

## Quantum ESPRESSO 5.4 for LX

### Webpage

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

### Version

5.4

### Build Environment

- Intel Parallel Studio 2017update4

### Files Required

- q-e-qe-5.4.tar.gz

### Build Procedure

```
#!/bin/sh

VERSION=5.4
BASEDIR=/home/users/${USER}/Software/QE/${VERSION}
TARBALL=${BASEDIR}/q-e-qe-${VERSION}.tar.gz

INSTDIR=/local/apl/lx/espresso54
#LIBXC=${INSTDIR}/libxc-4.2.3

# -----
umask 0022

module purge
module load intel_parallelstudio/2017update4

export LANG=
export LC_ALL=C

cd ${INSTDIR}
if [ -d q-e-qe-${VERSION} ]; then
  mv q-e-qe-${VERSION} q-e-qe-erase
  rm -rf q-e-qe-erase &
fi

tar xzf ${TARBALL}
mv q-e-qe-${VERSION}/* .
rmdir q-e-qe-${VERSION}

CC=icc FC=ifort F90=ifort F77=ifort MPIF90=mpiifort \
./configure --prefix=${INSTDIR} \
--with-scalapack=intel
echo "tsvdw.o: tsvdw.f90" >> ./Modules/Makefile
echo -e "\t$(MPIF90) $(FFLAGS_NOOPT) -nomodule -fpp $(DFLAGS) $(IFLAGS) $(MODFLAGS) -c <' >> ./Modules/Makefile

# libxc
#LIBXC_ESC=`echo ${LIBXC} | sed -e 's/\|\\|/g`
#sed -i -e "/^DFLAGS/s/$/ -D_${LIBXC}/" \
# -e "/^LD_LIBS/s/$/ -L${LIBXC_ESC}/lib -lxcf90 -lxc/" \
# -e "/^IFLAGS/s/$/ -I${LIBXC_ESC}/include/" \
# make.sys

make all

cd test-suite
make run-tests
cd ..
```

### Tests

- pw\_scf - scf-1.in: Unknown
  - The output values seem to be OK.
- pw\_scf - scf-disk\_io-1.in: Unknown
  - The output values seem to be OK.
- pw\_uspp - uspp1-coulomb.in: **\*\*FAILED\*\***
  - This does not work regardless of conditions (also tried with gcc(no MPI), gcc+openmpi, intel+openmpi, but failed to run). Empty PP\_PSWFC tag in "pseudo/H.coulomb-ae.UPF" might be the problem? (If dummy data is added in PP\_PSWFC tag, it works correctly.)

```
#####
# WARNING: there are pending errors
# PENDING ERROR (ierr=1)
# ERROR IN: iotk_getline (iotk_scan.f90:947)
# CVS Revision: 1.23
```

```
#
iostat=-1
# ERROR IN: iotk_scan_tag (iotk_scan.f90:593)
# CVS Revision: 1.23
# ERROR IN: iotk_open_read (iotk_files.f90:631)
# CVS Revision: 1.20
# PENDING ERROR (ierr=2)
# ERROR IN: iotk_close_read (iotk_files.f90:730)
# CVS Revision: 1.20
# FROM IOTK LIBRARY, VERSION 1.2.0
# UNRECOVERABLE ERROR (ierr=-3)
# ERROR IN: iotk_scan_begin (iotk_scan.f90:182)
# CVS Revision: 1.23
# Tag not found
name=PP_PSWFC
#####
```

- pw\_xdm - xdm.in: **\*\*FAILED\*\***
  - Numerical error (not significant).
  - This error also happens even for gfortran-4.8.5(serial) and gfortran-4.8.5/openmpi versions.
  - MKL is not concerned with this numerical error.