International HPC Summer School 2023: Performance analysis and optimization

Score-P – A Joint Performance Measurement Run-Time Infrastructure for Periscope, Scalasca, TAU, and Vampir

VI-HPS Team
Ilya Zhukov – Jülich Supercomputing Centre

Score-P
Scalable performance measurement infrastructure for parallel codes

Score-P:
Specialized Measurements and Analyses

Mastering build systems

- Hooking up the Score-P instrumenter `scorep` into complex build environments like *Autotools* or *CMake* was always challenging
- Score-P provides new convenience wrapper scripts to simplify this (since Score-P 2.0)
- *Autotools* and *CMake* need the used compiler already in the *configure step,* but instrumentation should not happen in this step, only in the *build step*

```
% SCOREP_WRAPPER=off \
> cmake .. \
> -DCMAKE_C_COMPILER=scorep-icc \
> -DCMAKE_CXX_COMPILER=scorep-icpc
```

Disable instrumentation in the *configure step*

Specify the wrapper scripts as the compiler to use

- Allows to pass addition options to the Score-P instrumenter and the compiler via environment variables without modifying the *Makefiles*
- Run `scorep-wrapper --help` for a detailed description and the available wrapper scripts of the Score-P installation

Mastering C++ applications

- Automatic compiler instrumentation greatly disturbs C++ applications because of frequent/short function calls => Use sampling instead
- Novel combination of sampling events and instrumentation of MPI, OpenMP, …
  - Sampling replaces compiler instrumentation (instrument with `--nocompiler` to further reduce overhead) => Filtering not needed anymore
  - Instrumentation is used to get accurate times for parallel activities to still be able to identifies patterns of inefficiencies
- Supports profile and trace generation

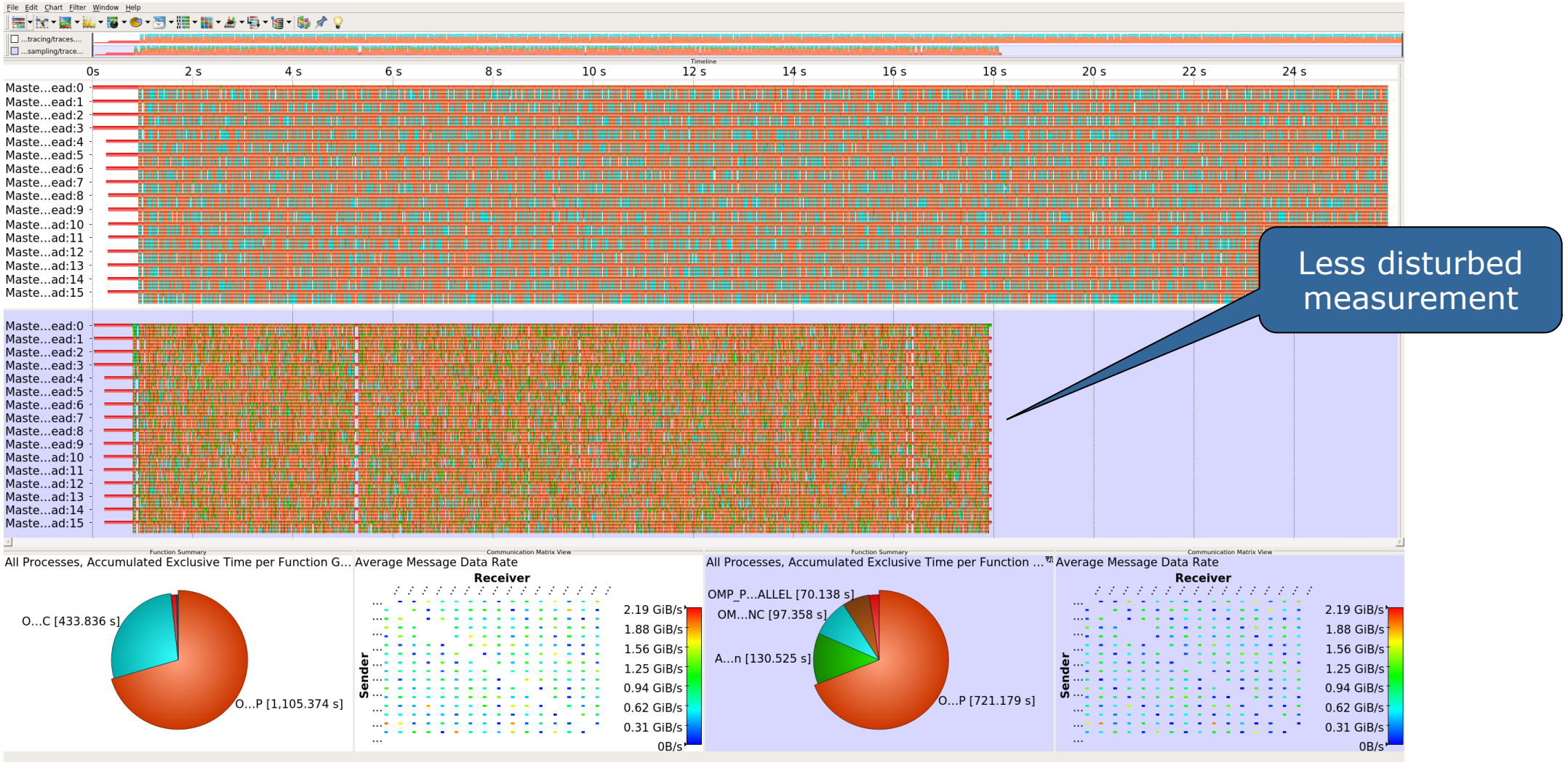
```
% export SCOREP_ENABLE_UNWINDING=true
% # use the default sampling frequency
% #export SCOREP_SAMPLING_EVENTS=perf_cycles@2000000

% OMP_NUM_THREADS=4 mpiexec -np 4 ./bt-mz_W.4
```

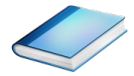
- Set new configuration variable to enable sampling

- Available since Score-P 2.0, only x86-64 supported currently

Mastering C++ applications



Wrapping calls to 3rd party libraries



- Enables users to install library wrappers for any C/C++ library
- Intercept calls to a library API
  - no need to either build the library with Score-P or add manual instrumentation to the application using the library
  - no need to access the source code of the library, header and library files suffice
- Score-P needs to be executed with `--libwrap=…`
- Execute `scorep-libwrap-init` for directions:

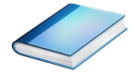
Step 1: Initialize the working directory
Step 2: Add library headers
Step 3: Create a simple example application
Step 4: Further configure the build parameters
Step 5: Build the wrapper
Step 6: Verify the wrapper
Step 7: Install the wrapper
Step 8: Verify the installed wrapper

Only once

Often

Step 9: Use the wrapper

Wrapping calls to 3rd party libraries



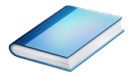
- Generate your own library wrappers by telling `scorep-libwrap-init` how you would compile and link an application, e.g. using FFTW

```
% scorep-libwrap-init          \
>   --name=fftw                 \
>   --prefix=$PREFIX            \
>   -x c                        \
>   --cppflags="-O3 -DNDEBUG -openmp -I$FFTW_INC" \
>   --ldflags="-L$FFTW_LIB"     \
>   --libs="-lfftw3f -lfftw3" \
>   working_directory
```

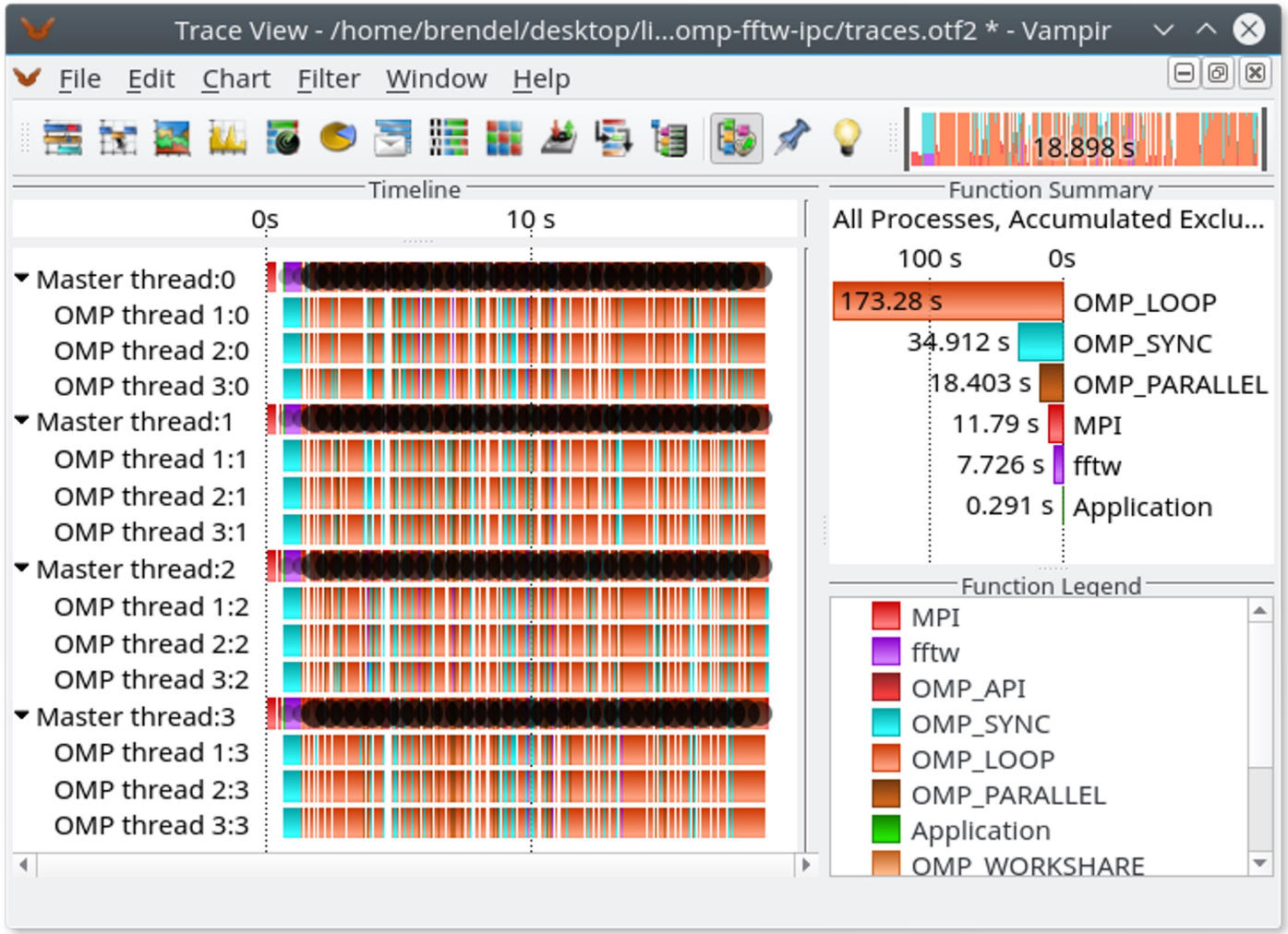
- Generate and build wrapper

```
% cd working_directory
% ls                    # (Check README.md for instructions)
% make                  # Generate and build wrapper
% make check            # See if header analysis matches symbols
% make install          #
% make installcheck     # More checks: Linking etc.
```

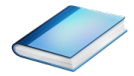
Wrapping calls to 3rd party libraries



- MPI + OpenMP
- Calls to FFTW library



Mastering application memory usage



- Determine the maximum heap usage per process
- Find high frequent small allocation patterns
- Find memory leaks
- Support for:
  - C, C++, MPI, and SHMEM (Fortran only for GNU Compilers)
  - Profile and trace generation (profile recommended)
    - Memory leaks are recorded only in the profile
    - Resulting traces are not supported by Scalasca yet

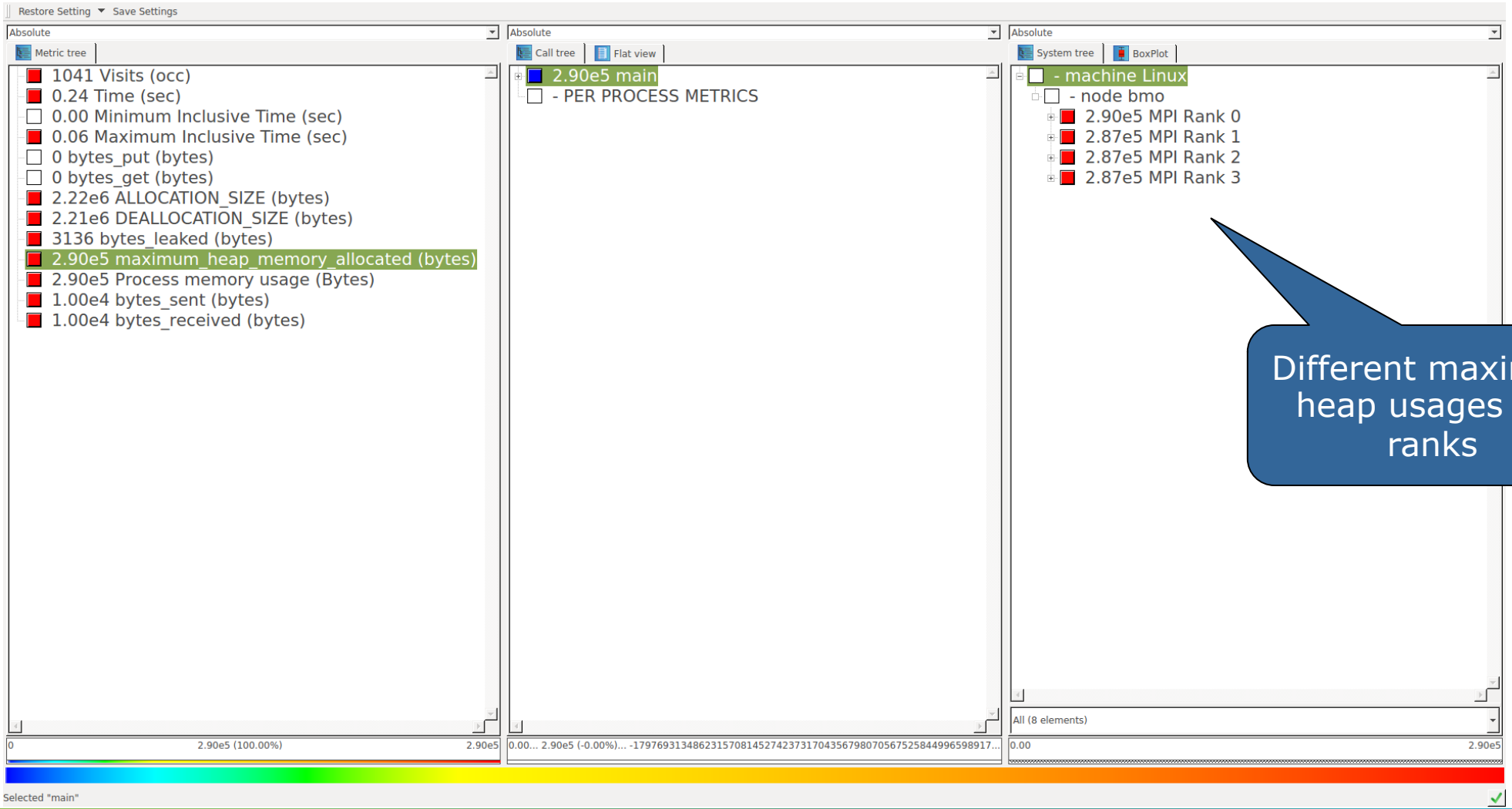
```
% export SCOREP_MEMORY_RECORDING=true
% export SCOREP_MPI_MEMORY_RECORDING=true

% OMP_NUM_THREADS=4 mpiexec -np 4 ./bt-mz_W.4
```

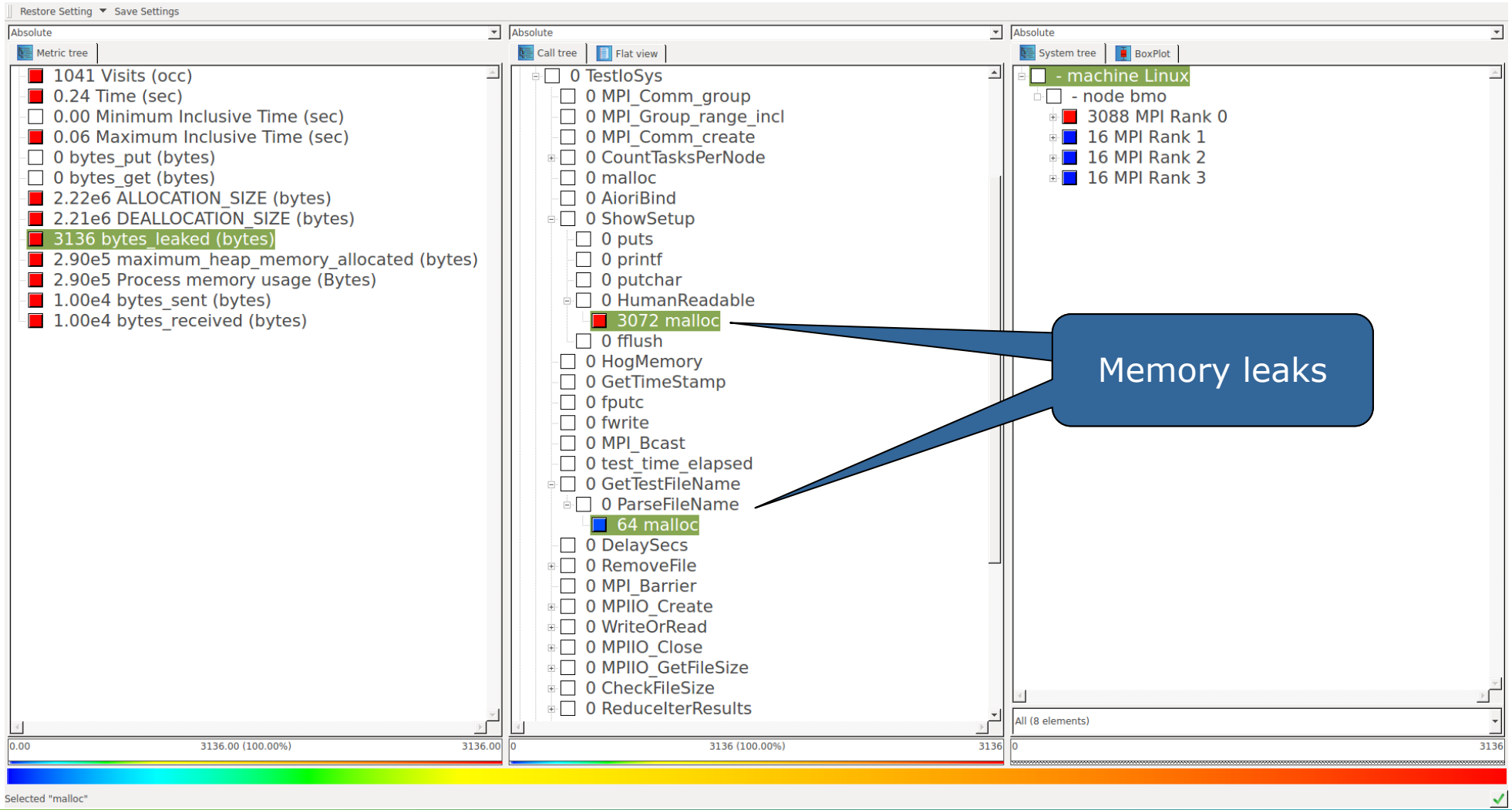
- Set new configuration variable to enable memory recording

- Available since Score-P 2.0

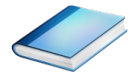
Mastering application memory usage



Mastering application memory usage

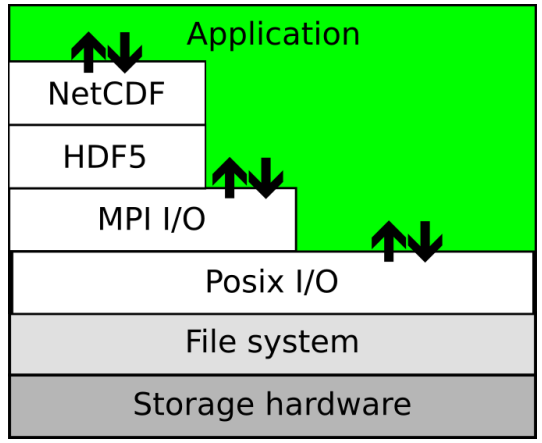


File I/O recording



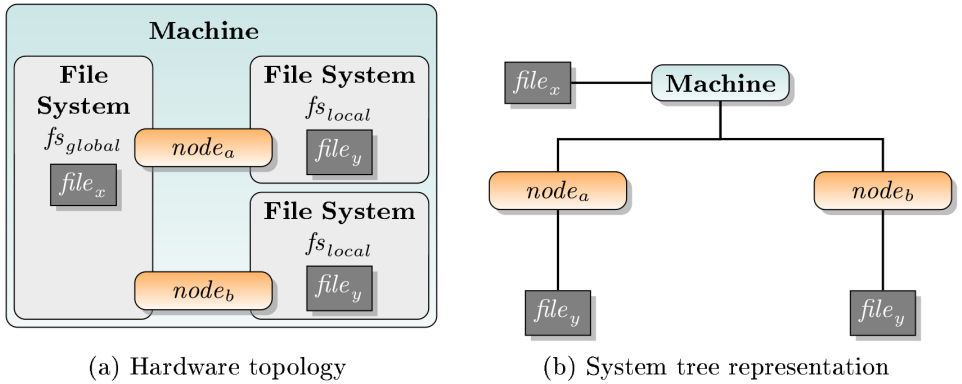
- Omnipresent in todays HPC applications

- Record interaction between multiple layers
  - MPI I/O (`MPI_File_open`)
  - ISO C I/O (`fopen`)
  - POSIX I/O (`open`, interface to OS)



- System tree information determine whether file resides in a shared filesystem

- High level of detail
  => Trace data might increase dramatically



(a) Hardware topology (b) System tree representation

NetCDF & HDF5 will be supported later

B_EFF I/O

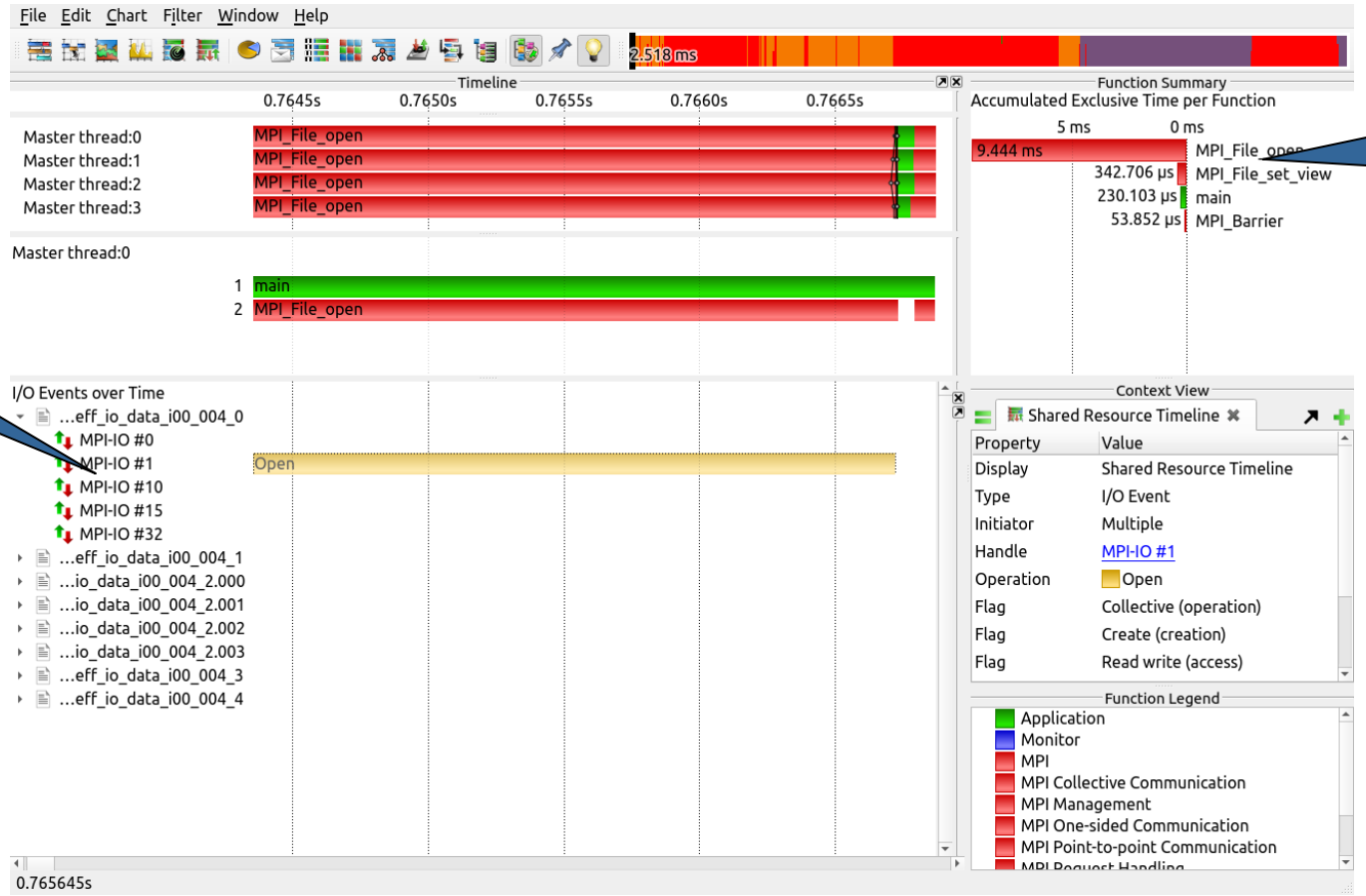
- MPI I/O benchmark
- fs.hlrs.de/projects/par/mpi/b_eff_io/

- MPI I/O is enabled by default

```
% scorep-mpicc -o b_eff_io b_eff_io.c
% export SCOREP_EXPERIMENT_DIRECTORY=scorep-b_eff_io-4-profile
% mpirun -n 4 -c 6 ./b_eff_io -MB 2048 -MT 98304 -rewrite -N 4 -T 60
% scorep-scorep –g scorep-b_eff_io-4-profile/profile.cubex
% export SCOREP_EXPERIMENT_DIRECTORY=scorep-b_eff_io-4-tracing
% export SCOREP_FILTERING_FILE=initial_scorep.filter
% export SCOREP_ENABLE_TRACING=true
% export SCOREP_TOTAL_MEMORY=31MB
% mpirun -n 4 -c 6 ./b_eff_io -MB 2048 -MT 98304 -rewrite -N 4 -T 60
```

Result visualization

Hierarchy of files and corresponding handles



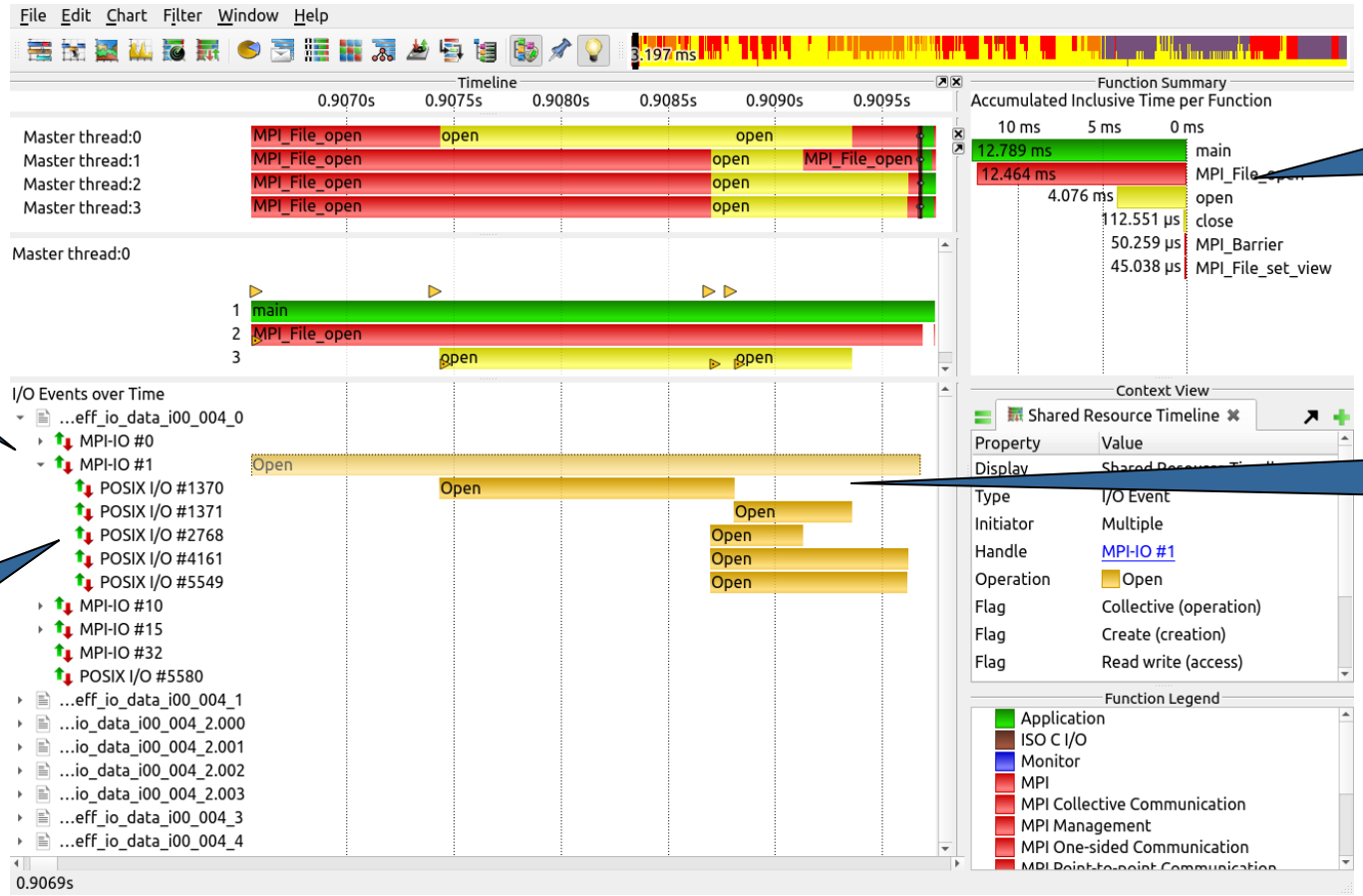
MPI I/O functions recorded

B_EFF I/O

- Enabling ISO C and POSIX I/O instrumentation
- Instrumentation might require threading support

```
% export SCOREP_WRAPPER_INSTRUMENTER_FLAGS=\
    '--io=runtime:posix --thread=pthread'
% scorep-mpicc -o b_eff_io b_eff_io.c
% export SCOREP_EXPERIMENT_DIRECTORY=scorep-b_eff_io-4-profile+posix
% export SCOREP_ENABLE_TRACING=false
% scorep-scorep scorep-b_eff_io-4-profile+posix/profile.cubex
% export SCOREP_EXPERIMENT_DIRECTORY=scorep-b_eff_io-4-tracing+posix
% export SCOREP_ENABLE_TRACING=true
% export SCOREP_TOTAL_MEMORY=61MB
% mpirun -n 4 -c 6 ./b_eff_io -MB 2048 -MT 98304 -rewrite -N 4 -T 60
```

Result visualization



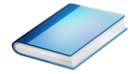
Increased hierarchy

Each rank operates on its own POSIX handle

MPI and POSIX I/O functions recorded

Rank 0 ensures file exists for all ranks

Mastering heterogeneous applications



- Record CUDA applications and device activities

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

- Record OpenCL applications and device activities

```
% export SCOREP_OPENCL_ENABLE=api,kernel
```

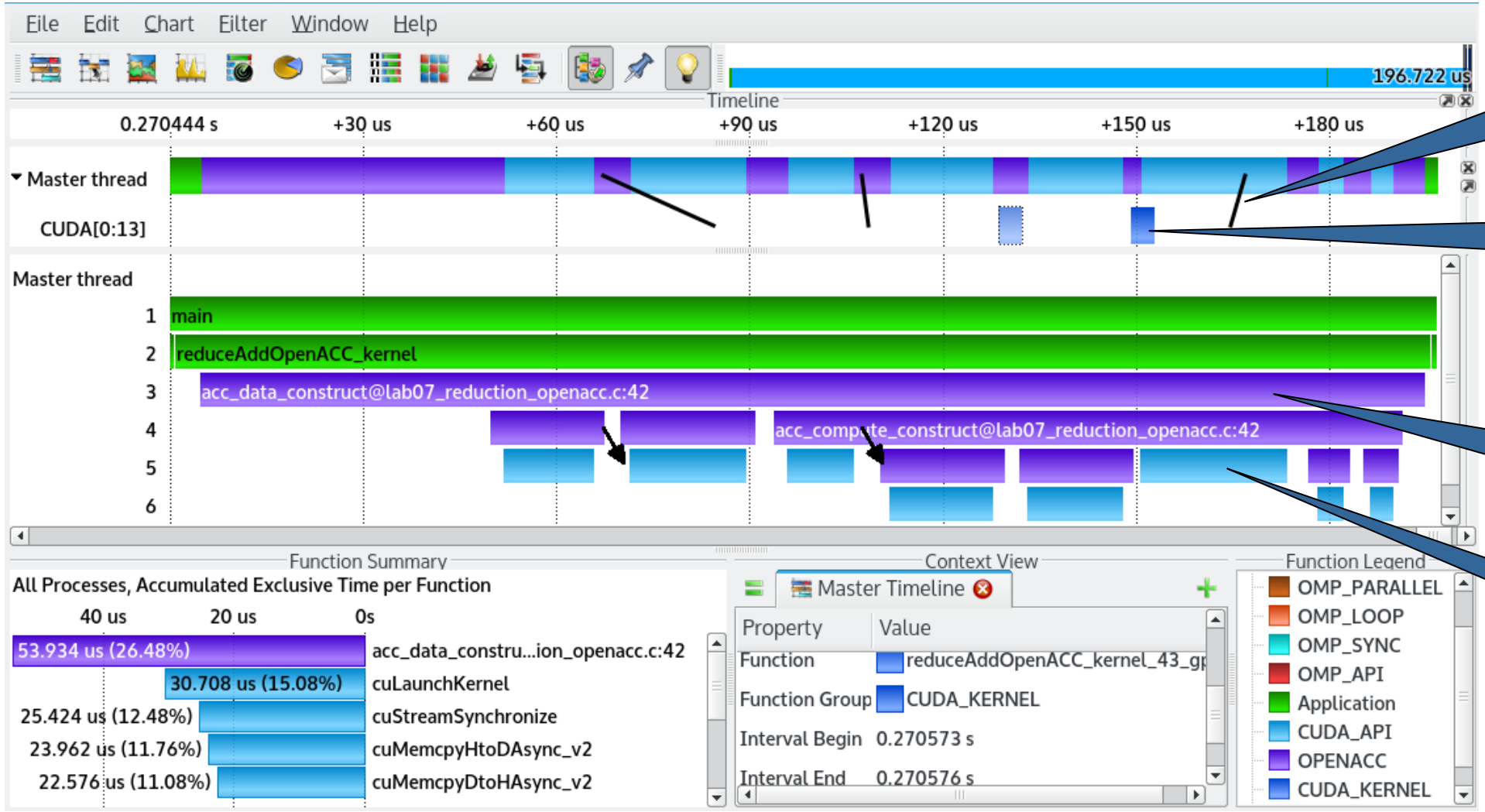
- Record OpenACC applications

```
% export SCOREP_OPENACC_ENABLE=yes
```

  - Can be combined with CUDA if it is a NVIDIA device

```
% export SCOREP_CUDA_ENABLE=kernel
```

Mastering heterogeneous applications



Enriching measurements with performance counters

- Record metrics from PAPI:

```
% export SCOREP_METRIC_PAPI=PAPI_TOT_CYC
% export SCOREP_METRIC_PAPI_PER_PROCESS=PAPI_L3_TCM
```

  - Use PAPI tools to get available metrics and valid combinations:

```
% papi_avail
% papi_native_avail
```

- Record metrics from Linux perf:

```
% export SCOREP_METRIC_PERF=cpu-cycles
% export SCOREP_METRIC_PERF_PER_PROCESS=LLC-load-misses
```

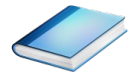
  - Use the `perf` tool to get available metrics and valid combinations:

```
% perf list
```

- Write your own metric plugin
  - Repository of available plugins: https://github.com/score-p

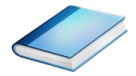
Only the master thread records the metric (assuming all threads of the process access the same L3 cache)

Score-P user instrumentation API



- No replacement for automatic compiler instrumentation
- Can be used to further subdivide functions
  - E.g., multiple loops inside a function
- Can be used to partition application into coarse grain phases
  - E.g., initialization, solver, & finalization
- Enabled with `--user` flag to Score-P instrumenter
- Available for Fortran / C / C++

Score-P user instrumentation API (Fortran)



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

subroutine foo(…)
  ! Declarations
  SCOREP_USER_REGION_DEFINE( solve )

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

- Requires processing by the C preprocessor
  - For most compilers, this can be automatically achieved by having an uppercase file extension, e.g., `main.F` or `main.F90`

Score-P user instrumentation API (C/C++)

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

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

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

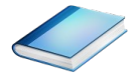
Score-P user instrumentation API (C++)

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

void foo()
{
  // Declarations

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

Score-P measurement control API



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

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

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

Fortran (requires C preprocessor)

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

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

C / C++

Further information

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