) MPI
      COM          9696        465.93    3.93 (summary) COM
      USR          9744      11235.64   94.82 (summary) USR
```

The line at the top of the table referring to `ALL` provides the aggregate information for all executed functions. In this table, the column `max_tbc` refers to the maximum of the trace buffer capacity requirements determined for each process in bytes. If `max_tbc` exceeds the buffer size available for the event stream in memory, intermediate flushes during measurement will occur. To prevent flushing, you can either increase the event buffer size or exclude a given set of functions from measurement.

To aid in setting up an appropriate filter file, this "scoring" functionality also provides a breakdown by different categories, determined for each region according to its type of call path. Type `MPI` refers to function calls to the MPI library and type `OMP` either to OpenMP regions or calls to the OpenMP API. User-program routines on paths that directly or indirectly call MPI or OpenMP provide valuable context for understanding the communication and synchronization behaviour of the parallel execution, and are distinguished with the `COM` type from other routines that are involved with purely local computation marked `USR`.

Routines with type `USR` are typically good candidates for filtering, which will effectively make them invisible to measurement and analysis (as if they were "inlined"). `COM` routines can also be filtered, however, this is generally undesirable since it eliminates context information. Since `MPI` and `OMP` regions are required by Scalasca analyses, these cannot be filtered.

By comparing the trace buffer requirements with the time spent in the routines of a particular group, the initial scoring report will already indicate what benefits can be expected from filtering. However, to actually set up the filter, a more detailed examination is required. This can be achieved by applying the `cube3_score` utility directly on the postprocessed summary report using the additional command-line option `-r`:

```
cube3_score -r epik_sor_vn128_sum/summary.cube

Reading summary.cube... done.
Estimated aggregate size of event trace (total_tbc): 25698304 bytes
Estimated size of largest process trace (max_tbc):   215168 bytes
(When tracing set ELG_BUFFER_SIZE > max_tbc to avoid intermediate flushes
 or reduce requirements using a file listing USR regions to be filtered.)

flt  type      max_tbc         time       % region
      ANY       215168     11849.04  100.00 (summary) ALL
      MPI       195728       147.47    1.24 (summary) MPI
      COM         9696       465.93    3.93 (summary) COM
      USR         9744     11235.64   94.82 (summary) USR

      MPI        80000         2.14    0.02 MPI_Irsend
      MPI        73600         1.07    0.01 MPI_Irecv
      MPI        16040        20.77    0.18 MPI_Allreduce
      MPI        16000        14.32    0.12 MPI_Barrier
      MPI         9600        87.25    0.74 MPI_Waitall
      COM         9600       304.28    2.57 get_halo
      USR         4800      5432.60   45.85 update_red
      USR         4800      5432.87   45.85 update_black
      MPI          240         0.54    0.00 MPI_Gather
      MPI          200         3.63    0.03 MPI_Bcast
      USR           48       368.66    3.11 TRACING
      USR           48         0.50    0.00 looplimits
      MPI           24         0.52    0.00 MPI_Finalize
      USR           24         0.54    0.00 init_boundary
      USR           24         0.48    0.00 init_red_black
      COM           24         2.88    0.02 sor_iter
      COM           24       156.25    1.32 init_field
      COM           24         0.82    0.01 setup_grid
      MPI           24        17.23    0.15 MPI_Init
      COM           24         1.70    0.01 main
```

(The basic form of this command is reported when running `scalasca -examine -s`.) As the maximum trace buffer required on a single process for the SOR example is approx. 215 KB, there is no need for filtering in this case.

Note:

Filtering will not prevent the function from being instrumented. Hence, measurement overhead can currently not be completely eliminated on filtered functions when automatic compiler-based instrumentation is used.

> Once the configuration of buffer sizes and/or filters have been determined, make sure they are specified for subsequent (tracing) measurements, via environment variables or an EPIK.CONF measurement configuration file in the working directory. A filter file can also be specified with `-f filter_file` to measurements with `scalasca -analyze`.
> Before initiating a trace measurement experiment, ensure that the filesystem where the experiment will be created is appropriate for parallel I/O (typically /scratch or /work rather than /home) and that there will be sufficient capacity (and/or quota) for the expected trace.

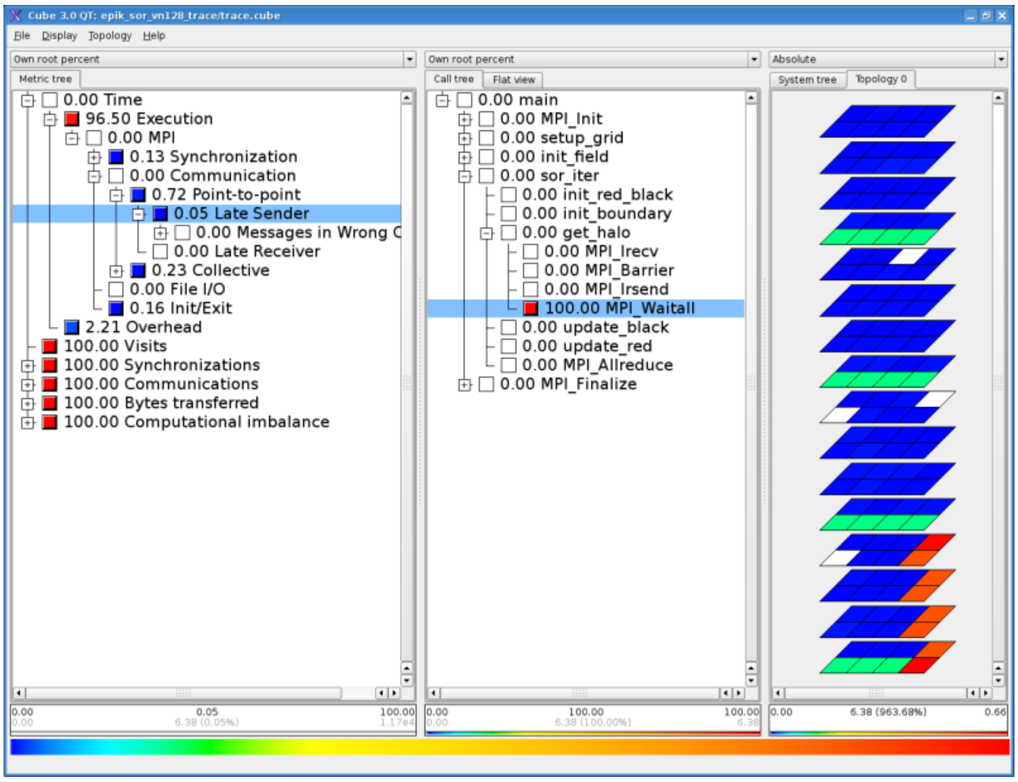
When all options of the Scalasca measurement system are set in a way that measurement overhead and space requirements are minimized, a new run of the instrumented application can be performed, passing the `-t` option to `scalasca -analyze`. This will enable the tracing mode of the Scalasca measurement system. Additionally, the parallel post-mortem trace analyzer searching for patterns of inefficient communication behaviour is automatically started after application completion.

```
scalasca -analyze -t mpirun -mode vn -np 128 ./sor.x

S=C=A=N: Scalasca 1.2 trace collection and analysis
S=C=A=N: ./epik_sor_vn128_trace experiment archive
S=C=A=N: Collect start
mpirun -mode vn -np 128 ./sor.x
[00000]EPIK: Created new measurement archive ./epik_sor_vn128_trace
[00000]EPIK: Activated ./epik_sor_vn128_trace [10000000 bytes]

            [... Application output ...]

[00000]EPIK: Closing experiment ./epik_sor_vn128_trace
[00000]EPIK: Flushed file ./epik_sor_vn128_trace/ELG/00000
...
[00013]EPIK: Flushed file ./epik_sor_vn128_trace/ELG/00013
[00000]EPIK: Closed experiment ./epik_sor_vn128_trace
S=C=A=N: Collect done
S=C=A=N: Analysis start
mpirun -mode vn -np 128 scout.mpi ./epik_sor_vn128_trace
            [... SCOUT output ...]
S=C=A=N: Analysis done
S=C=A=N: ./epik_sor_vn128_trace complete.
```

This creates an experiment archive directory `epik_sor_vn128_trace`, distinguishing it from the previous summary experiment through the suffix `_trace`. A separate trace file per MPI rank is written directly into a subdirectory when measurement is closed, and the parallel trace analyzer SCOUT is automatically launched to analyze these trace files and produce an analysis report. This analysis report can then be examined using the same commands and tools as the summary experiment.

```
scalasca -examine epik_sor_vn128_trace
INFO: Post-processing trace analysis report ...
INFO: Displaying ./epik_sor_vn128_trace/trace.cube ...
```

The screenshot in Figure 2.2 shows that the trace analysis result at first glance provides the same information as the summary result. However, the trace analysis report is enriched with additional performance metrics which show up as sub-metrics of the summary properties, such as the fraction of Point-to-point Communication Time potentially wasted due to Late Sender situations where early receives had to wait for sends to be initiated. That is, the trace analysis can reveal detail of inefficient execution behaviour.



```
0.00 Time
  96.50 Execution
    0.00 MPI
      0.13 Synchronization
      0.00 Communication
        0.72 Point-to-point
          0.05 Late Sender
            0.00 Messages in Wrong C
          0.00 Late Receiver
        0.23 Collective
      0.00 File I/O
      0.16 Init/Exit
  2.21 Overhead
100.00 Visits
100.00 Synchronizations
100.00 Communications
100.00 Bytes transferred
100.00 Computational imbalance
```

```
0.00 main
  0.00 MPI_Init
  0.00 setup_grid
  0.00 init_field
  0.00 sor_iter
    0.00 init_red_black
    0.00 init_boundary
    0.00 get_halo
      0.00 MPI_Irecv
      0.00 MPI_Barrier
      0.00 MPI_Irsend
      100.00 MPI_Waitall
    0.00 update_black
    0.00 update_red
    0.00 MPI_Allreduce
  0.00 MPI_Finalize
```

```
0.00        0.05              100.00
0.00        6.38 (0.05%)      1.17e4

0.00        100.00            100.00
0.00        6.38 (100.00%)    6.38

0.00        6.38 (963.68%)    0.66
```

Figure 2.2: Determine a Late Sender in CUBE3.

The filesystem requirements for an EPILOG event trace and its analysis are much higher than for a runtime summary. The runtime of a batch job will also increase due to additional file I/O at the end of measurement and for analysis. After successful tracing, the Scalasca measurement has created a directory containing the event trace and its analysis files. The default behaviour of Scalasca in tracing mode is to create a runtime summary report (stored in `summary.cube`) as well as a trace analysis report (stored in `trace.cube`).

After successful trace analysis, and before moving the experiment archive, the trace files can be removed by deleting the `ELG` subdirectory in the experiment archive.

3 Application instrumentation

Scalasca provides several possibilities to instrument user application code. Besides the automatic compiler-based instrumentation (Section 3.1), it provides manual instrumentation using the EPIK API (Section 3.2) and semi-automatic instrumentation using POMP directives (Section 3.3). Additionally, Scalasca provides a filtering model for excluding instrumented functions from measurement (Section 3.4).

Besides the instrumentation of user functions, Scalasca currently supports the following kinds of events:

- **MPI calls**:

  Instrumentation is accomplished using the standard MPI profiling interface PMPI. To enable it, the application program has to be linked against the EPIK MPI (or hybrid) measurement library plus MPI-specific libraries. Note that the EPIK libraries must be linked *before* the MPI library to ensure interposition will be effective.

- **OpenMP directives & API calls**:

  The Scalasca measurement system uses the OPARI tool for instrumentation of OpenMP constructs. See the OPARI documentation on how to instrument OpenMP source code. In addition, the application must be linked with the EPIK OpenMP (or hybrid) measurement library.

The Scalasca instrumenter command `scalasca -instrument` takes care of correct linking. When compiling without the Scalasca instrumenter, the `kconfig` command can be used to simplify determining the appropriate linker flags and libraries:

```
kconfig [--mpi|--omp|--hybrid] [--otf] [--for] [--32|--64] --libs
```

The `--mpi`, `--omp`, or `--hybrid` switch selects whether MPI, OpenMP or hybrid MPI/OpenMP measurement support is desired. By default, `kconfig` assumes a C or C++ program is being linked, Fortran applications have to be explicitly flagged with the `--for` switch. The `--32` or `--64` switch selects the 32-bit or 64-bit version of the measurement libraries, if necessary.

Note:

A particular installation of Scalasca may not offer all measurement configurations!

The `kconfig` command can also be used to determine the right compiler flags for specifying the include directory of the `epik_user.h` or `epik_user.inc` header files when compiling without using the Scalasca instrumenter:

```
kconfig --cflags
```

The following table gives an overview of the different possible calls of the Scalasca instrumenter and which API calls or directives are instrumented by each call.

Option	MPI	OpenMP	POMP	EPIK API	Compiler-based
none (MPI)	X	—	—	—	X
none (OpenMP)	—	X	—	—	X
none (hybrid)	X	X	—	—	X
`-user` (MPI)	X	—	—	X	X
`-user` (OpenMP)	—	X	—	X	X
`-user` (hybrid)	X	X	—	X	X
`-pomp`	X	X	X	—	—
`-pomp` `-user`	X	X	X	X	—

Table 3.1: Scalasca instrumenter option overview

3.1 Automatic function instrumentation

Most current compilers support automatic insertion of instrumentation calls at function entry and exit(s), and Scalasca can use this capability to determine which functions are executed in an instrumented measurement.

Note:

Depending on the compiler, and how it performs instrumentation, insertion of instrumentation may disable inlining and other significant optimizations, or inlined functions may not be instrumented at all (and therefore "invisible").

Automatic compiler-based instrumentation has been tested with a number of different compilers:

- GCC (UNIX-like operating systems, not tested with Windows)
- IBM xlc, xlC (version 7 or later, IBM Blue Gene and AIX)
- IBM xlf (version 9.1 or later, IBM Blue Gene and AIX)
- PGI (Cray XT and Linux)
- Intel compilers (version 10 or later, Cray XT and Linux, not tested with Windows)
- SUN Studio compilers (Linux and Solaris, Fortran only)
- PathScale compilers (Cray XT and SiCortex)
- CCE/Cray compiler (Cray XT)
- NEC compiler (NEC SX)

In all cases, Scalasca supports automatic instrumentation of C, C++ and Fortran codes, except for the SUN Studio compilers which only provide appropriate compiler support for Fortran.

Note:

> The automatic compiler instrumentation might create a significant relative measurement overhead on short function calls. This can impact the overall application performance during measurement. C++ applications are especially prone to suffer from this, depending on application design and whether C++ STL functions are also instrumented by the compiler. Currently, it is not possible to prevent the instrumentation of specific functions on all platforms when using automatic compiler instrumentation. See Section 3.4 on how to manually instrument applications if you encounter significant overheads.

Names provided for instrumented functions depend on the compiler, which may add underscores and other decorations to Fortran and C++ function names, and whether name "demangling" has been enabled when Scalasca was installed and could be applied successfully.

3.2 Manual region instrumentation

If the automatic compiler-based instrumentation (see Section 2.1) or semi-automatic instrumentation (see Section 3.3) procedure fails, instrumentation can be done manually.

Manual instrumentation can also be used to augment automatic instrumentation with region or phase annotations, which can improve the structure of analysis reports. Generally, the main program routine should be instrumented, so that the entire execution is measured and included in the analyses.

Instrumentation can be performed in the following ways, depending on the programming language used.

Fortran:

```
#include "epik_user.inc"

subroutine foo(...)
    !declarations
    EPIK_FUNC_REG("foo")
    EPIK_USER_REG(r_name,"iteration loop")
    EPIK_FUNC_START()
    ...
    EPIK_USER_START(r_name)
    do i= 1, 100
        ...
    end do
    EPIK_USER_END(r_name)
    ...
    EPIK_FUNC_END()
end subroutine foo
```

C/C++:

```
#include "epik_user.h"

void foo(...)
{
    /* declarations */
    EPIK_USER_REG(r_name,"iteration loop");
    EPIK_FUNC_START();
    ...
    EPIK_USER_START(r_name);
    for (i = 0; i < 100; ++i)
    {
       ...
    }
    EPIK_USER_END(r_name);
    ...
```

```
        EPIK_FUNC_END();
    }
```

C++ only:

```
    #include "epik_user.h"

    void foo(...)
    {
        EPIK_TRACER("foo");
        ...
    }
```

Region identifiers (`r_name`) should be registered in each annotated function/subroutine prologue before use within the associated body, and should not already be declared in the same program scope. For C and C++, function names are automatically provided by the `EPIK_FUNC_BEGIN` and `EPIK_FUNC_END` macros (so don't need registering), whereas annotated Fortran functions and subroutines should call `EPIK_FUNC_REG` with an appropriate name.

The source files instrumented in this way have to be compiled with `-DEPIK` otherwise `EPIK_*` calls expand to nothing and are ignored. If the Scalasca instrumenter `-user` flag is used, the `EPIK` symbol will be defined automatically. Also note, that Fortran source files instrumented this way have to be preprocessed with the C preprocessor (CPP).

Manual function instrumentation in combination with automatic source code instrumentation by the compiler leads to double instrumentation of user functions, i.e., usually only user region instrumentation is desired in this case.

For examples of how to use the EPIK user API, see the `*-epik.*` files in the example directory of the Scalasca installation.

3.3 Semi-automatic instrumentation

If you manually instrument the desired user functions and regions of your application source files using the POMP `INST` directives described below, the Scalasca instrumenter `-pomp` flag will generate instrumentation for them. POMP instrumentation directives are supported for Fortran and C/C++. The main advantages are that

- being directives, the instrumentation is ignored during "normal" compilation and
- this semi-automatic instrumentation procedure can be used when fully automatic compiler instrumentation is not supported.

The `INST BEGIN/END` directives can be used to mark any user-defined sequence of statements. If this block has several exit points (as is often the case for functions), all but the last have to be instrumented by `INST ALTEND`.

Fortran:

```
subroutine foo(...)
    !declarations
    !POMP$ INST BEGIN(foo)
    ...
    if (<condition>) then
        !POMP$ INST ALTEND(foo)
        return
    end if
    ...
    !POMP$ INST END(foo)
end subroutine foo
```

C/C++:

```
void foo(...)
{
    /* declarations */
    #pragma pomp inst begin(foo)
    ...
    if (<condition>)
    {
        #pragma pomp inst altend(foo)
        return;
    }
    ...
    #pragma pomp inst end(foo)
}
```

At least the main program function has to be instrumented in this way, and additionally, one of the following should be inserted as the first executable statement of the main program:

Fortran:

```
program main
    ! declarations
    !POMP$ INST INIT
    ...
end program main
```

C/C++:

```
    int main(int argc, char** argv)
    {
        /* declarations */
        #pragma pomp inst init
        ...
    }
```

For an example of how to use the POMP directives, see the `*-pomp.*` files in the example directory of the Scalasca installation.

3.4 Selective instrumentation and measurement

Scalasca experiments contain by default only summarized metrics for each call path and process/thread. More detailed analyses, providing additional metrics regarding wait states and other inter-process inefficiencies, require that event traces are collected in buffers on each process that must be adequately sized to store events from the entire execution.

Instrumented functions which are executed frequently, while only performing a small amount of work each time they are called, have an undesirable impact on measurement. The measurement overhead for such functions is large in comparison to the execution time of the uninstrumented function, resulting in measurement dilation. Recording such events requires significant space and analysis takes longer with relatively little improvement in quality.

Ideally, such functions (or regions) should not be instrumented, to entirely remove their impact on measurement. Uninstrumented functions are still executed, but become "invisible" in measurement and subsequent analyses (as if inlined). Manual annotations (see Section 3.2) or POMP directives (see Section 3.3) should be removed or disabled.

Automatic function instrumentation, working at the level of source modules, can be disabled by selectively compiling such sources normally, i.e., without preprocessing with the Scalasca instrumenter.

Note:

The instrumenter is, however, still required when linking.

If only some functions within a source module should be instrumented and others left uninstrumented, the module can be split into separate files, or compiled twice with conditional preprocessor directives selecting the separate parts and producing separate object files.

Alternatively, a measurement filtering capability is supported for most (but not all) compilers. A file containing the names of functions (one per line) to be excluded from measurement can be specified using the EPIK configuration variable `EPK_FILTER` or alternatively via the `-f <filter_file>` option of the `scalasca -analyze` command (and will be archived in `epik_<title>/epik.filt` as part of the experiment). Filter function names can include wildcards (`"*"`) and, if name demangling is not supported, then linker names must be used. On the other hand, if C++ name demangling is supported, `"*"` characters indicating pointer variables have to be escaped using a backslash.

Whenever a function marked for filtering is executed, the measurement library skips making a measurement event, thereby substantially reducing the overhead and impact of such functions. In some cases, even this minimal instrumentation processing may be undesirable, and the function should be excluded from instrumentation as described previously.

4 Measurement Collection & Analysis

The Scalasca measurement collection and analysis nexus manages the configuration and processing of performance experiments with an instrumented executable. Many different experiments can typically be performed with a single instrumented executable without needing to re-instrument, by using different measurement and analysis configurations. The default runtime summarization mode directly produces an analysis report for examination, whereas event trace collection and analysis are automatically done in two steps.

The distinctive feature of Scalasca is the automatic analysis of event traces in order to find performance bottlenecks. Internally, performance problems are specified in terms of execution patterns that represent standard situations of inefficient behaviour. These patterns are used during the analysis process to recognize and quantify the inefficient behaviour in the application.

The analysis of traces from pure MPI or hybrid MPI/OpenMP programs can be performed in parallel (with as many processes and threads as the original application execution), see section 4.4. Pure OpenMP traces are still analyzed sequentially, see section 4.5.

Scalasca not only supports the analysis of function calls and user-defined source-code regions (cf. chapter 3), but also the analysis of hardware performance counter metrics, see section 4.3.

4.1 Nexus configuration

The Scalasca measurement collection and analysis nexus (SCAN) is a command prefixed to the command used to launch and run the application executable. Arguments can be given to specify whether tracing should be enabled (`-t`), a filter that should be applied (`-f filter_file`, and hardware counters that should be included in the measurement (`-m metric_list`).

The target executable is examined to determine whether MPI and/or OpenMP instrumentation is present, and the number of MPI processes and OpenMP threads are determined from the launch environment and command-line specification. These are used to generate a default name for the experiment, unless a title has been explicitly specified with `-e expt_title` (or `EPK_TITLE`). (Where the number of processes and/or threads are omitted, or were otherwise not determined, the number is replaced with the letter '`O`' is used to indicate this.)

Note:

Configuration specified on the nexus command-line takes precedence over that specified as environment variables or in a configuration file.

Environment variables with the `SCAN_` prefix may be used to configure the nexus itself (which is a serial workflow manager process), as distinct from the instrumented application process or processes which will be measured, which are also configured via environment variables discussed in the following section 4.2.

Serial and OpenMP programs are typically executed directly, whereas MPI (and hybrid OpenMP/MPI) programs usually require a special launcher (such as `mpiexec`) which might also specify the number of processes to be created. Many MPI launchers are automatically recognized, but if not, the MPI launcher name can be specified with the environment variable `SCAN_MPI_LAUNCHER`. When the MPI launch command is being parsed, unrecognized flags might be reported as ignored, and unrecognized options with required arguments might need to be quoted.

Note:

Launcher-specific configuration files which augment the launch command are currently not handled by Scalasca.

If the target executable isn't specified as one of the launcher arguments, it is expected to be the immediately following part of the command line. It may be necessary to use a double-dash specification (`--`) to explicitly separate the target from the preceding launcher specification.

If there is an imposter executable or script, e.g., used to specify placement, that precedes the instrumented target, it may be necessary to explcitly identify the target with the environment variable `SCAN_TARGET`.

If environment variables aren't automatically forwarded to MPI processes by the launcher, it may be necessary to specify the syntax that the launcher requires for this as `SCAN_SETENV`. For example, if an environment variable VAR and value VAL must be exported with "--export VAR VAL" use `SCAN_SETENV=--export`, or use `SCAN_SETENV=-setenv=` for "-setenv VAR=VAL" syntax.

Trace analysis is done with different trace analyzers according to availability and the type of experiment. An alternate trace analyzer can be specified with `SCAN_TRACE_ANALYZER`. Options to be given to the trace analyzer can be specified with `SCAN_ANALYZE_OPTS`. Trace data can be automatically removed after successful trace analysis by setting `SCAN_CLEAN`.

4.2 Measurement configuration

A number of configuration variables can be used to control the EPIK measurement runtime configuration: for an annotated list of configuration variables, and their current settings, run the `epik_conf` command. Configuration variables can be specified via environment variables or in a configuration file called `EPIK.CONF`: by default the current directory is searched for this file, or an alternative location can be specified with the `EPK_CONF` environment variable.

The values for configuration variables can contain (sub)strings of the form `$XYZ` or `${XYZ}` where `XYZ` is the name of another configuration variable. Evaluation of the configuration variable is done at runtime when measurement is initiated.

When tracing (large-scale) MPI applications it is recommended to set the `EPK_LDIR` and `EPK_GDIR` variables to the same location, as in such cases intermediate file writing is avoided and can greatly improve performance. Therefore, this is the default setting.

4.3 Measurement and analysis of hardware counter metrics

If the Scalasca measurement library EPIK has been built with hardware counter support enabled (see `INSTALL` file), it is capable of processing hardware counter information as part of event handling. (This can be checked by running `epik_conf` and seeing whether `EPK_METRICS_SPEC` is set.)

Counters are processed into counter metrics during runtime summarization, and recorded as part of event records in collected traces. Note that the number of counters recorded determines measurement and analysis overheads, as well as the sizes of measurement storage datastructures, event traces and analysis reports. Counter metrics recorded in event traces are currently ignored by the Scalasca parallel trace analyzer, and it is generally recommended that they should only be specified for summarization measurements.

To request the measurement of certain counters, set the variable `EPK_METRICS` to a colon-separated list of counter names, or a predefined platform-specific group. Alternatively specify the desired metrics with `-m <metriclist>` argument to the Scalasca measurement collection and analysis system (`scalasca -analyze`). Hardware counter measurement is disabled by default.

Metric names can be chosen from the list contained in file `doc/METRICS.SPEC` or may be PAPI preset names or platform-specific "native" counter names. `METRICS.SPEC` also contains specifications of groups of (related) counters which may conveniently be measured simultaneously on various platforms. The installed `doc/METRICS.SPEC` specification is overridden by a file named `METRICS.SPEC` in the current working directory, or specified by the EPIK configuration variable `EPK_METRICS_SPEC`.

If any of the requested counters are not recognized or the full list of counters cannot be recorded due to hardware-resource limits, measurement of the program execution will be aborted with an error message.

Counter metrics appear in the Performance Metrics pane of the CUBE3 browser. Relationships between counter metrics which define hierarchies are also specified in the file `METRICS.SPEC` — those without specified relationships are listed separately.

Experiments with subsets of the counter metrics required for a full hierarchy could previously be combined into composite experiments using the `cube_merge` utility. Note that a replacement for this utility is still under development and not yet available. Generally several measurement experiments are required, and the groupings of counters provided in METRICS.SPEC can act as a guide for these.

The default `doc/METRICS.SPEC` provides generic metric specifications which can be used for analysis on any platform. Additional platform-specific example metric specifications are provided in the examples directory. If desired, an example `METRICS.SPEC` appropriate for the platform where the measurements will be (or have been) recorded can be used instead of the default `doc/METRICS.SPEC` via setting the `EPK_METRICS_-SPEC` configuration variable or replacing the installed file.

EXPERT analysis (see Section 4.5) can further be customized using additional environment variables: `EPT_INCOMPLETE_COMPUTATION` can be set to accept metric computations which are missing one or more component measurement (while not generally useful on its own, it can allow more detailed metric hierarchies to be created when experiments are combined); `EPT_MEASURED_METRICS` modifies the handling of unparented measured metrics, such that they can be ignored (value 0), listed separately (value 1, the default) or listed together with parented metrics (value 2).

4.4 Automatic parallel event trace analysis

SCOUT is Scalasca's automatic MPI-based analyzer for EPIK event traces. It is used internally by the Scalasca measurement collection and analysis system (`scalasca -analyze`) on MPI and hybrid MPI/OpenMP event traces, or can be explicitly executed on event traces in EPIK measurement archives. Depending on the build configuration and the capabilities of the target platform, SCOUT may be available in two forms:

scout.mpi is built whenever Scalasca is configured with MPI support. It is used to analyze event traces generated by pure MPI applications. It can also be used on traces from hybrid MPI/OpenMP applications, however, it will then only provide information about the master thread of each process and its MPI activities.

scout.hyb is built in addition to `scout.mpi` if Scalasca is configured with hybrid MPI/OpenMP support. It is used to analyze event traces generated by hybrid

MPI/OpenMP applications, providing information about all OpenMP threads of each MPI process.

The appropriate SCOUT variant can be explicitly executed on event traces in EPIK measurement archives using

```
$MPIEXEC $MPIEXEC_FLAGS <scout.type> [-s] epik_<title>
```

which produces an (intermediate) analysis report `epik_<title>/scout.cube`.

Event traces collected on clusters without a synchronized clock may contain logical clock condition violations [2] (such as a receive completing before the corresponding send is initiated). When SCOUT detects this, it reports a warning that the analysis may be inconsistent and recommends (re-)running trace analysis with its integrated timestamp synchronization algorithm (based on the controlled logical clock [1]) activated: this auxilliary trace processing is specified with the optional `-s` flag to SCOUT.

Alternatively, event trace analysis can be (re-)initiated using the `scalasca -analyze` command, e.g.,

```
scalasca -analyze -a -e epik_<title> $MPIEXEC $MPIEXEC_FLAGS
```

where `MPIEXEC` is the command used to configure and launch MPI applications, and is typically identical to that used to launch the user MPI application. In the second case, the `scalasca -analyze` command will automatically figure out which SCOUT variant should be used and/or is available. To activate the integrated timestamp synchronization algorithm when using the `scalasca -analyze` command, the environment variable `SCAN_ANALYZE_OPTS` needs to be set to `-s`.

Note:

The number of MPI processes for SCOUT must be identical to the number of MPI processes for the original application! Furthermore, if SCOUT is executed on hybrid MPI/OpenMP traces, the `OMP_NUM_THREADS` environment variable must be set to the value used for the original application.

Warning:

The `scout.hyb` analyzer requires hybrid OpenMP/MPI applications to use the same number of threads during all parallel regions. A dynamically changing number of threads is not supported, and typically will result in deadlock!

When running the SCOUT analyzer on (back-end) compute nodes with a different architecture to their system front-end, remember to specify the path to the appropriate (back-end) version (e.g., `$SCALASCA_RTS/<scout.type>`).

If your MPI library doesn't automatically support passing command-line arguments to all MPI processes, the name of the experiment to analyze may need to be passed in a special form (e.g., `-args "epik_<title>"`) or can be specified via the `EPK_TITLE` configuration variable (in a `EPIK.CONF` file or set in the environment for each MPI process, e.g., `-env "EPK_TITLE=<title>"`).

Note:

SCOUT processes may require three times the memory of the largest MPI-rank trace file to complete analysis without paging to disk. Hardware counters recorded in event traces are currently ignored by SCOUT, however, hardware counter metrics can be found in the runtime summarization analysis report (summary.cube) which is also produced by default when tracing is enabled.

4.5 Automatic sequential event trace analysis

EXPERT is an automatic serial analyzer for *merged* EPILOG event traces. It is used internally by the Scalasca collection and analysis system (`scalasca -analyze`) on pure OpenMP event traces, and it can also be manually applied to MPI and hybrid MPI/OpenMP traces in EPIK experiment archives after they have been merged via

```
elg_merge epik_<title>
```

to produce `epik_<title>/epik.elg`.

Note:

It may take quite a long time to merge large event traces, and the resulting `epik.elg` will typically be more than three times as large as the unmerged process traces!

Explicit execution of EXPERT on a merged EPILOG event trace in an EPIK experiment archive via

```
expert epik_<title>
```

produces an analysis report `epik_<title>/expert.cube`.

Note:

Bear in mind, that both merging of MPI rank traces and EXPERT analysis are sequential operations that might take a long time for large experiments!

Warning:

> The EXPERT analyzer requires the event trace to represent a call tree with a single root. Therefore you should instrument the entry and exit of the application's "main" function if necessary. Also note that EXPERT requires OpenMP applications to use the same number of threads during all parallel regions. A dynamically changing number of threads is not supported!

Integrated merged trace analysis and results presentation is provided by the KOJAK analysis command:

```
kanal epik_<title>
```

or

```
kanal <file>[.elg|.cube]
```

The command takes as argument either an EPIK experiment archive (containing a merged trace), a merged trace `<file>.elg` or a generated analysis report `<file>.cube`. If `<file>.cube` already exists (and is newer than `<file>.elg`), CUBE3 is used to present it and browse the analysis. If the trace `<file>.elg` is newer (or no analysis file exists), then EXPERT is run to generate `<file>.cube` before it is presented with CUBE3. Where generation of a new `<file>.cube` would overwrite an existing (older) file with the same name, a prompt will confirm whether to continue or not.

The EXPERT event trace analysis and CUBE analysis visualization can also be executed separately, which is particularly appropriate when the CUBE viewer is installed on a separate system (e.g., desktop) from the measurement system (e.g., a remote HPC system or cluster).

EXPERT analysis performance for particular trace files can be tuned via EARL environment variables which trade efficiency and memory requirements.

In order to analyze a trace file, EXPERT reads the trace file once from the beginning to the end. After accessing a particular event, EXPERT might request other events usually from the recent past of the event or ask for state information related to one of those events. Random access to events as well as the calculation of state information is done inside the EARL event accessor library, a component used by EXPERT.

During the analysis process, EARL dynamically builds up a sparse index structure on the trace file. At fixed intervals the state information is stored in so-called bookmarks to speed up random access to events. If a particular event is requested, EARL usually needs not start reading from the beginning of the trace file in order to find it. Instead, the interpreter looks for the nearest bookmark and takes the state information from there which is required to correctly interpret the subsequent events from the file. Then it starts reading the trace from there until it reaches the desired event. The distance of bookmarks can be set using the following environment variable:

```
    EARL_BOOKMARK_DISTANCE (default 10000)
```

To gain further efficiency, EARL automatically caches the most recently processed events in a history buffer. The history buffer always contains a contiguous subsequence of the event trace and the state information referring to the beginning of this subsequence. So all information related to events in the history buffer can be completely generated from the buffer including state information. The size of the history buffer can be set using another environment variable:

```
    EARL_HISTORY_SIZE (default 1000 * number of processes or threads)
```

Note:

Choosing the right buffer parameters is usually a trade-off decision between access efficiency and memory requirements. In particular, for very long traces with many events or very wide traces with many processes or threads, adjustment of these parameters might be recommended.

5 Additional Utilities

5.1 Additional EPILOG event trace utilities

Process-local EPILOG traces in EPIK experiment archives can be *merged* by executing

```
elg_merge epik_<title>
```

in order to produce a single merged trace file `epik_<title>/epik.elg`.

Note:

It may take quite a long time to merge large event traces, and the resulting `epik.elg` will typically be more than three times as large as the unmerged process traces!

Two utility programs are provided to check the *correctness* and to *summarize* the contents of EPILOG trace files:

```
elg_print <file>.elg
```

Prints the contents of the EPILOG trace file `<file>.elg` to the standard output stream. `elg_print` creates a readable representation of the EPILOG low-level record format. This is mainly provided for debugging purposes to check the correct structure and content of the EPILOG trace records.

```
elg_stat <file>.elg
```

By default, `elg_stat` calculates and reports some very simple event statistics to standard output. In addition, options `-d` (definition records) and `-e` (event records) enable the printing of a human-readable representation of the trace contents on the event level.

5.2 Trace converters

The following utility programs can be used to *convert* merged EPILOG trace file into other formats.

If support for the trace formats OTF and/or VTF3 were included during configuration and installation, merged EPILOG event traces can be converted for visual analysis with the VAMPIR trace visualizer from TU Dresden ZIH [5].

To convert a merged trace to the VampirTrace Open Trace Format (OTF) use

```
elg2otf epik_<title>
```

and to convert to the older VAMPIR version 3 format (VTF3) use

```
elg2vtf3 epik_<title>/<file>.elg
```

which stores the resulting trace in <`file`>`.vpt`.

Experimental support is provided to convert merged EPILOG traces to the format used by the PARAVER trace visualizer from the Barcelona Supercomputing Center [3] via

```
elg2prv epik_<title>
```

5.3 Recording user-specified virtual topologies

A virtual topology defines the mapping of processes and threads onto the application domain, such as a weather model simulation area. In general, a virtual topology is specified as a graph (e.g., a ring) or a Cartesian topology such as two- or higher-dimensional grids. Virtual topologies can include processes, threads or a combination of both, depending on the programming model.

Virtual topologies can be useful to identify performance problems. Mapping performance data onto the topology can help uncover inefficient interactions between neighbors and suggest algorithmic improvements. EPIK supports the recording of 3D Cartesian grids as the most common case. To do this, the user has two options:

1. Using MPI Cartesian-topology functions
2. Manual recording using the EPILOG topology API

If an application uses MPI topology functions to set up a Cartesian grid, EPIK automatically includes this information in the measurement experiment.

In addition, EPIK provides users who do not use MPI topologies with an API to define a one-, two- or three- dimensional Cartesian topology. These functions are available in C and Fortran. To use the C API, include `elg_topol.h`. Whereas in C all functions start with the prefix `elg_`, they start with `elgf_` in Fortran. Here are the signatures of these two functions:

1. `elg(f)_cart_create(size_0, size_1, size_2,`
   `                    period_0, period_1, period_2);`

   defines a Cartesian grid topology of up to 3 dimensions where

   - `size_X` is an integer describing the number of locations in dimension X and
   - `period_X` is an integer describing the periodicity in dimension X. It should be
     - *zero* if dimension is not periodic, and
     - *non-zero* if dimension is periodic.

   To specify a grid with less than three dimensions, set `size_X` to zero for the dimensions not being used. At least one process/thread must call this function. Redundant calls done by other processes/threads will be ignored.

2. `elg(f)_cart_coords(coord_0, coord_1, coord_2);`

   defines the coordinates of the calling process or thread (i.e., location) in the previously defined grid where

   - `coord_X` is an integer describing the coordinate of a location in dimension `X` with $X \in [0, \text{size\_X} - 1]$

   This function must be called exactly once by every process/thread that is part of the Cartesian topology.

Note:

Presently, the user can define only one topology per measurement, and this topology is ignored if a physical machine topology is defined. This is currently the case for IBM Blue Gene systems.

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