Quantum Espresso 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:

Quantum ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials (both norm-conserving and ultrasoft).

For further information, see http://www.pwscf.org

3. Version Information:

Quantum ESPRESSO 4.1.2

Download from http://www.quantum-espresso.org/previousVersion.php

4. Prerequisites:

4.1 Hardware:

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

Intel® Xeon 5570 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 Red Hat Enterprise Linux 5.3

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® MKL 11.1.064

   Intel MPI 4.0.0.028 or Open MPI 1.3.3 (compiled by Intel® compiler)

   FFTW 3.2.2 (compiled by Intel® compiler)

5. Building FFTW

1. Steps to build FFTW 3.2.2:

./configure --prefix=<path to FFTW-3.2.2> F77=ifort CC=icc CFLAGS=-O3 FFLAGS="-O3 --enable-shared --enable-threads" --enable-type-prefix --enable-float

make

make install

This will create FFTW single-precision library which is needed by Quantum ESPRESSO.

6. Building Quantum ESPRESSO:

1. Compile Quantum ESPRESSO

   export CC=icc

   export F77=ifort

   export F90=ifort

   export MPIF90="mpif90"

   export CFLAGS="-O3 -xSSE4.2 -openmp "

   export FFLAGS="-O3 -xSSE4.2 -openmp "

   export FFTW_LIB=-L<path to FFTW-3.2.2>/lib

   export FFTW_INC=-L<path to FFTW-3.2.2> / include

   export MKL="-L/opt/intel/11.1/064/mkl/lib/em64t -lmkl_em64t -lpthread -lguide"

   #./configure BLAS_LIBS="$MKL" LAPACK_LIBS="$MKL" FFT_LIBS="-L$FFTW_LIB -lfftw3f" INCLUDEFFTW="$FFTW_INC"

   # make pw

   Executable pw.x will be generated under bin directory

7. Building Quantum ESPRESSO:

1. Download benchmark dataset from

   http://qe-forge.org/frs/?group_id=10&release_id=47

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2. Untar any data files you picked

   For example: tar -vzxf AUSURF112.tgz

3. Run benchmark

   mpirun --mca mpi_affinity_alone 1 --mca coll_tuned_use_dynamic_rules 1 --mca coll_tuned_alltoallv_algorithm 2 --mca coll_tuned_barrier_algorithm 6 -np 64 -hostfile hosts ../bin/pw.x -input ausurf.in -npool 2

   Benchamrk time is the wall time printed near the end of the output file like: PWSCF : 49m43.18s CPU time, 17m49.12s wall time

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