



NPB-MZ-MPI / BT

Demo/Hands-on: Reference execution

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 analysis & report examination

Compiler and MPI modules (COSMA)

- Select modules for the GCC + OpenMPI tool chain

```
% module load gnu_comp/14.1.0 openmpi/5.0.3
```

- Copy tutorial sources to your WORK directory

```
% export WORK=/cosma/apps/do009/$USER  
% cd $WORK  
% tar xf /cosma/apps/do009/shared/Scalasca/NPB3.4-MZ-MPI.tar.gz  
% cd NPB3.4-MZ-MPI
```

NPB-MZ-MPI Suite

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

- Available from:

<https://www.nas.nasa.gov/Software/NPB>

- 3 benchmarks in Fortran90
- 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 generic MPI with GCC or Intel compiler
#-----
COMPFLAGS = -fopenmp           # GCC compiler
#COMPFLAGS = -qopenmp          # Intel compiler
...
#-----
# The Fortran compiler used for MPI programs
#-----
FC = mpif90
...

```

Uncomment COMPILER flags
according to current environment

Default (no instrumentation)

Building an NPB-MZ-MPI Benchmark

```

% make
=====
=      NAS PARALLEL BENCHMARKS 3.4      =
=      MPI+OpenMP Multi-Zone Versions   =
=      F90                               =
=====

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 cluster: *
*      make bt-mz CLASS=B                                *
*****

```

- Type "make" for instructions

Shortcut: `% make suite`

Building an NPB-MZ-MPI Benchmark

```
% make bt-mz CLASS=B
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 B
make[2]: Entering directory `../BT-MZ'
mpif90 -g -c -O3 -fopenmp          bt_scorep_user.F90
[...]
mpif90 -g -c -O3 -fopenmp          mpi_setup.f90
cd ../common; mpif90 -g -c -O3 -fopenmp  print_results.f90
cd ../common; mpif90 -g -c -O3 -fopenmp  timers.f90
mpif90 -g -O3 -fopenmp      -o ../bin/bt-mz_B.x  bt_scorep_user.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_B.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=B**

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 Fortran90 source modules

- Uses MPI & OpenMP in combination
 - 4 processes each with 6 threads should be reasonable for 2 compute nodes of 'bluefield1'
 - bt-mz_B.x should run in ~30 seconds with the GCC + OpenMPI toolchain

NPB-MZ-MPI / BT Reference Execution

```
% cd bin
% cp ../jobscript/bluefield1/reference.sbatch .
% less reference.sbatch
% sbatch reference.sbatch

% less slurm-<job_id>.out
NAS Parallel Benchmarks (NPB3.4-MZ MPI+OpenMP) - BT-MZ 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:   24 ( 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 = 30.23
```

- 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