

Quantum Espresso 7.4.1 with GPU support

Webpage

<https://www.quantum-espresso.org/>
<https://gitlab.com/QEF/q-e>

Version

7.4.1

Build Environment

- NVIDIA HPC SDK 24.9 (nompri version)
- Open MPI 4.1.6 (CUDA-aware)

Files Required

- q-e-qe-7.4.1.tar.gz (downloaded from gitlab)
- (some of files were downloaded in the installation procedure)

Build Procedure

```
#!/bin/sh

QE_VERSION=7.4.1
BASEDIR=/home/users/${USER}/Software/QE/${QE_VERSION}
TARBALL=${BASEDIR}/q-e-qe-${QE_VERSION}.tar.gz

#D3Q_ID="808acba012468f42147d8d6af452ec64b9e5ab0"
#GIPAW_ID="3bbf5a931fc195503c3f01565ac43cac8c05db44"

WORKDIR=/gwork/users/${USER}

INSTDIR=/apl/qe/7.4.1-gpu
PARALLEL=24

# -----
umask 0022

module -s purge
module -s load nvhpc/24.9-nompri
module -s load openmpi/4.1.6/nv24
## gui; not necessary while building
#module -s load itcl/3.4.4
#module -s load itk/3.4.2
#module -s load iwidgets/4.1.1

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

if [ ! -d ${WORKDIR} ]; then
  mkdir -p ${WORKDIR}
fi

cd ${WORKDIR}
if [ -d q-e-qe-${QE_VERSION} ]; then
  mv q-e-qe-${QE_VERSION} qe-erase
  rm -rf qe-erase &
fi
tar xzf ${TARBALL}

QE_WORKDIR=${WORKDIR}/q-e-qe-${QE_VERSION}
```

```

# QE
cd ${QE_WORKDIR}
sed -i -e "s/wget -O/wget --trust-server-names -O/" \
    -e "s/curl -o/curl -L -o/" test-suite/check_pseudo.sh
sed -i -e "s/[^ ]* qe-gipaw/${GIPAW_ID} qe-gipaw/" \
    external/submodule_commit_hash_records

mkdir build && cd build
cmake .. \
-DMAKE_INSTALL_PREFIX=${INSTDIR} \
-DMAKE_Fortran_COMPILER=mpif90 \
-DMAKE_C_COMPILER=mpicc \
-DMAKE_CXX_COMPILER=mpicxx \
-DMAKE_PREFIX_PATH="${MAKE_PREFIX_PATH}" \
-DESPRESSO_PSEUDO=${INSTDIR}/pseudo \
-DQE_ENABLE_CUDA=ON \
-DNVFORTRAN_CUDA_CC=80 \
-DNVFORTRAN_CUDA_VERSION=12.6 \
-DQE_ENABLE_OPENACC=ON \
-DQE_ENABLE_OPENMP=ON \
-DQE_ENABLE_MPI=ON \
-DQE_ENABLE_MPI_GPU_AWARE=ON \
-DQE_ENABLE_SCALAPACK=OFF \
-DQE_ENABLE_ELPA=OFF \
-DQE_ENABLE_LIBXC=OFF \
-DQE_ENABLE_HDF5=OFF \
-DQE_ENABLE_PLUGINS="pw2qmcpack;gipaw" \
-DQE_ENABLE_FOX=ON \
-DQE_WANNIER90_INTERNAL=ON \
-DQE_MBD_INTERNAL=ON \
-DQE_DEVICE_LIB_INTERNAL=ON \
-DQE_ENABLE_ENVIRON=OFF \
-DQE_ENABLE_OSCDFT=OFF

make -j${PARALLEL}
make install
ln -s ${INSTDIR}/bin ${QE_WORKDIR}/bin
cp -r ${QE_WORKDIR}/pseudo ${INSTDIR}/pseudo
mv ${QE_WORKDIR}/pseudo ${QE_WORKDIR}/pseudo.org
ln -s ${INSTDIR}/pseudo ${QE_WORKDIR}/pseudo
make test # to run "system--pw-pseudo" test for pseudo files

```

Tests

Tests were submitted as a job [in the case of 7.4](#). In 7.4.1, "184:system--pw_md-correctness" test was additionally failed with numerical error.

Notes

- [The same procedure as 7.4](#).