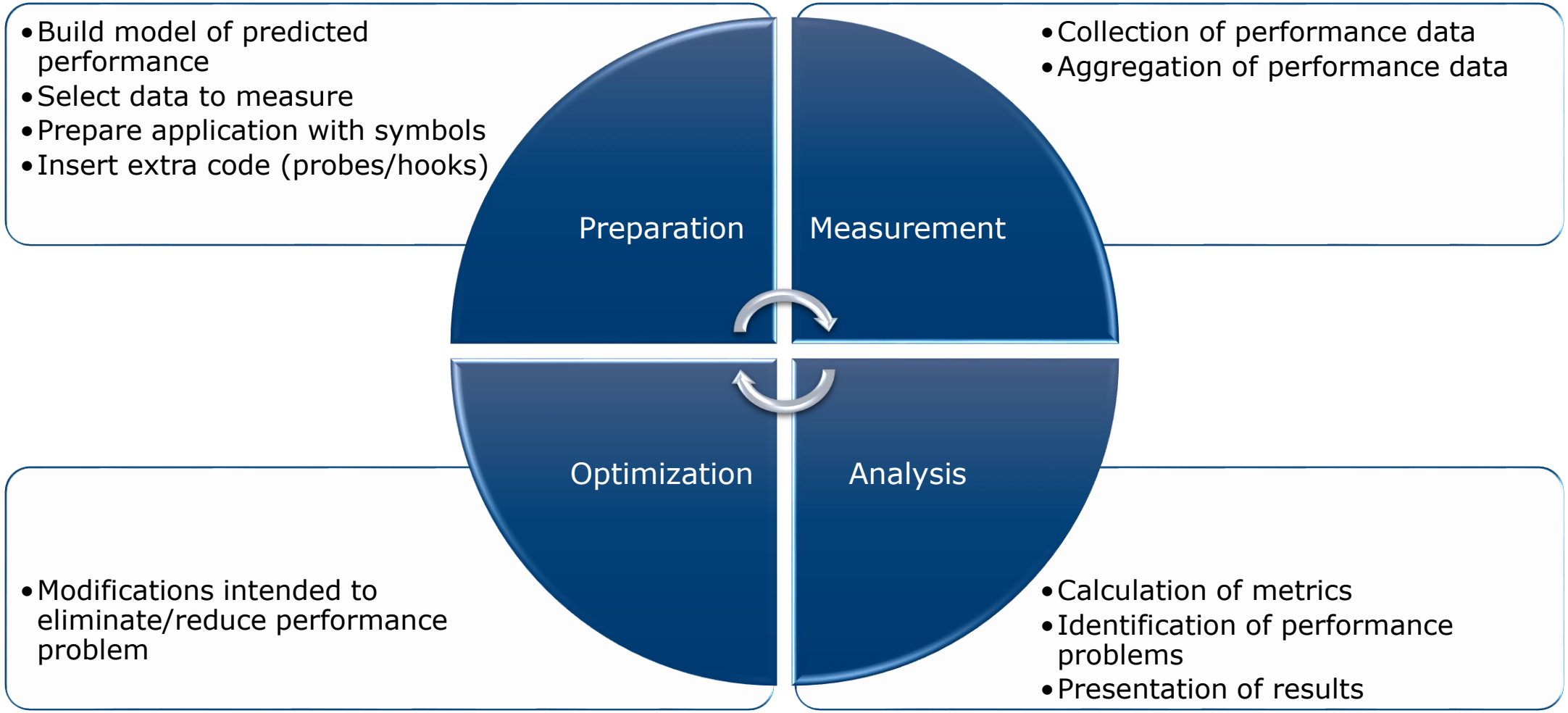
Score-P – Joint instrumentation & measurement infrastructure for Scalasca, TAU, and Vampir

VI-HPS Team

Score-P
Scalable performance measurement infrastructure for parallel codes

Performance engineering workflow



Score-P

- Infrastructure for instrumentation and performance measurements
- Instrumented application can be used to produce several results:
  - Call-path profiling: CUBE4 data format used for data exchange
  - Event-based tracing: OTF2 data format used for data exchange

- Supported parallel paradigms:
  - Multi-process: MPI, SHMEM
  - Thread-parallel: OpenMP, Pthreads
  - Accelerator-based: CUDA, OpenCL, OpenACC, Kokkos

- Open Source; portable and scalable to all major HPC systems
- Initial project funded by BMBF
- Further developed in multiple 3rd-party funded projects

GEFÖRDERT VOM
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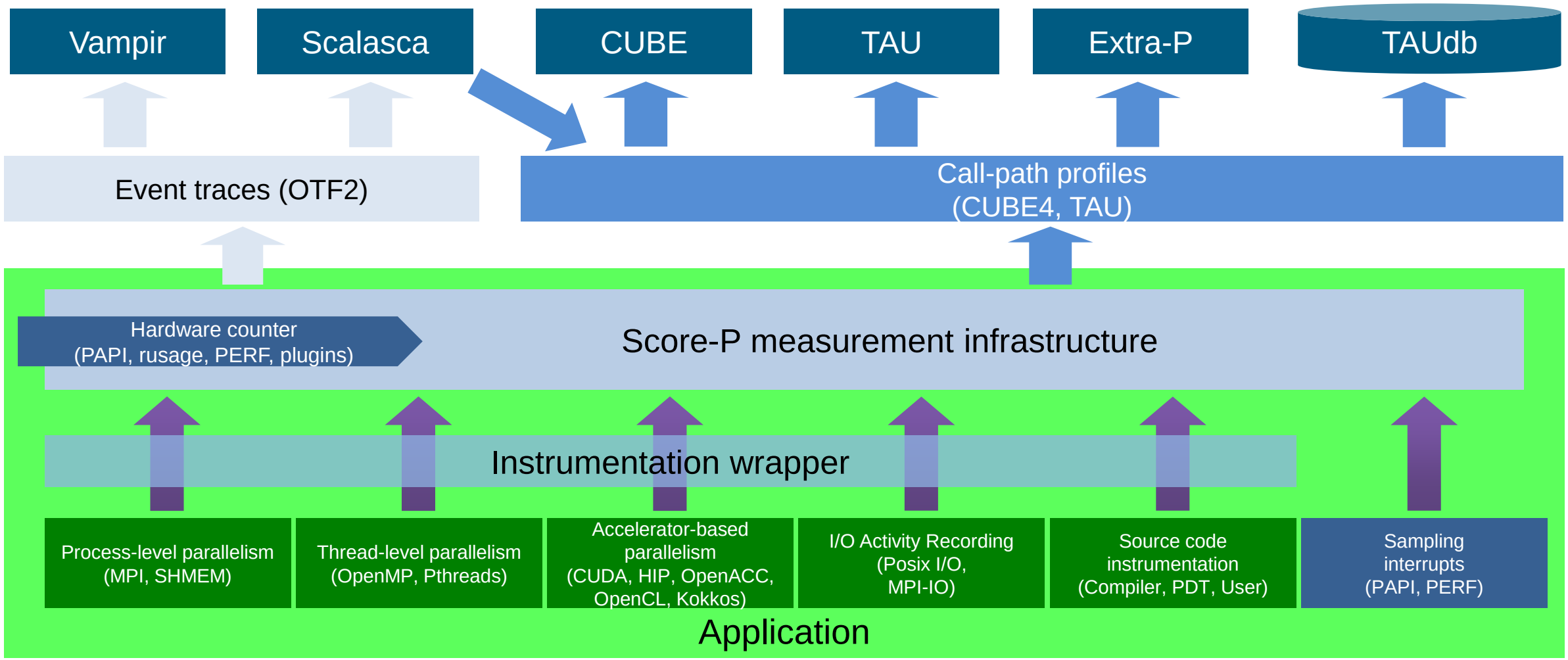
Score-P overview



Partners

- Forschungszentrum Jülich, Germany
- Gesellschaft für numerische Simulation mbH Braunschweig, Germany
- RWTH Aachen, Germany
- Technische Universität Darmstadt, Germany
- Technische Universität Dresden, Germany
- Technische Universität München, Germany
- University of Oregon, Eugene, USA

Performance analysis steps

- 0.0 Reference preparation for validation

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

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

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

Local installation (Karolina)

- Set account and environment (e.g. NVHPC + OpenMPI) via modules:

```
% module load nvompi
```

- Load the *corresponding* modules for the tool environment:

```
% module load Scalasca/2.6.1-NVHPC-24.3-CUDA-12.3.0
```

Scalasca module loads Score-P & CUBE module dependencies

- Copy example sources to your WORK directory (or your personal workspace)
  - Only required if not done already (for opening exercise)

```
% cd $WORK
% cp -r /mnt/proj2/dd-24-88/jsc/examples/CloverLeaf_OpenACC   .
% cd CloverLeaf_OpenACC
```

Score-P instrumenter

- `scorep` instrumenter is used as a preposition to compile & link commands

```
% scorep  ftn -fopenmp -c solve.f90
% scorep  cc -c timer.c
% scorep  mpif90 -o a.out solve.o timer.o -fopenmp -lfft -lcuda
```

- Instrumenter uses heuristics to determine when MPI & OpenMP are employed to perform source processing, direct compilers' function instrumentation and link measurement libraries
  - no heuristics yet for CUDA, Kokkos, OpenACC, …

- Instrumenter is highly configurable via flags: see `scorep --help`
  - should be used when heuristics fail or for custom instrumentation options

```
% scorep --cuda --nomemory  mpif90 -o a.out solve.o timer.o -fopenmp -lfft -lcuda
```

CloverLeaf_OpenACC: Makefile

```
#Crown Copyright 2012 AWE
#
# This file is part of CloverLeaf.
#
# CloverLeaf is free software...
#
# Agnostic, platform independent Makefile for the CloverLeaf benchmark code.
# It is not meant to be clever in any way, just a simple build script.
#
# this works as well:-
#
# make COMPILER=PGI [OPENMP=1]
#

...

#PREP=scorep --openacc --cuda --user

MPI_COMPILER=$(PREP) mpif90

# No preposition for C/CXX_MPI_COMPILER!
C_MPI_COMPILER=mpicc
CXX_MPI_COMPILER=mpic++

...
```

Specify the suite of compilers (and optionally OpenMP)

No instrumentation by default

Set/uncomment PREP macro for instrumenter preposition

Instrumenting clover_leaf

Score-P instrumenter options:
--compiler: source code routines (default)
--mpp=mpi: MPI determined by heuristics
--openacc: enable OpenACC
--cuda: enable CUDA
--user: enable Score-P user API (optional)

```
% make clean
% make PREP="scorep --openacc --cuda --user"

mpicc -c timer_c.c
scorep --openacc --cuda --user  mpif90 -O3 -acc=gpu -ta=nvidia \
    data.f90 definitions.f90 pack_kernel.f90 clover.F90 report.f90 timer.f90 \
    parse.f90 read_input.f90 initialise_chunk_kernel.f90 initialise_chunk.f90 build_field.f90 \
    update_tile_halo_kernel.f90 update_tile_halo.f90 update_halo_kernel.f90 update_halo.f90 \
    ideal_gas_kernel.f90 ideal_gas.f90 start.f90 generate_chunk_kernel.f90 generate_chunk.f90 \
    initialise.f90 field_summary_kernel.f90 field_summary.f90 viscosity_kernel.f90 viscosity.f90 \
    calc_dt_kernel.f90 calc_dt.f90 timestep.f90 accelerate_kernel.f90 accelerate.f90 \
    revert_kernel.f90 revert.f90 PdV_kernel.f90 PdV.f90 flux_calc_kernel.f90 flux_calc.f90 \
    advec_cell_kernel.f90 advec_cell_driver.f90 advec_mom_kernel.f90 advec_mom_driver.f90 \
    reset_field_kernel.f90 reset_field.f90 hydro.F90 clover_leaf.F90 visit.f90 \
    timer_c.o \
    -o bin.scorep/clover_leaf
```

Mastering build systems

- Hooking up the Score-P instrumenter `scorep` into complex build environments like *Autotools* or *CMake* was always challenging
- Score-P provides convenience wrapper scripts to simplify this
- *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 \
> -DCMAKE_Fortran_COMPILER=scorep-ifort
```

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 *Makefile*s (**`SCOREP_WRAPPER_INSTRUMENTER_FLAGS`** & **`SCOREP_WRAPPER_COMPILER_FLAGS`**)
- Run `scorep-wrapper --help` for a detailed description and the available wrapper scripts of each Score-P installation (depends on configured compilers)

Measurement configuration: scorep-info

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

- Score-P measurements are configured via environmental variables

Required for OpenACC measurements. [yes|default] recommended to start. Additional CUDA measurement optional.

Score-P filtering

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

% export SCOREP_FILTERING_FILE=\
../config/scorep.filt
```

Region name filter block using wildcards

Apply filter

- Filtering by source file name
  - All regions in files that are excluded by the filter are ignored
- Filtering by region name
  - All regions that are excluded by the filter are ignored
  - Overruled by source file filter for excluded files
- Apply filter by
  - exporting **`SCOREP_FILTERING_FILE`** environment variable
- Apply filter at
  - Run-time
  - Compile-time (GCC-plugin and Intel only)
    - Add cmd-line option **`--instrument-filter`**
    - No overhead for filtered regions but recompilation

Source file name filter block

- Keywords
  - Case-sensitive
  - `SCOREP_FILE_NAMES_BEGIN`, `SCOREP_FILE_NAMES_END`
    - Define the source file name filter block
    - Block contains `EXCLUDE`, `INCLUDE` rules
  - `EXCLUDE`, `INCLUDE` rules
    - Followed by one or multiple white-space separated source file names
    - Names can contain bash-like wildcards `*`, `?`, `[]`
    - Unlike bash, `*` may match a string that contains slashes
- `EXCLUDE`, `INCLUDE` rules are applied in sequential order
- Regions in source files that are excluded after all rules are evaluated, get filtered

```
# This is a comment
SCOREP_FILE_NAMES_BEGIN
  # by default, everything is included
  EXCLUDE */foo/bar*
  INCLUDE */filter_test.c
SCOREP_FILE_NAMES_END
```

Region name filter block

- Keywords
  - Case-sensitive
  - `SCOREP_REGION_NAMES_BEGIN`, `SCOREP_REGION_NAMES_END`
    - Define the region name filter block
    - Block contains `EXCLUDE`, `INCLUDE` rules
  - `EXCLUDE`, `INCLUDE` rules
    - Followed by one or multiple white-space separated region names
    - Names can contain bash-like wildcards `*`, `?`, `[]`
- `EXCLUDE`, `INCLUDE` rules are applied in sequential order
- Regions that are excluded after all rules are evaluated, get filtered

```
# This is a comment
SCOREP_REGION_NAMES_BEGIN
  # by default, everything is included
  EXCLUDE *
  INCLUDE bar foo
          baz
          main
SCOREP_REGION_NAMES_END
```

Region name filter block, mangling

- Name mangling
  - Filtering based on names seen by the measurement system
    - Dependent on compiler
    - Actual name may be mangled
- `scorep-score` names as starting point (e.g. `matvec_sub_`)
  - Use `*` for Fortran trailing underscore(s) for portability
  - Use `?` and `*` as needed for full signatures or overloading
  - Use `\` to escape special characters

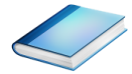
```
void bar(int* a) {
    *a++;
}
int main() {
    int i = 42;
    bar(&i);
    return 0;
}
```

```
# filter bar:
# for gcc-plugin, scorep-score
# displays 'void bar(int*)',
# other compilers may differ

SCOREP_REGION_NAMES_BEGIN
  EXCLUDE void?bar(int?)
SCOREP_REGION_NAMES_END
```

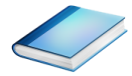
New: generate initial filter file

```
% score-scorep --help
[…]
 -g [<list>] Generation of an initial filter file with the name
             'initial_scorep.filter'. A valid parameter list has the form
             KEY=VALUE[,KEY=VALUE]*. By default, uses the following control
             parameters:

                 `bufferpercent=1,timepervisit=1`

             A region is included in the filter file (i.e., excluded from
             measurement) if it matches all of the given conditions, with the
             following keys:
             - `bufferpercent`       : estimated memory requirements exceed the
                                       given threshold in percent of the total
                                       estimated trace buffer requirements
             - `bufferabsolute`      : estimated memory requirements exceed
                                       the given absolute threshold in MB
             - `visits`              : number of visits exceeds the given
                                       threshold
             […]
```

Score-P:
Specialized Measurements and Analyses

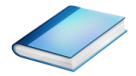


Score-P user instrumentation API



- Can be used to partition application into coarse grain phases
  - E.g., initialization, solver, & finalization
- Can be used to further subdivide functions
  - E.g., multiple loops inside a function
- Enabled with `--user` flag to Score-P instrumenter
- Available for Fortran / C / C++

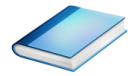
Score-P user instrumentation API (Fortran)



```
#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++)

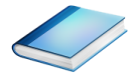


```
#include "scorep/SCOREP_User.h"

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

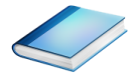
```
#include "scorep/SCOREP_User.inc"

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++

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
```

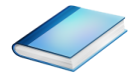
  - Use the `perf` tool to get available metrics and valid combinations:

```
% 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)

Mastering heterogeneous applications



- Record CUDA applications and device activities

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

Idle is an artificial region defined as outside of kernel time

- Record OpenCL applications and device activities

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

- Record OpenACC applications

```
% export SCOREP_OPENACC_ENABLE=yes
```

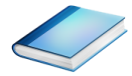
  - Can be combined with CUDA if it is a NVIDIA device

```
% export SCOREP_CUDA_ENABLE=kernel
```

Adding options will increase overhead to a varying degree

  - Check `scorep-info config-vars --full` for a wide range of further options and default values

HIP/ROCm instrumentation

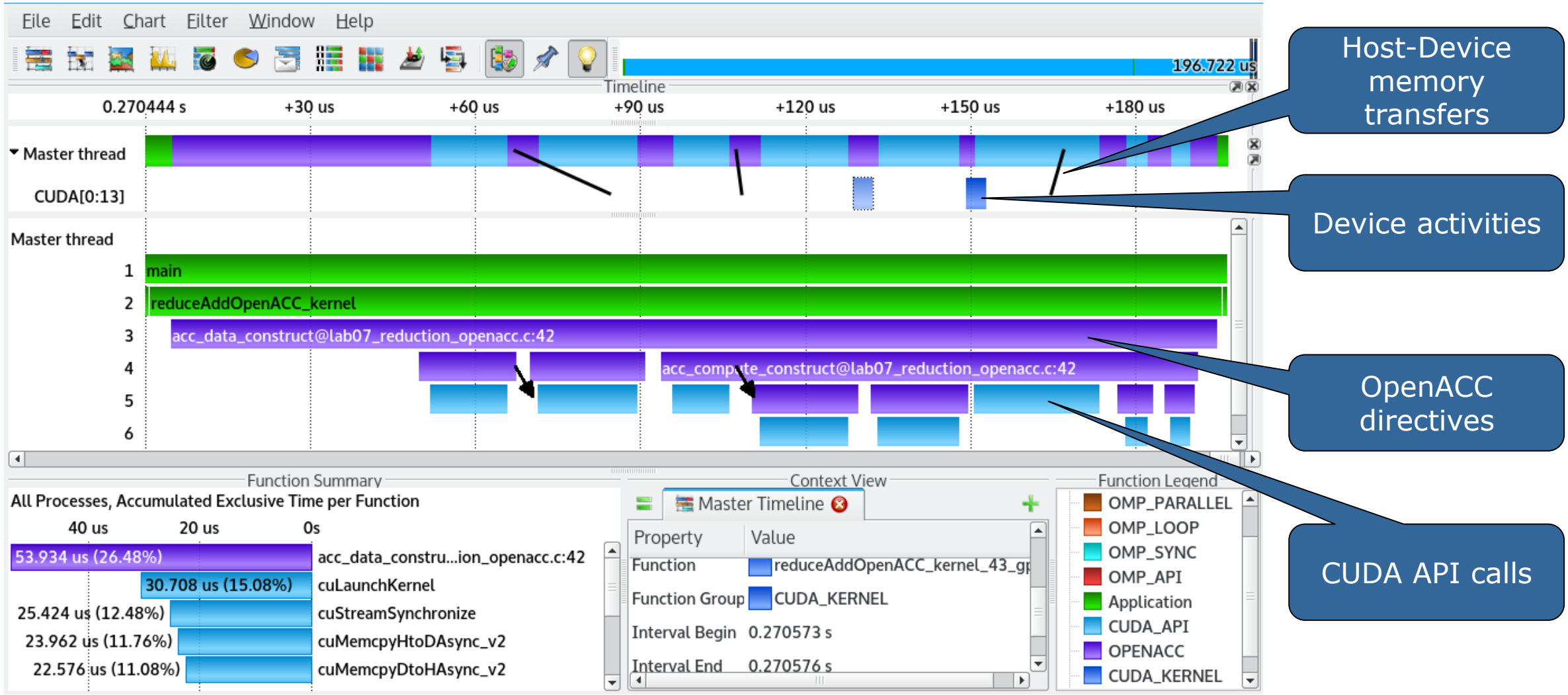


- Instrument with "scorep **--hip**" to ensure ROCm adapter is included
  - alternatively SCOREP_WRAPPER_INSTRUMENTER_FLAGS="--hip …"

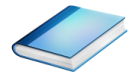
- For measurement execution set SCOREP_HIP_ENABLE
  - api: all HIP API calls
  - kernel: HIP kernels
    - kernel_callsite: additional tracking of kernel callsites between launch and execution
  - malloc: HIP-managed host and device allocations
  - memcpy: H2D, D2H, H2H copies through HIP memcpy functions (not yet for D2D)
  - sync: device/stream synchronization calls
  - user: ROCTx support

  - default/yes/1/true: all of the above
  - none/no: disable feature

Mastering heterogeneous applications



Mastering application memory usage



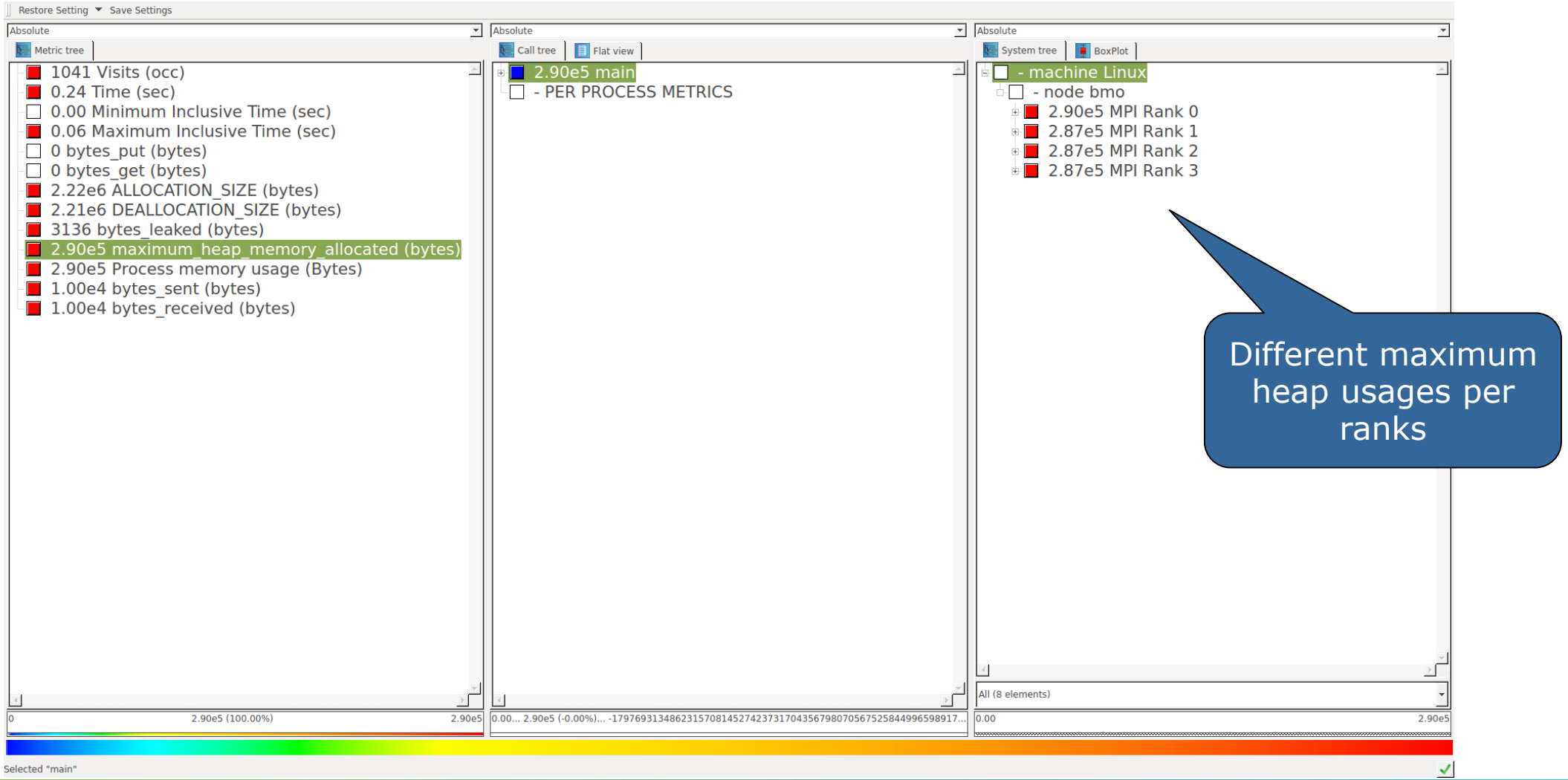
- Determine the maximum heap usage per process
- Find high frequent small allocation patterns
- Find memory leaks
- Support for:
  - C, C++, MPI, and SHMEM (Fortran only for GNU Compilers)
  - Profile and trace generation (profile recommended)
    - Memory leaks are recorded only in the profile
    - 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
```

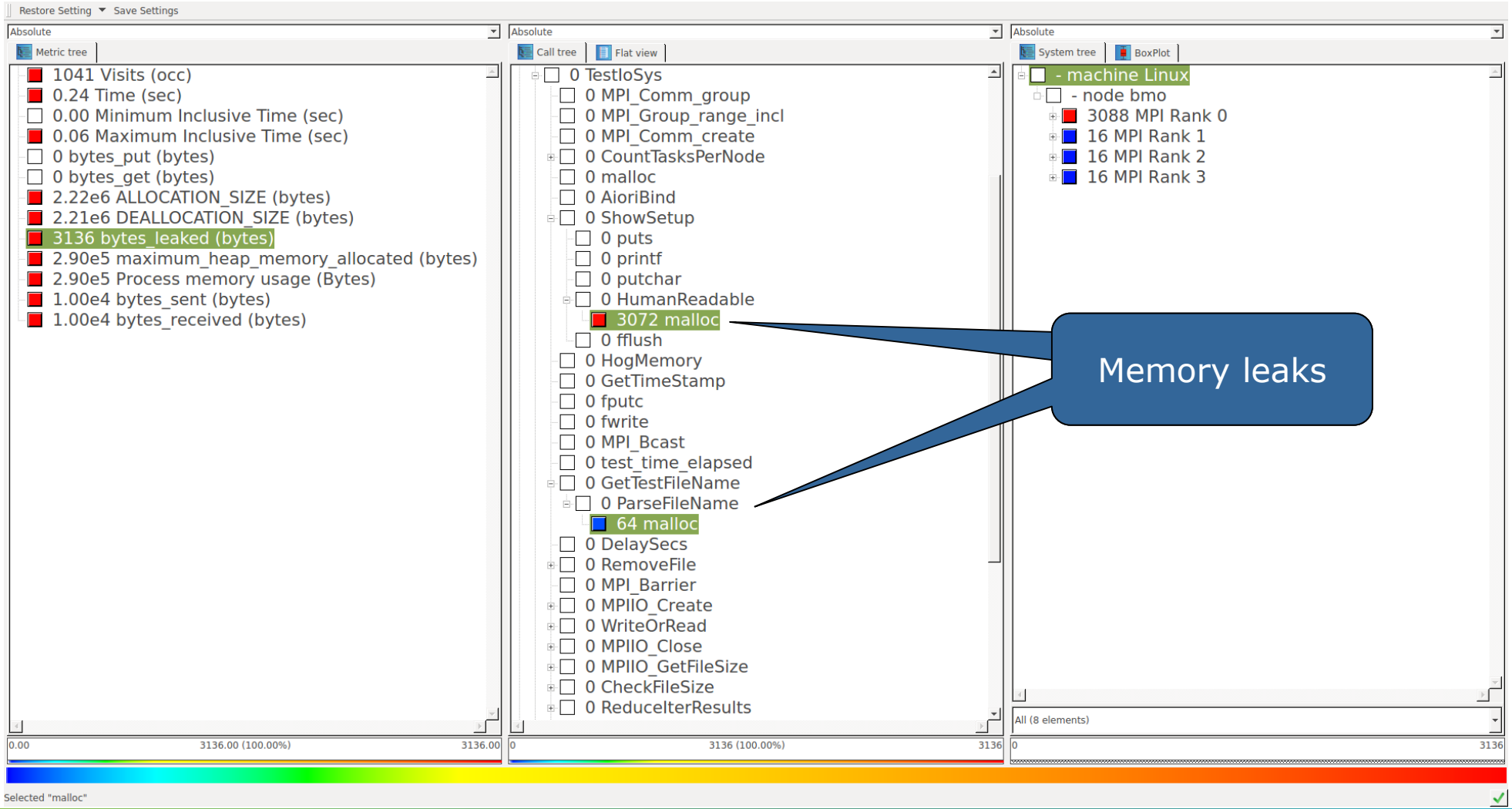
- Set new configuration variable to enable memory recording

- Available since Score-P 2.0

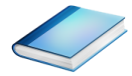
Mastering application memory usage



Mastering application memory usage



Mastering C++ applications



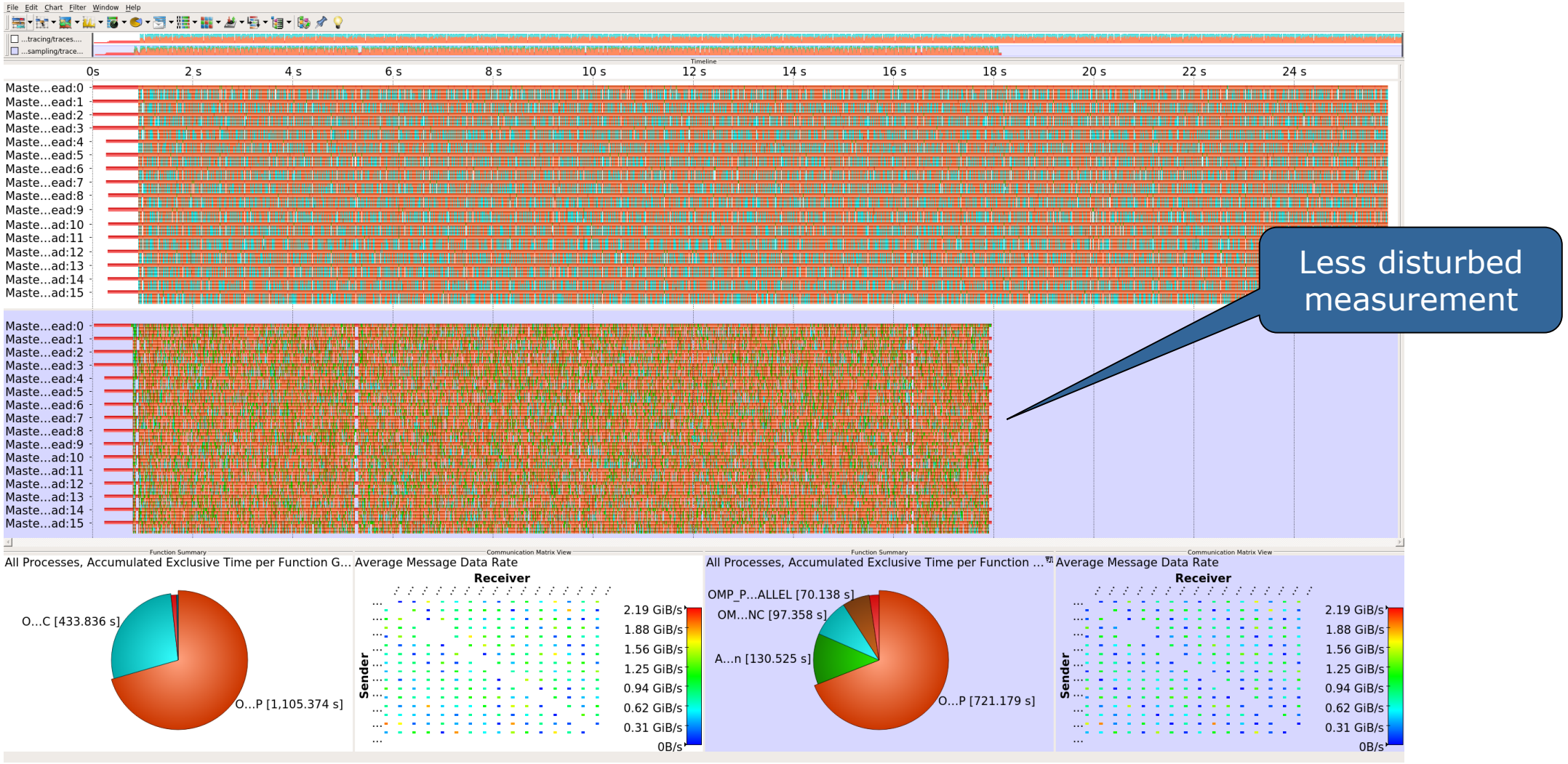
- Automatic compiler instrumentation greatly disturbs C++ applications because of frequent/short function calls => Use sampling instead
- Novel combination of sampling events and instrumentation of MPI, OpenMP, …
  - Sampling replaces compiler instrumentation (instrument with `--nocompiler` to further 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
```

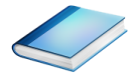
- Set new configuration variable to enable sampling

- 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:

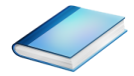
Step 1: Initialize the working directory
Step 2: Add library headers
Step 3: Create a simple example application
Step 4: Further configure the build parameters
Step 5: Build the wrapper
Step 6: Verify the wrapper
Step 7: Install the wrapper
Step 8: Verify the installed wrapper

Only once

Often

Step 9: Use the wrapper

Wrapping calls to 3rd party libraries



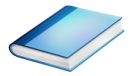
- Generate your own library wrappers by telling `scorep-libwrap-init` how you would compile and link an application, e.g. using FFTW

```
% 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
```

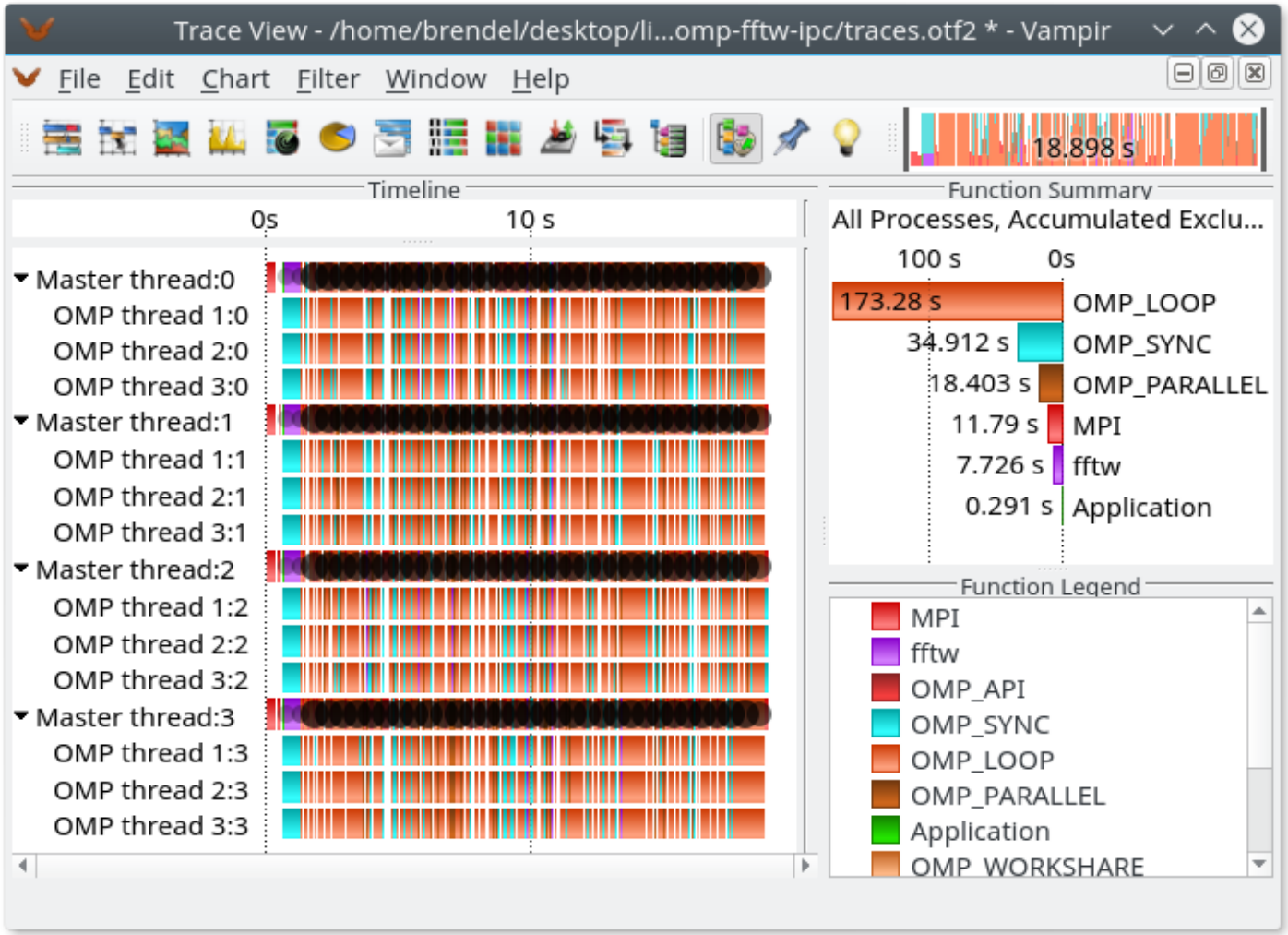
- Generate and build wrapper

```
% 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



Further information

- Community instrumentation & measurement infrastructure
  - Instrumentation (various methods) and sampling
  - Basic and advanced profile generation
  - Event trace recording
- Available under 3-clause 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