

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 $(FDFLAGS) $(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.