QUANTUM ESPRESSO Installation Best Practices

HPC ADVISORY COUNCIL
NETWORK OF EXPERTISE
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).

3. Version Information:

Download QUANTUM ESPRESSO v5.1.1 (or newer) at:

http://www.quantum-espresso.org

4. Prerequisites:

4.1

The instructions from this best practice have been tested on the following configuration:

Hardware:

- Dell PowerEdge R730 32-node (896-core) "Thor" cluster.
- Dual-Socket 14-Core Intel E5-2697v3 @ 2.60 GHz CPUs
- Mellanox Connect-IB FDR InfiniBand adapters
- Mellanox SwitchX SX6036 VPI InfiniBand and Ethernet switches

Software:

- RHEL 6.5, OFED 2.3-2.0.2 InfiniBand SW stack
- MPI: Mellanox HPC-X v1.2.0-318
- Compilers: Intel Composer XE 2015.1.133
- Application: Quantum ESPRESSO 5.1.1
- Benchmarks:
  - » Unified European Application Benchmark Suite (UEABS) DEISA pw benchmark Test Case A AUSURF112 - Gold surface (112 atoms) DEISA pw benchmark

5. Installation

5.1 Building Quantum ESPRESSO

The following makefile is used for compiling Quantum ESPRESSO

```
.SUFFIXES :
.SUFFIXES : .o .c .f .f90
.f90.o:
	$(MPIF90) $(F90FLAGS) -c $<
.f.o:
	$(F77) $(FFLAGS) -c $<
.c.o:
	$(CC) $(CFLAGS)  -c $<
TOPDIR = /home/qe/espresso-5.3.0-intel-hpcx
MANUAL_DFLAGS  =
DFLAGS         =  -D__INTEL -D__FFTW -D__MPI -D__PARA -D__SCALAPACK -D__ELPA -D__OPENMP $(MANUAL_DFLAGS)
FDFLAGS        = $(DFLAGS) $(MANUAL_DFLAGS)
IFLAGS         = -I../include
MOD_FLAG       = -I
MPIF90         = mpif90
CC             = icc
F77            = ifort
CPP            = cpp
CPPFLAGS       = -P -C -traditional $(DFLAGS) $(IFLAGS)
CFLAGS         = -O3 $(DFLAGS) $(IFLAGS) -xHOST -fno-alias -ansi-alias -g -mkl -openmp -fimf-arch-consistency=true -fp-model precise
F90FLAGS       = $(FFLAGS) -nomodule -openmp -fpp $(FDFLAGS) $(IFLAGS) $(MODFLAGS)
FFLAGS         = -O3 -xHOST -fno-alias -ansi-alias -g -mkl -openmp -fimf-arch-consistency=true -fp-model precise
FFLAGS_NOOPT   = -O0 -assume byterecl -g -traceback
FFLAGS_NOMAIN  =
LD             = mpif90
LDFLAGS        =  -g -pthread -parallel
LD_LIBS        =
BLAS_LIBS      = -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core
```

BLAS_LIBS_SWITCH = external

LAPACK_LIBS = -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core

LAPACK_LIBS_SWITCH = external

ELPA_LIBS_SWITCH = enabled

SCALAPACK_LIBS = $(TOPDIR)/ELPA/libelpa.a -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64

FFT_LIBS =

MPI_LIBS =

MASS_LIBS =

AR = ar

ARFLAGS = ruv

RANLIB = ranlib

FLIB_TARGETS = all

LIBOBJS = ../flib/ptools.a ../flib/flib.a ../clib/clib.a ../iotk/src/libiotk.a

LIBS = $(SCALAPACK_LIBS) $(LAPACK_LIBS) $(FFT_LIBS) $(BLAS_LIBS) $(MPI_LIBS) $(MASS_LIBS) $(LD_LIBS)

WGET = wget -O

PREFIX = /usr/local

Compile Quantum ESPRESSO by doing:

$ make pw

6. Running QUANTUM ESPRESSO

Benchmark input cases can be downloaded from PRACE:

http://www.prace-ri.eu/ueabs/#Quantum_Espresso

$ source /opt/intel/compilers_and_libraries_2016.1.150/linux/bin/compilervars.sh intel64

$ module use /opt/hpcx-v1.5.370-icc-MLNX_OFED_LINUX-3.2-2.0.0.0-redhat6.5-x86_64/modulefiles

$ module load hpcx

$ mpirun --map-by slot --report-bindings --display-map -x MKL_NUM_THREADS -x OMP_NUM_THREADS -x HCOLL_MAIN_IB=mlx5_0:1 -mca pml yalla -x MXM_TLS=self,shm,ud -x MALLOC_MMAP_MAX_=0 -x MALLOC_TRIM_THRESHOLD_=-1 -mca coll_hcoll_enable 1 -mca coll_hcoll_np 0 -mca coll_fca_np 0 -x HCOLL_ML_LARGE_BUFFER_COUNT=28 -mca coll_fca_enable 0 -hostfile /home/qe/hostfile/nodes.12351 -np 224 /home/qe/espresso-5.3.0-intel-hpcx/bin/pw.x -inp /home/qe/espresso-5.3.0-intel-hpcx/benchmark/AUSURF/ausurf.in -npool 2

PWSCF : 53.98s CPU 58.37s WALL

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