International HPC Summer School 2023: Performance analysis and optimization

Hands-on:
NPB-MZ-MPI/BT Reference run

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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

- 3.0 Trace measurement with filtering
- 3.1 Event trace examination & analysis

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Tutorial exercise objectives

- Familiarize with a typical **workflow**
- Prepare to apply tools productively to *your* application(s)
- Exercise is based on a small portable benchmark code
  - Unlikely to have significant optimization opportunities

- Optional (recommended) exercise extensions
  - Investigate reproducibility of measurements: CPU frequency/Turboboost
  - Analyze performance of alternative configurations
  - Investigate effectiveness of system-specific compiler/MPI optimizations and/or placement/binding/affinity capabilities
  - Investigate scalability and analyze scalability limiters
  - Compare performance on different HPC platforms
  - …

Access to Bridges2

```
# Connect to the Bridges2 login node
% ssh -X userid@bridges2.psc.edu
```

- Logging in to Bridges2

```
$HOME
/jet
…

/jet/home/zhukov/ihpcss23/tutorial
```

- File systems & directories
  - Use $HOME for the tutorial

Tutorial materials

- More extensive documentation:
  - https://www.psc.edu/resources/bridges-2/user-guide-2

Compiling & job submission

- Development environment: GNU compiler with OpenMPI
  - Use OpenMPI compiler wrappers
    - `mpicc`
    - `mpicxx`
    - `mpif77`

- Bridges2 uses the SLURM batch system
  - Jobs submitted from tutorial accounts will need to specify our reservation

```
% sbatch jobscript.sbatch
% squeue -u $USER
% scancel <jobid>
```

← Submit job
← View job queue
← Cancel job

Local installation

- VI-HPS tools not yet installed system-wide
  - Enable and load local tool installations
  - Required for each shell session

```
% module use /jet/home/zhukov/ihpcss23/modules/
% module load openmpi/4.0.2-intel20.4 likwid/5.2.0
```

- Copy tutorial sources to a working directory, e.g. $HOME

```
% cd $HOME
% tar zxvf /jet/home/zhukov/ihpcss23/tutorial/NPB3.3-MZ-MPI.tar.gz
% cd NPB3.3-MZ-MPI
```

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 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 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
  - Proposed hands-on setup on Bridges2:
    - 2 compute nodes with 2 x AMD EPYC 7742 64-Core Processor
      - 64 cores per CPU, 128 cores per node
      - 256GB RAM each
      - Get more details using likwid-topology
    - 8 MPI processes with 6 OpenMP threads each, not utilizing all cores
  - bt-mz_C.8 should run ~15 seconds on Bridges2

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 Bridges2:      *
 *       make bt-mz CLASS=C NPROCS=8                           *
 ***********************************************************
```

- Type "make" for instructions

Building an NPB-MZ-MPI benchmark

```
% make bt-mz CLASS=C NPROCS=8
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'
mpif77 -c  -O3 -fopenmp       bt.f
[…]
mpif77 -c  -O3 -fopenmp       mpi_setup.f
cd ../common;  mpif77 -c  -O3 -fopenmp       print_results.f
cd ../common;  mpif77 -c  -O3 -fopenmp       timers.f
mpif77  -O3 -fopenmp   -o ../bin/bt-mz_B.30 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 number of MPI processes: NPROCS=**8**
  - the benchmark class (S, W, A, B, C, D, E): CLASS=**C**
  - Or use "**make suite**"

System topology

```
% likwid-topology
--------------------------------------------------------------------------------
CPU name:         AMD EPYC 7742 64-Core Processor
CPU type:         AMD K17 (Zen2) architecture
CPU stepping:     0
********************************************************************************
Hardware Thread Topology
********************************************************************************
Sockets:          2
Cores per socket: 64
Threads per core: 2
--------------------------------------------------------------------------------
HWThread        Thread        Core        Die        Socket        Available
0               0             0           0          0             *
1               0             1           0          0             *
…
```

- likwid-topology: thread and cache topology on x86 CPUs
- 128 cores available per node
- Hyperthreading deactivated

NPB-MZ-MPI / BT reference execution

```
% cd bin
% cp ../jobscript/bridges2/reference.sbatch.C.8 .
% less reference.sbatch.C.8
#!/bin/bash
#SBATCH -J mzmpibt           # job name
#SBATCH -o ref-C.8-%j.out    # stdout output file
#SBATCH -e ref-C.8-%j.err    # stderr output file
#SBATCH --nodes=2            # requested nodes
#SBATCH --ntasks=8           # requested MPI tasks
#SBATCH --cpus-per-task=6    # requested logical CPUs/threads per task
#SBATCH --partition RM       # partition to use
#SBATCH --account=tra210016p # account to charge
#SBATCH --export=ALL         # export env varibales
#SBATCH --time=00:10:00      # max wallclock time (hh:mm:ss)

# setup modules, add tools to PATH
set -x
module load openmpi/4.0.2-intel20.4
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

# benchmark configuration
export NPB_MZ_BLOAD=0
CLASS=C
PROCS=$SLURM_NTASKS
EXE=./bt-mz_$CLASS.$PROCS
SOCKETS=2
TASKS_PER_SOCKET=$(( $SLURM_NTASKS / $SLURM_NNODES ) / $SOCKETS ))

mpirun -report-bindings --map-by ppr:$TASKS_PER_SOCKET:socket:pe=$SLURM_CPUS_PER_TASK \
       -n $SLURM_NTASKS $EXE
```

- Examine jobscript

NPB-MZ-MPI / BT reference execution (cont)

```
% sbatch reference.sbatch.C.8
% less ref-C.8-<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
 Total number of threads:       48   (   6.0 threads/process)

 Time step    1
 Time step   20
 Time step   40

  [...]

 Time step  180
 Time step  200
 Verification Successful

 BT-MZ Benchmark Completed.
 Time in seconds = 14.25
```

- Copy jobscript and launch as a hybrid MPI+OpenMP application
- Reproducible? CPU frequency constant? Turboboost?

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

NPB-MZ-MPI / BT reference execution (cont)

```
% less ref-C.8-<job_id>.err
[...]

node r164 [...] rank 0 bound to socket 0 [...]: [B/B/B/B/B/B/./././././././…][./././././././././././././././…]
node r164 [...] rank 1 bound to socket 0 [...]: [././././././B/B/B/B/B/B/./…][./././././././././././././././…]
node r164 [...] rank 2 bound to socket 1 [...]: [././././././././././././././…][B/B/B/B/B/B/././././././././…]
node r164 [...] rank 3 bound to socket 1 [...]: [././././././././././././././…][././././././B/B/B/B/B/B/./…]
node r172 [...] rank 4 bound to socket 0 [...]: [B/B/B/B/B/B/././././././././…][././././././././././././././…]
node r172 [...] rank 5 bound to socket 0 [...]: [././././././B/B/B/B/B/B/./…][././././././././././././././…]
node r172 [...] rank 6 bound to socket 1 [...]: [././././././././././././././…][B/B/B/B/B/B/././././././././…]
node r172 [...] rank 7 bound to socket 1 [...]: [././././././././././././././…][././././././B/B/B/B/B/B/./…]

[...]
```

- **--report-bindings** makes each rank print to its standard error output the affinity mask that apply to itapplication
- Each socket is represented as a set of square brackets with each core represented by a dot. The core(s) that each rank is bound to is/are denoted by the letter B.