BQCD Best Practices for Intel® Cluster Ready

HPC ADVISORY COUNCIL
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BEST PRACTICES

1. Introduction:

The following best practices document is provided as courtesy of the HPC Advisory Council.

2. Application Description:

BQCD (Berlin Quantum ChromoDynamics program) is a hybrid Monte-Carlo code that simulates Quantum Chromodynamics with dynamical standard Wilson fermions. The computations take place on a four-dimensional regular grid with periodic boundary conditions. The kernel of the program is a standard conjugate gradient solver with even/odd pre-conditioning.

For further information, see http://www.deisa.eu/science/benchmarking/codes/bqcd

3. Version Information:

Download BQCD

http://www.deisa.eu/science/benchmarking

4. Prerequisites:

4.1 Hardware:

The instructions from this best practice have been tested on Dell PowerEdge M610 blade server

- Intel® Xeon 5670 processors
- Mellanox QDR InfiniBand HCA (Driver: MLNX_OFED 1.5.1)
- Mellanox QDR InfiniBand switch

4.2 Software:

1. OS

   Intel® Cluster Ready Platform, using CentOS 5.4

2. Compilers

   The Intel® C and C++ Compiler for Linux; We used Intel® version 11.1.064

3. Libraries in addition to Intel® Cluster Ready configuration

   Intel MPI 4.0.0.028 or Open MPI 1.4.1 (compiled by Intel® compiler)

5. Building BQCD

1. Compile BQCD

   export FPP = ifort -E

   export FPP2 = icc -E -C -P

   export F90 = mpif90 -fc=ifort

   export CC = mpicc -cc=icc

   # make -j 8

   Executable bqcd will be generated under bin directory

6. Building BQCD:

1. Create benchmark input file, for example:

   run 0

   lattice 48 6 12 48

   processes 1 1 2 4

   boundary_conditions_fermions 1 1 1 -1

   beta 5

   kappa 0.13

   csw 2.3327

   h 0

   hmc_test 0

   hmc_model C

   hmc_rho 0.1

   hmc_trajectory_length 0.2

   hmc_steps 10

   hmc_accept_first 1

   hmc_m_scale 3

   start_configuration cold

   start_random default

   mc_steps 1

```
mc_total_steps          100
solver_rest             1e-99
solver_maxiter          50
solver_ignore_no_convergence 2
solver_mre_vectors      7
```

In this input file, line lattice specifies lattice size and line processes specifies total number of processes (8 process in this example)

2. Running benchmark

   mpirun --mca mpi_affinity_alone 1 -np 8 -hostfile host bqcd ./input

   Benchamrk performance is the line CG printed in the middle of the output file.

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350 Oakmead Pkwy, Sunnyvale, CA 94085
Tel: 408-970-3400 • Fax: 408-970-3403
www.hpcadvisorycouncil.com