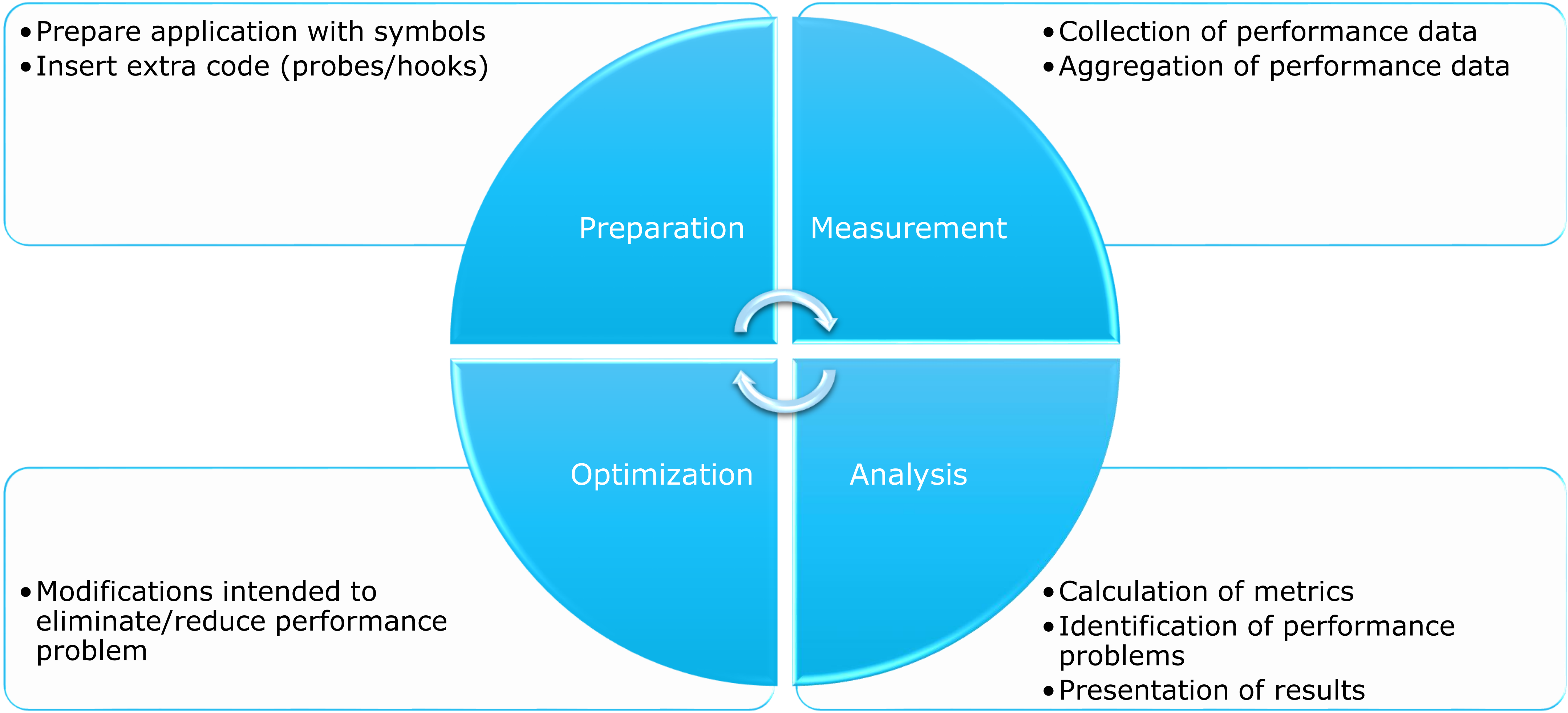
Score-P – A Joint Performance Measurement Run-Time Infrastructure for Scalasca, TAU, and Vampir

VI-HPS Team

Score-P

Scalable performance measurement infrastructure for parallel codes

Performance engineering workflow



- Prepare application with symbols
- Insert extra code (probes/hooks)

- Collection of performance data
- Aggregation of performance data

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

- Modifications intended to eliminate/reduce performance problem

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, HIP, 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

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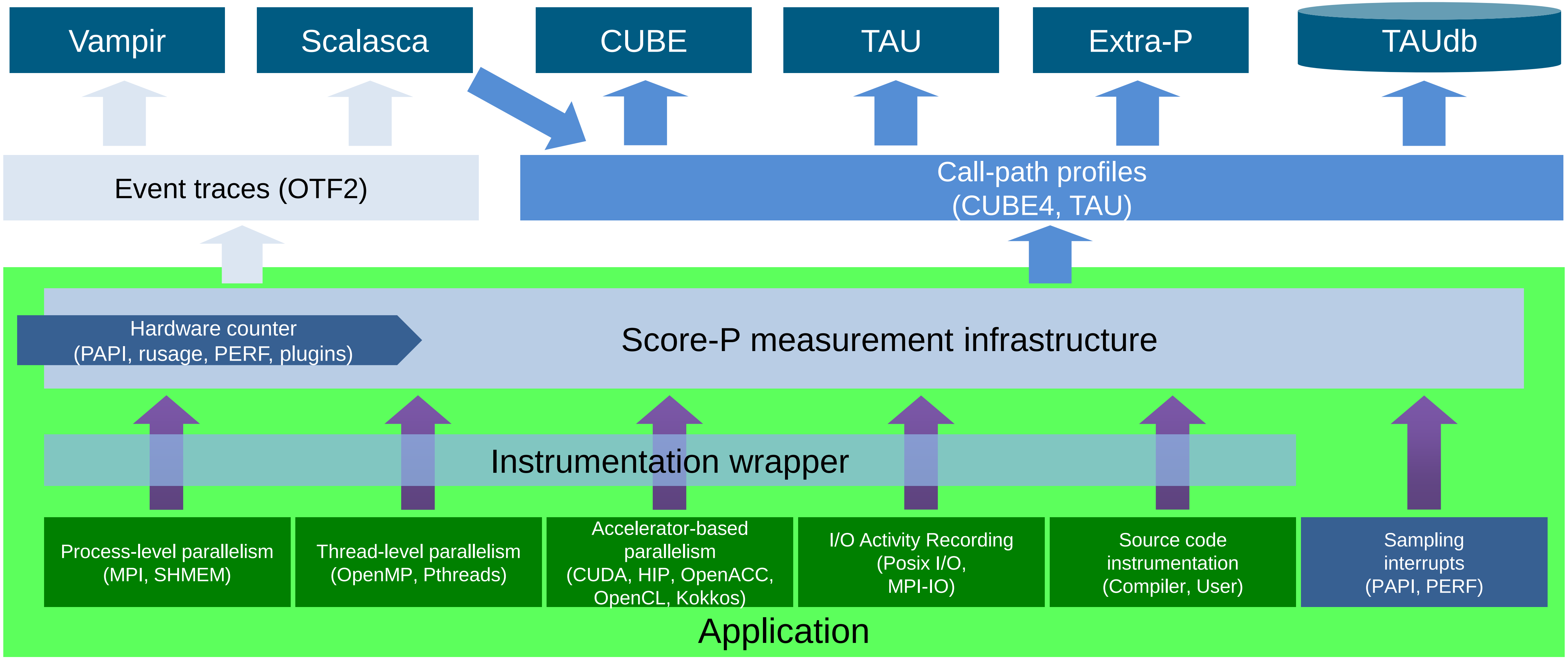
Score-P overview


Vampir
Scalasca
CUBE
TAU
Extra-P
TAUdb
Event traces (OTF2)
Call-path profiles (CUBE4, TAU)
Hardware counter (PAPI, rusage, PERF, plugins)
Score-P measurement infrastructure
Instrumentation wrapper
Process-level parallelism (MPI, SHMEM)
Thread-level parallelism (OpenMP, Pthreads)
Accelerator-based parallelism (CUDA, HIP, OpenACC, OpenCL, Kokkos)
I/O Activity Recording (Posix I/O, MPI-IO)
Source code instrumentation (Compiler, User)
Sampling interrupts (PAPI, PERF)
Application

Score-P user commands

`scorep` – instrument your software by prepending to your compile command:

```
scorep <scorep-options> <compiler> <compiler-options>
```

`scorep-cc/CC/ftn` – alt. instrumentation, replaces compiler command (CMake, autotools):

```
SCOREP_WRAPPER_INSTRUMENTER_FLAGS=<scorep-options> scorep-CC <compiler-options>
```

See `scorep-wrapper --help` for details.

`scorep-info` – List (measurement) configuration options, open issues, license, and more

`scorep-score` – *Score* a profile measurement, create a filter (prepare trace measurement):

```
scorep-score [-g] [-r] [-f <filter>] profile.cubex
```

All commands support `--help`

Contributing Partners

- Forschungszentrum Jülich, Germany
- RWTH Aachen, Germany
- Technische Universität Darmstadt, Germany
- Technische Universität Dresden, Germany
- Technische Universität München, Germany
- University of Oregon, Eugene, USA
- German Aerospace Center (DLR)

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

Score-P

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 (Archer2)

- Select modules for the PrgEnv-gnu tool chain

```
% module swap PrgEnv-cray PrgEnv-gnu
```

Default is PrgEnv-cray
Alternatives PrgEnv-aocc & PrgEnv-gnu

- Copy tutorial sources to your “WORK” directory

```
% cd /work/ta115/ta115/$USER
% tar zxvf /work/y23/shared/tutorial/NPB3.4-MZ-MPI.tar.gz
% cd NPB3.4-MZ-MPI
```

Use “WORK” filesystem
for building and submitting

- Directory for data exchange during the workshop

```
/work/ta115/ta115/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 Fortran90 (older versions Fortran77)
  - Configurable for various sizes & classes
- Move into the NPB3.4-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 HPE/Cray systems with PrgEnv compiler-specific OpenMP
#---------------------------------------------------------------------------
#COMPFLAGS = -fopenmp # aocc/flang
#COMPFLAGS = -homp -G2 # cce
COMPFLAGS = -fopenmp -fallow-argument-mismatch # gnu
...

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

# Alternative variants to perform instrumentation
...
#FC = $(PREP) ftn
#FC = scorep --user  ftn
#FC = scorep-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 3.4        =
  =      MPI+OpenMP Multi-Zone Versions     =
  =      MPI/Fortran                        =
  ===========================================

  To make a NAS multi-zone benchmark type

         make <benchmark-name> CLASS=<class>

  where <benchmark-name> is “bt-mz”, “lu-mz”, or “sp-mz”
        <class>          is “S”, “W”, “A” through “F”

  [...]

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

- Type “make” for instructions

Building an NPB-MZ-MPI Benchmark

```
% make bt-mz CLASS=C
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 C
make[2]: Entering directory `../BT-MZ'
ftn -g -c  -O3 -fopenmp   bt.f90
[…]
ftn -g -c  -O3 -fopenmp   setup_mpi.f90
cd ../common; ftn -g -c  -O3 -fopenmp       print_results.f90
cd ../common; ftn -g -c  -O3 -fopenmp       timers.f90
ftn -g -O3 -fopenmp        -o ../bin/bt-mz_C.x  bt.o bt_data.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 setup_mpi.o mpinpb.o error_cond.o
 ../common/print_results.o ../common/timers.o
make[2]: Leaving directory `BT-MZ'
Built executable ../bin/bt-mz_C.x
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**

Shortcut: `% make suite`

NPB-MZ-MPI / BT (Block Tri-diagonal 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
  - Includes verification of solution
- Implemented in 20 or so Fortran90 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.x should run in less than 15 seconds
  - Benchmark time reported as “Time in seconds”

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 (NPB3.4-MZ MPI+OpenMP) - BT-MZ 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

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Local installation (ARCHER2)

- Setup access to Scalasca and associated tools, accessible via “other-software”
  - Required for each shell session
  - Score-P and Scalasca installations are toolchain specific (GCC11 default)

```
% module swap PrgEnv-cray PrgEnv-gnu
% module load load-epcc-module other-software
% module load scalasca/2.6.1-gcc11
```

PrgEnv-cray
PrgEnv-aocc
PrgEnv-gnu

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

- Copy tutorial sources to your personal workspace (if not already done)

```
% cd /work/ta115/ta115/$USER
% tar zxvf /work/y23/shared/tutorial/NPB3.4-MZ-MPI.tar.gz
% cd NPB3.4-MZ-MPI
```

NPB-MZ-MPI / BT instrumentation

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

# Alternative variants to perform instrumentation
...
# PREP is a generic macro for instrumentation preparation
# e.g. PREP="scorep --user"
FC = $(PREP) ftn

# Alternative via Score-P compiler wrapper
# configured via SCOREP_WRAPPER_INSTRUMENTER_FLAGS="--user"
# FC = scorep-ftn

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

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

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
cd BT-MZ; make CLASS=C VERSION=
make: Entering directory 'BT-MZ'
cd ../sys; cc  -o setparams setparams.c -lm
../sys/setparams bt-mz C
scorep --user ftn -g -c  -O3 -fopenmp bt.f90
 [...]
cd ../common;  scorep --user ftn -g -c  -O3 -fopenmp timers.f90
 [...]
scorep --user ftn -g -O3 -fopenmp -o ../bin.scorep/bt-mz_C.x \
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.x
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_TOTAL_MEMORY=100M
#export SCOREP_ENABLE_TRACING=true

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

% 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 (NPB3.4-MZ MPI+OMP) - BT-MZ 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_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/y23/shared/tutorial/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
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

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
- Download sources, subscribe to news mailing list:
  - http://www.score-p.org
- User guide part of installation or available online:
  - <prefix>/share/doc/scorep/{pdf,html}/
  - Online HTML / Online PDF
- Support and feedback: support@score-p.org