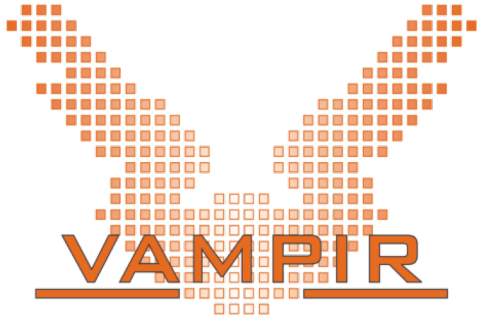
Vampir hands-on:
Visualizing and analyzing NPB-MZ-MPI / BT



Demo example code: NPB-MZ-MPI / BT

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

```
% cd tutorial; 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's ready to “make” one or more of the benchmarks and install them into a (tool-specific) “bin” subdirectory

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

- What does it do?
  - Solves a discretized version of 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
  - 4 processes with 4 threads each should be reasonable
    - don’t expect to see speed-up when run on a laptop!
  - bt-mz_W.4 should run in around 13 seconds on a laptop
  - bt-mz_C.4 is more suitable for dedicated HPC compute nodes
    - Each class step takes around 10-15x longer

Building an NPB-MZ-MPI benchmark

- Type "make" for instructions

```
% 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 LiveISO/DVD:  *
 *       make bt-mz CLASS=W NPROCS=4                           *
 ***********************************************************
```

Hint: the recommended build configuration is available via
`% make suite`

Building an NPB-MZ-MPI benchmark

- Specify the benchmark configuration
  - benchmark name: **bt-mz**, lu-mz, sp-mz
  - the number of MPI processes: NPROCS=**4**
  - the benchmark class (S, W, A, B, C, D, E): CLASS=**W**

```
% make bt-mz CLASS=W NPROCS=4
cd BT-MZ; make CLASS=W NPROCS=4 VERSION=
make: Entering directory 'BT-MZ'
cd ../sys; cc  -o setparams setparams.c
../sys/setparams bt-mz 4 W
mpif77 -c  -O3 -fopenmp bt.f
 [...]
cd ../common;  mpif77 -c  -O3 -fopenmp timers.f
mpif77 -O3 -fopenmp -o ../bin/bt-mz_W.4 \
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/bt-mz_W.4
make: Leaving directory 'BT-MZ'
```

NPB-MZ-MPI / BT reference execution

- Launch as a hybrid MPI+OpenMP application

```
% cd bin
% OMP_NUM_THREADS=4  mpiexec -np 4 ./bt-mz_W.4
 NAS Parallel Benchmarks (NPB3.3-MZ-MPI) - BT-MZ MPI+OpenMP Benchmark
 Number of zones:    4 x    4
 Iterations:  200    dt:    0.000800
 Number of active processes:     4
 Total number of threads:     16   (   4.0 threads/process)

 Time step    1
 Time step   20
 Time step   40
  [...]
 Time step  160
 Time step  180
 Time step  200
 Verification Successful

 BT-MZ Benchmark Completed.
 Time in seconds = 5.57
```

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

Profile NPB-MZ-MPI / BT

NPB-MZ-MPI / BT Instrumentation

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

```
#            SITE- AND/OR PLATFORM-SPECIFIC DEFINITIONS
#----------------------------------------------------------------------
# Items in this file may need to be changed for each platform.
#----------------------------------------------------------------------
...
#----------------------------------------------------------------------
# The Fortran compiler used for MPI programs
#----------------------------------------------------------------------
#MPIF77 = mpif77

# Alternative variants to perform instrumentation
...
MPIF77 = scorep mpif77

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

Uncomment the Score-P compiler wrapper specification

NPB-MZ-MPI / BT Instrumented Build

- Return to root directory and clean-up

```
% make clean
```

- Re-build executable using Score-P compiler wrapper

```
% make bt-mz CLASS=W NPROCS=4
cd BT-MZ; make CLASS=W NPROCS=4 VERSION=
make: Entering directory 'BT-MZ'
cd ../sys; cc  -o setparams setparams.c -lm
../sys/setparams bt-mz 4 B
scorep mpif77 -c  -O3 -fopenmp bt.f
 [...]
cd ../common;  scorep mpif77 -c  -O3 -fopenmp timers.f
scorep mpif77 -O3 -fopenmp -o ../bin.scorep/bt-mz_W.4 \
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_W.4
make: Leaving directory 'BT-MZ'
```

Measurement Configuration: scorep-info

- Score-P measurements are configured via environmental variables:

```
% 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 ...]
```

Summary Measurement Collection

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

```
% cd bin.scorep
% export OMP_NUM_THREADS=4
% export SCOREP_EXPERIMENT_DIRECTORY=scorep_bt-mz_W_4x4_sum
% mpiexec -np 4 ./bt-mz_W.4

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

 Number of zones:   8 x   8
 Iterations: 200    dt:   0.000300
 Number of active processes:     4

 Use the default load factors with threads
 Total number of threads:     16   (  4.0 threads/process)

 Calculated speedup =     15.96

 Time step    1

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

BT-MZ Summary Analysis Report Examination

- Creates experiment directory ./scorep_bt-mz_W_4x4_sum containing
  - A record of the measurement configuration (scorep.cfg)
  - The analysis report that was collated after measurement (profile.cubex)

```
% ls
bt-mz_B.4  scorep_bt-mz_W_4x4_sum
% ls scorep_bt-mz_W_4x4_sum
profile.cubex  scorep.cfg
```

Congratulations!?

- If you made it this far, you successfully used Score-P to
  - instrument the application
  - analyze its execution with a summary measurement, and
  - examine it with one the interactive analysis report explorer GUIs
- ... revealing the call-path profile annotated with
  - the "Time" metric
  - Visit counts
  - MPI message statistics (bytes sent/received)
- ... but how ***good*** was the measurement?
  - The measured execution produced the desired valid result
  - however, the execution took longer than expected!
    - even when ignoring measurement start-up/completion
    - ☞ it was probably dilated by instrumentation/measurement overhead

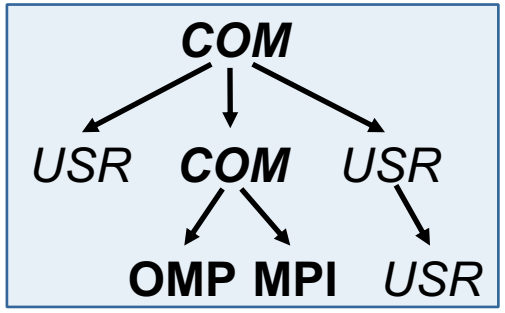
BT-MZ Summary Analysis Result Scoring

- Report scoring as textual output

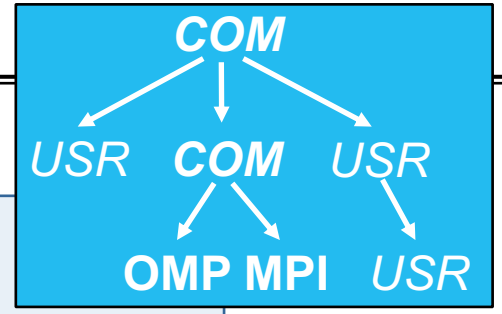
```
% scorep-score scorep_bt-mz_W_4x4_sum/profile.cubex
Estimated aggregate size of event trace:                   35965836622 bytes
Estimated requirements for largest trace buffer (max_tbc): 9046029930 bytes
(hint: When tracing set SCOREP_TOTAL_MEMORY > max_tbc to avoid intermediate flushes
 or reduce requirements using file listing names of USR regions to be filtered.)

flt type         max_tbc         time      % region
     ALL      9046029930       799.89   100.0 ALL
     USR      9025830154       383.72    48.0 USR
     OMP        19113728       411.49    51.4 OMP
     COM          997150         0.75     0.1 COM
     MPI           88898         3.92     0.5 MPI
```

33.5 GB total memory
8.4 GB per rank!

- Region/callpath classification
  - MPI (pure MPI library functions)
  - OMP (pure OpenMP functions/regions)
  - USR (user-level source local computation)
  - COM ("combined" USR + OpenMP/MPI)
  - ANY/ALL (aggregate of all region types)



BT-MZ Summary Analysis Report Breakdown



- Score report breakdown by region

```
% scorep-score -r scorep_bt-mz_W_4x4_sum/profile.cubex
  [...]
flt type          max_tbc         time      % region
     ALL       9046029930       799.89  100.0 ALL
     USR       9025830154       383.72   48.0 USR
     OMP         19113728       411.49   51.4 OMP
                   997150         0.75    0.1 COM
                    88898         3.92    0.5 MPI

                2894950740       152.50   19.1 binvcrhs_
                2894950740        98.73   12.3 matvec_sub_
     USR        2894950740       117.78   14.7 matmul_sub_
     USR         127716204         5.01    0.6 binvrhs_
     USR         127716204         6.62    0.8 lhsinit_
     USR          94933520         3.07    0.4 exact_solution_
     OMP           1183488         0.04    0.0 !$omp parallel @exch_...
     OMP           1183488         0.04    0.0 !$omp parallel @exch_...
     OMP           1183488         0.04    0.0 !$omp parallel @exch_...
 [...]
```

More than 8 GB just for these 6 regions

BT-MZ Summary Analysis Score

- Summary measurement analysis score reveals
  - Total size of event trace would be ~34 GB
  - Maximum trace buffer size would be ~8.5 GB per rank
    - smaller buffer would require flushes to disk during measurement resulting in substantial perturbation
  - 99.8% of the trace requirements are for USR regions
    - purely computational routines never found on COM call-paths common to communication routines or OpenMP parallel regions
  - These USR regions contribute around 32% of total time
    - however, much of that is very likely to be measurement overhead for frequently-executed small routines
- Advisable to tune measurement configuration
  - Specify an adequate trace buffer size
  - Specify a filter file listing (USR) regions not to be measured

BT-MZ Summary Analysis Report Filtering

- Report scoring with prospective filter listing
  6 USR regions

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

% scorep-score -f ../config/scorep.filt scorep_bt-mz_W_4x4_sum/profile.cubex
Estimated aggregate size of event trace:                   80814262 bytes
Estimated requirements for largest trace buffer (max_tbc): 20203582 bytes
(hint: When tracing set SCOREP_TOTAL_MEMORY > max_tbc to avoid intermediate flushes
 or reduce requirements using file listing names of USR regions to be f
```

77 MB of memory in total,
20 MB per rank!

BT-MZ Summary Analysis Report Filtering

- Score report break-down by region

```
% scorep-score -r -f ../config/scorep.filt \
> scorep_bt-mz_W_4x4_sum/profile.cubex
flt type         max_tbc         time      % region
 *   ALL        20203582       416.17   52.0 ALL-FLT
 +   FLT      9025826370       383.72   48.0 FLT
 -   OMP        19113728       411.49   51.4 OMP-FLT
 *   COM          997150         0.75    0.1 COM-FLT
 -   MPI           88898         3.92    0.5 MPI-FLT
 *   USR            3806         0.00    0.0 USR-FLT

 +   USR      2894950740       152.50   19.1 binvcrhs_
 +   USR      2894950740        98.73   12.3 matvec_sub_
 +   USR      2894950740       117.78   14.7 matmul_sub_
 +   USR       127716204         5.01    0.6 binvrhs_
 +   USR       127716204         6.62    0.8 lhsinit_
 +   USR        94933520         3.07    0.4 exact_solution_
 -   OMP         1183488         0.04    0.0 !$omp parallel @exch_...
 -   OMP         1183488         0.04    0.0 !$omp parallel @exch_...
 -   OMP         1183488         0.04    0.0 !$omp parallel @exch_...
 [...]
```

Filtered routines marked with '+'

BT-MZ Filtered Summary Measurement

- Set new experiment directory and re-run measurement with new filter configuration
  - Adjust configuration and re-run measurement
  - Submit job

```
% export OMP_NUM_THREADS=4
% export SCOREP_EXPERIMENT_DIRECTORY=scorep_bt-mz_W_4x4_sum_with_filter
% export SCOREP_FILTERING_FILE=../config/scorep.filt
% mpiexec -np 4 ./bt-mz_W.4

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

 Number of zones:   8 x   8
 Iterations: 200    dt:   0.000300
 Number of active processes:     4

 Use the default load factors with threads
 Total number of threads:     16   (  4.0 threads/process)

 Calculated speedup =     15.96

 Time step    1

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

BT-MZ Tuned Summary Analysis Report Score

- Scoring of new analysis report as textual output

```
% scorep-score scorep_bt-mz_W_4x4_sum_with_filter/profile.cubex
Estimated aggregate size of event trace:                   80814262 bytes
Estimated requirements for largest trace buffer (max_tbc): 20203582 bytes
(hint: When tracing set SCOREP_TOTAL_MEMORY > max_tbc to avoid intermediate flushes
 or reduce requirements using file listing names of USR regions to be filtered.)

flt type         max_tbc         time      % region
     ALL        20203582       218.95  100.0 ALL
     OMP        19113728       216.94   99.1 OMP
     COM          997150         0.73    0.3 COM
     MPI           88898         1.27    0.6 MPI
     USR            3806         0.00    0.0 USR
```

- Significant reduction in runtime (measurement overhead)
  - Not only reduced time for USR regions, but MPI/OMP reduced too!
- Further measurement tuning (filtering) may be appropriate
  - E.g., use “timer_*” to filter timer_start_, timer_read_, etc.

Advanced Measurement Configuration: Metrics

- Recording hardware counters via PAPI

```
% export SCOREP_METRIC_PAPI=PAPI_L2_TCM,PAPI_FP_OPS
```

- Also possible to record them only per rank

```
% export SCOREP_METRIC_PAPI_PER_PROCESS=PAPI_L3_TCM
```

- Recording operating system resource usage

```
% export SCOREP_METRIC_RUSAGE_PER_PROCESS=ru_maxrss,ru_stime
```

Advanced Measurement Configuration: Metrics

- Available PAPI metrics
  - Preset events: common set of events deemed relevant and useful for application performance tuning
    - Abstraction from specific hardware performance counters, mapping onto available events done by PAPI internally

```
% papi_avail
```

  - Native events: set of all events that are available on the CPU (**platform dependent**)

```
% papi_native_avail
```

Note:
Due to hardware restrictions
- number of concurrently recorded events is limited
- there may be invalid combinations of concurrently recorded events

Advanced Measurement Configuration: Metrics

- Available resource usage metrics

```
% man getrusage
 [... Output ...]

struct rusage {
     struct timeval ru_utime; /* user CPU time used */
     struct timeval ru_stime; /* system CPU time used */
     long   ru_maxrss;        /* maximum resident set size */
     long   ru_ixrss;         /* integral shared memory size */
     long   ru_idrss;         /* integral unshared data size */
     long   ru_isrss;         /* integral unshared stack size */
     long   ru_minflt;        /* page reclaims (soft page faults) */
     long   ru_majflt;        /* page faults (hard page faults) */
     long   ru_nswap;         /* swaps */
     long   ru_inblock;       /* block input operations */
     long   ru_oublock;       /* block output operations */
     long   ru_msgsnd;        /* IPC messages sent */
     long   ru_msgrcv;        /* IPC messages received */
     long   ru_nsignals;      /* signals received */
     long   ru_nvcsw;         /* voluntary context switches */
     long   ru_nivcsw;        /* involuntary context switches */
};

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

Note:
(1) Not all fields are maintained on each platform.
(2) Check scope of metrics (per process vs. per thread)

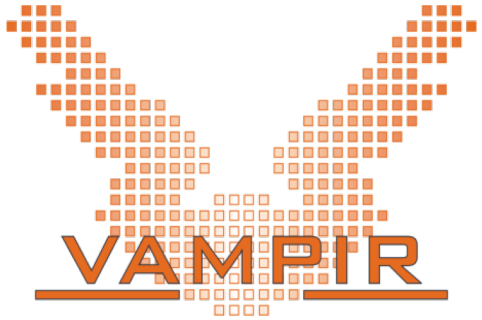
BT-MZ Trace Measurement Collection...

- Adjust configuration and re-run the application using the tracing mode of Score-P

```
% export OMP_NUM_THREADS=4
% export SCOREP_EXPERIMENT_DIRECTORY=scorep_bt-mz_W_4x4_trace
% export SCOREP_FILTERING_FILE=../config/scorep.filt
% export SCOREP_ENABLE_TRACING=true
% export SCOREP_ENABLE_PROFILING=false
% export SCOREP_TOTAL_MEMORY=30M
% mpiexec -np 4 ./bt-mz_W.4

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

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

- Separate trace file per thread written straight into new experiment directory ./scorep_bt-mz_B_4x4_trace

Visualize NPB-MZ-MPI/BT with Vampir

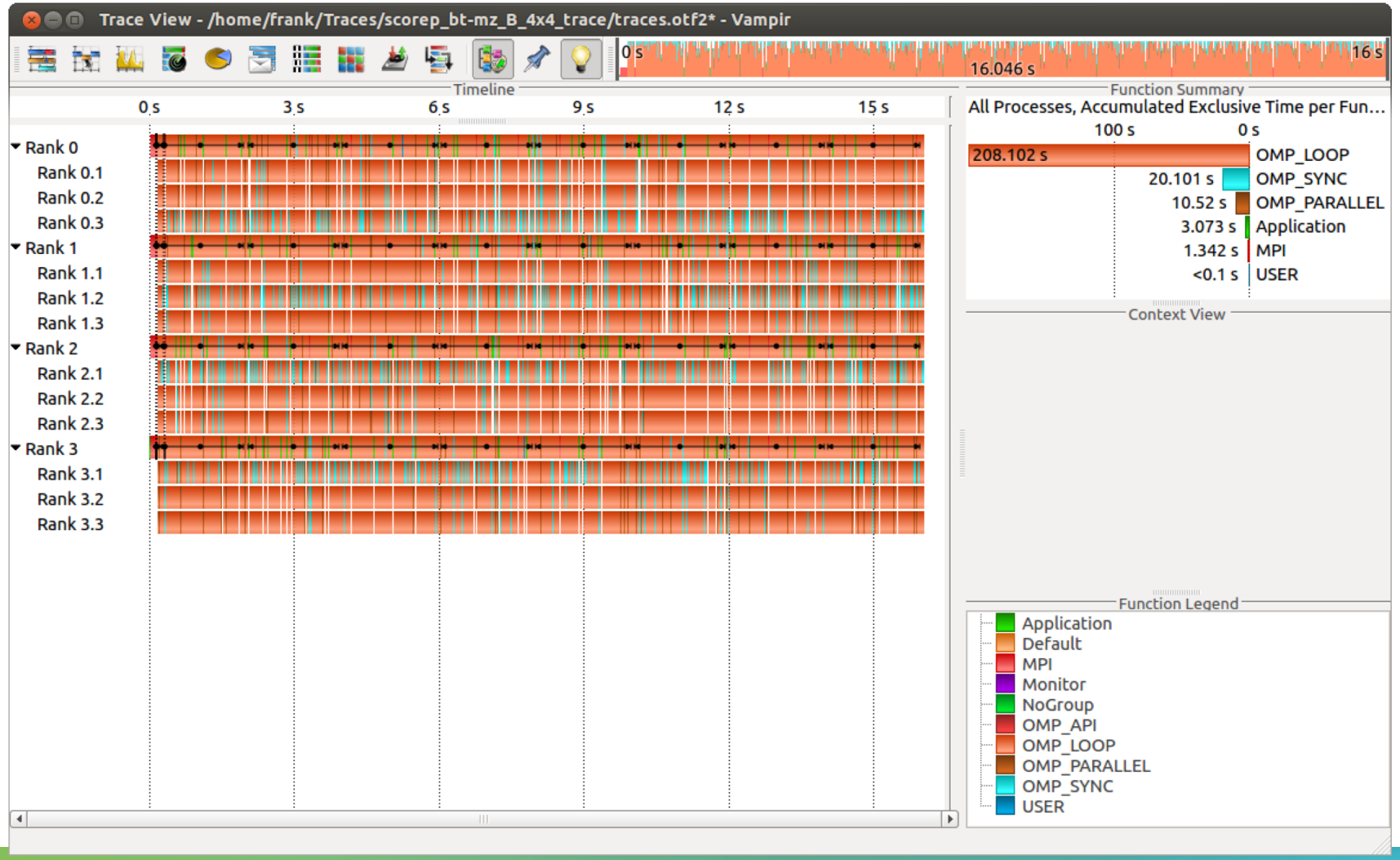


Start Vampir

```
% vampir <tracefile>

% vampir scorep_bt-mz_W_4x4_trace/traces.otf2
```

- Start Vampir and load trace

Visualization of the NPB-MZ-MPI / BT trace



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