

Quantum Espresso 6.7.0

Webpage

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

Version

6.7.0

Build Environment

- ▶ Intel Parallel Studio 2018 update 4

Files Required

- ▶ q-e-qe-6.7.0.tar.gz

Build Procedure

```
#!/bin/sh
VERSION=6.7.0
BASEDIR=/home/users/${USER}/Software/QE/${VERSION}
TARBALL=${BASEDIR}/q-e-qe-${VERSION}.tar.gz
INSTDIR=/local/apl/lx/espresso670
PARALLEL=12

# -----
umask 0022

module purge
module load intel_parallelstudio/2018update4

export LANG=C
export LC_ALL=C
ulimit -s unlimited

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}/* .
mv q-e-qe-${VERSION}/.[a-z]* .
rmdir q-e-qe-${VERSION}

export MPIF90=mpiifort
export MPICF=mpiifort
export MPIF77=mpiifort
export MPICC=mpicc
export MPICXX=mpicpc

FC=ifort F90=ifort F77=ifort CC=icc CXX=icpc \
FFLAGS="-O3 -assume byterecl -ip -g" \
./configure --enable-parallel --with-scalapack=intel

# pwall(pw neb ph pp pwcond acfd) cp ld1 tddft hp xspectra gw
echo "==== all ===="
make -j${PARALLEL} all

for i in epw w90 couple; do
  echo "==== $i ===="
  make -j${PARALLEL} $i
done

for i in yambo; do
  echo "==== $i ===="
  make $i
done

cd test-suite
make run-tests-serial
make clean
make run-tests-parallel
cd ..
```

Notes

- ▶ All the tests have been passed.
- ▶ Intel 2020u2 failed to compile yambo (fftw part). This is a known issue of this compiler version.
 - ▶ <https://community.intel.com/t5/Intel-C-Compiler/icc-and-fftw-and-INT-MAX/m-p/1219856?profile.language=en>

- ▶ Intel 2019u5 and 2019u5(compilers and MKL) + 2020u2(MPI) couldn't pass tests.
 - ▶ Intel 18 version shows slightly better performance than GCC version (tested with Au surf system).
 - ▶ plumed option seems to be removed from Makefile (obsolete?).
 - ▶ gipaw is not available for this version (at least for now; Jan 4, 2021).
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