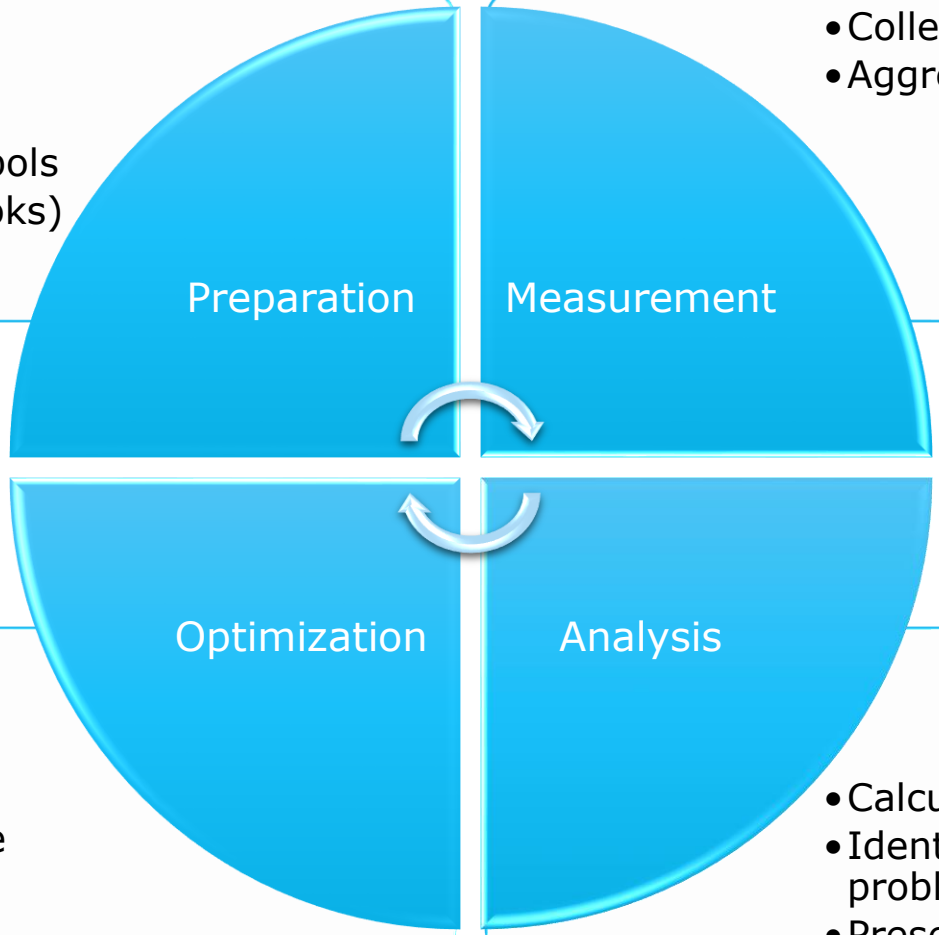
Score-P – A Joint Performance Measurement Run-Time Infrastructure for Scalasca, TAU, and Vampir

VI-HPS Team

Score-P
Scalable performance measurement infrastructure for parallel codes

Performance engineering workflow

- Build model of predicted performance
- Select data to measure
- Prepare application with symbols
- Insert extra code (probes/hooks)



- Collection of performance data
- Aggregation of performance data

- Modifications intended to eliminate/reduce performance problem

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

Score-P

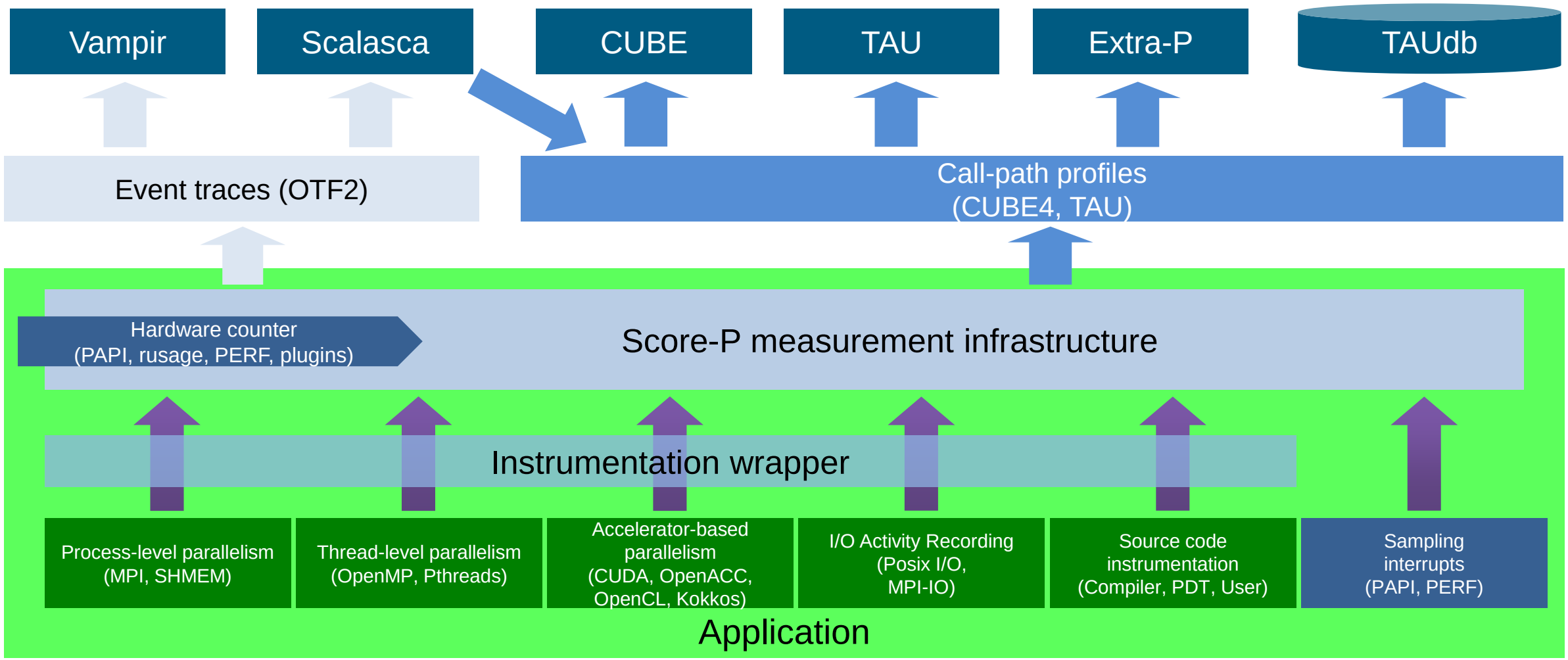
- Infrastructure for instrumentation and performance measurements
- Instrumented application can be used to produce several results:
  - Call-path profiling: CUBE4 data format used for data exchange
  - Event-based tracing: OTF2 data format used for data exchange

- 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
Bundesministerium für Bildung und Forschung

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

Hands-on:
NPB-MZ-MPI / bt-mz_C.8

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

Tutorial exercise objectives

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

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

Compiler and MPI modules (IvyMUC)

- Select modules for the PrgEnv-gnu tool chain

```
% module -s restore PrgEnv-gnu
```

Default is PrgEnv-cray

- Copy tutorial sources to your "WORK" directory

```
% cd /work/ta031/ta031/$USER
% tar zxvf /work/y23/shared/tutorial/NPB3.3-MZ-MPI.tar.gz
% cd NPB3.3-MZ-MPI
```

Use "WORK" for building and submitting

- Directory for data exchange during the workshop

```
% /work/ta031/ta031/shared/
```

NPB-MZ-MPI Suite

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

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

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

- Subdirectories contain source code for each benchmark
  - plus additional configuration and common code
- The provided distribution has already been configured for the tutorial, such that it is ready to "make" one or more of the benchmarks
  - but config/make.def may first need to be adjusted to specify appropriate compiler flags

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

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

#-----------------------------------------------------------------------
# Configured for PrgEnv-gnu
#-----------------------------------------------------------------------
#COMPFLAGS = -homp -G2 -N 255 # cce
COMPFLAGS = -fopenmp -fallow-argument-mismatch -ffixed-line-length-none # gnu
...

#-----------------------------------------------------------------------
# The Fortran compiler used for MPI programs
#-----------------------------------------------------------------------
MPIF77 = ftn

# Alternative variants to perform instrumentation
...

#MPIF77 = scorep --user  ftn
...
```

Uncomment COMPILER flags according to current environment

Default (no instrumentation)

Hint: uncomment a compiler wrapper to do instrumentation

Building an NPB-MZ-MPI Benchmark

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

  To make a NAS multi-zone benchmark type

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

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

  [...]

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

- Type "make" for instructions

Building an NPB-MZ-MPI Benchmark

```
% make bt-mz CLASS=B NPROCS=28
make[1]: Entering directory `BT-MZ'
make[2]: Entering directory `sys'
cc  -o setparams setparams.c -lm
make[2]: Leaving directory `sys'
../sys/setparams bt-mz 8 C
make[2]: Entering directory `../BT-MZ'
ftn -g -c  -O3 -fopenmp   bt.f
[…]
ftn -g -c  -O3 -fopenmp   mpi_setup.f
cd ../common; ftn -g -c  -O3 -fopenmp       print_results.f
cd ../common; ftn -g -c  -O3 -fopenmp       timers.f
ftn -g -O3 -fopenmp        -o ../bin/bt-mz_C.8 bt.o
 initialize.o exact_solution.o exact_rhs.o set_constants.o adi.o
 rhs.o zone_setup.o x_solve.o y_solve.o  exch_qbc.o solve_subs.o
 z_solve.o add.o error.o verify.o mpi_setup.o ../common/print_results.o
 ../common/timers.o
make[2]: Leaving directory `BT-MZ'
Built executable ../bin/bt-mz_C.8
make[1]: Leaving directory `BT-MZ'
```

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

Shortcut: % **make suite**

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

- What does it do?
  - Solves a discretized version of the unsteady, compressible Navier-Stokes equations in three spatial dimensions
  - Performs 200 time-steps on a regular 3-dimensional grid
- Implemented in 20 or so Fortran77 source modules

- Uses MPI & OpenMP in combination
  - 8 processes each with 6 threads should be reasonable for 1 compute node of ARCHER2
  - bt-mz_C.8 should run in less than 12 seconds with the PrgEnv-gnu toolchain

NPB-MZ-MPI / BT Reference Execution

```
% cd bin
% cp ../jobscript/archer2/run.sbatch .
% less run.sbatch
% sbatch run.sbatch

% cat slurm-<job_id>.out
 NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:  16 x  16
 Iterations:  200   dt:   0.000300
 Number of active processes:    8
 Use the default load factors with threads
 Total number of threads:    48   (  6.0 threads/process)

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

 BT-MZ Benchmark Completed.
 Time in seconds = 11.67
```

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

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

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 (ARCHER2)

- Latest/recent versions/combinations of VI-HPS tools not yet installed system-wide
  - Source `module use /work/y23/shared/tutorial/modulefiles` to prepare the environment
  - Required for each shell session
  - Score-P/Scalasca installation only for PrgEnv-gnu (PrgEnv-cray available soon)

```
% module restore PrgEnv-gnu
% module load scalasca/2.6-gcc10
```

  - Check `module avail scalasca` for alternate Scalasca/Score-P modules available

- Copy tutorial sources to your "WORK" directory (should be done already)

```
% cd /work/ta031/ta031/$USER
% tar zxvf /work/y23/shared/tutorial/NPB3.3-MZ-MPI.tar.gz
% cd NPB3.3-MZ-MPI
```

NPB-MZ-MPI / BT instrumentation

```
#--------------------------------------------------------------
# The Fortran compiler used for MPI programs
#--------------------------------------------------------------
#MPIF77 = ftn

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

#MPIF77 = SCOREP_WRAPPER_INSTRUMENTER_FLAGS="--user" \
# SCOREP_WRAPPER_COMPILER_FLAGS="-fopenmp -fallow-argument-mismatch -ffixed-line-length-none" \
# scorep-ftn

# This links MPI Fortran programs; usually the same as ${MPIF77}
FLINK   = $(MPIF77)
...
```

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

Uncomment the Score-P compiler wrapper specification
Alternatively, use compiler wrapper `scorep-ftn`

NPB-MZ-MPI / BT instrumented build

```
% make clean

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

- Return to root directory and clean-up
- Re-build executable using Score-P compiler wrapper

Measurement configuration: scorep-info

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

- Score-P measurements are configured via environmental variables

Summary measurement collection

```
% cd bin.scorep
% cp ../jobscript/archer2/scorep.sbatch .
% cat scorep.sbatch
...
# Score-P measurement configuration
export SCOREP_EXPERIMENT_DIRECTORY=scorep_bt-mz_sum
#export SCOREP_FILTERING_FILE=../config/scorep.filt
#export SCOREP_METRIC_PAPI=PAPI_TOT_INS,PAPI_TOT_CYC,…
#export SCOREP_METRIC_PAPI_PER_PROCESS=PAPI_L2_TCM
#export SCOREP_METRIC_RUSAGE=ru_stime
#export SCOREP_METRIC_RUSAGE_PER_PROCESS=ru_maxrss
#export SCOREP_TIMER=gettimeofday

# Run the application
srun./bt-mz_C.8

% sbatch scorep.sbatch
```

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

Leave these lines commented out for the moment

- Submit job

Summary measurement collection

```
% less slurm-<job_id>.out

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

 Number of zones:  16 x  16
 Iterations: 200    dt:   0.000100
 Number of active processes:     8
 Use the default load factors with threads
 Total number of threads:    48   (  6.0 threads/process)

 Calculated speedup = 47.97

 Time step    1

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

- Check the output of the application run

BT-MZ summary analysis report examination

```
% ls
Slurm-<job_id>.out scorep_bt-mz_sum/
% ls -1 scorep_bt-mz_sum
MANIFEST.md
profile.cubex
scorep.cfg


% cube scorep_bt-mz_sum/profile.cubex
# alternatively
% square scorep_bt-mz_sum/
 [CUBE GUI showing summary analysis report]

% paraprof scorep_bt-mz_A_4x4_sum/profile.cubex
 [TAU ParaProf GUI showing summary analysis report]
```

- Creates experiment directory including
  - A brief content overview (MANIFEST.md)
  - A record of the measurement configuration (scorep.cfg)
  - The analysis report that was collated after measurement (profile.cubex)
- Interactive exploration with Cube

Hint:
Copy ‘profile.cubex’ to local system (laptop) using ‘scp’ to improve responsiveness of GUI

Reference results available:
/work/ta031/shared/examples

BT-MZ summary analysis report remapping

```
% ls -1 scorep_bt-mz_sum/
MANIFEST.md
profile.cubex
scorep.cfg

# remap the Score-P way
% cube_remap2 -d -o scorep_bt-mz_sum/summary.cubex \
  scorep_bt-mz_sum/profile.cubex


# remap the Scalasca way
% square scorep_bt-mz_sum/profile.cubex
INFO: Post-processing runtime summarization report (profile.cubex)...
INFO: Displaying ./scorep_bt-mz_sum/summary.cubex...

  [CUBE GUI showing summary analysis report]
```

- `profile.cubex` contains raw measurement data
- Enhance by *remapping,* i.e., transform given metric tree into metric hierarchy
  - Score-P way:
    `cube_remap2 -d profile.cubex`
  - Scalasca way:
    `square profile.cubex`

Further information

- Community instrumentation & measurement infrastructure
  - Instrumentation (various methods)
  - 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