

## Quantum ESPRESSO-6.1 for PRIMERGY

### Webpage

<http://www.quantum-espresso.org/>

### Version

6.1

### Tools for Compiling

- ▶ Intel Compiler 17.0.2.174
- ▶ Intel MPI 2017.2.174
- ▶ Intel MKL 2017.2.174

### Necessary Files for Compiling

- ▶ espresso-6.1.tar.gz
- ▶ qe-6.1-test-suite.tar.gz
- ▶ qe-6.1-examples.tar.gz

### Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_qe=/home/users/${USER}/build/espresso61/qe-6.1.tar.gz
set file_test=/home/users/${USER}/build/espresso61/qe-6.1-test-suite.tar.gz
set file_examples=/home/users/${USER}/build/espresso61/qe-6.1-examples.tar.gz
set prefix=/local/apl/pg/espresso61
set work=/work/users/${USER}
#-----
cd ${work}
if (-d qe-6.1) then
  mv qe-6.1 qe-6.1-erase
  rm -rf qe-6.1-erase &
endif
setenv LANG C
setenv CPP cpp
setenv CC icc
setenv CXX icpc
setenv F77 ifort
setenv F90 ifort
setenv FC ifort
setenv MPIF90 mpiifort
tar xzf ${file_qe}
cd qe-6.1
tar xzf ${file_test}
tar xzf ${file_examples}
sed -i '/unset ac_cv_lib_mkl_intel_lp64_DftiComputeForward/a\\ttdir="none" install/configure
sed -i '/try_incdire/vopt/intel/Compiler/,/opt/intel/mkl/*d' install/configure
./configure --with-scalapack --prefix=${prefix} BLAS_LIBS="-mkl=sequential" LAPACK_LIBS="-mkl=sequential" FFT_LIBS="-mkl=sequential" SCALAPACK_LIBS="-lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64"
cd install; make -f plugins_makefile uncompress-yambo; cd ../
sed -i 's/tp7/xHost/ YAMBO/configure
# To pass the test 'pw_vdw/vdw-ts', the optimization for tsvdw.f90 must be -O0.
echo "tsvdw.o: tsvdw.f90" >> ./Modules/Makefile
echo ' $(MPIF90) $(FFLAGS_NOOPT) -nomodule -fpp $(FDFLAGS) $(IFLAGS) $(MODFLAGS) -c $<' >> ./Modules/Makefile
#
foreach i (pw ph pp pwcond neb cp ld1 upf tddft)
echo "==== $i ====="
make -j 12 $i || exit 1
end
foreach i (want gipaw yambo)
echo "==== $i ====="
make $i || exit 1
end
foreach i (epw w90 west d3q)
echo "==== $i ====="
make -j 12 $i || exit 1
end
cd test-suite
make run-tests-serial
make clean
make run-tests-parallel
cd ..
```