Quantum Espresso 7.4.1

ウェブページ

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

バージョン

7.4.1

ビルド環境

- GCC 12.2.1 (gcc-toolset-12)
- Open MPI 4.1.6
- OpenBLAS 0.3.29 (lp64)
- Scalapack 2.2.2

ビルドに必要なファイル

- q-e-qe-7.4.1.tar.gz (gitlab よりダウンロード)
- (qe 7.4 用の hdf5, libxc, elpa を再利用)
- (以下の手順内でもダウンロードしている)

ビルド手順

```
#!/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="808acbaf012468f42147d8d6af452ec64b9e5ab0"
GIPAW_ID="3bbf5a931fc195503c3f01565ac43cac8c05db44"
ENVIRON_URL="https://github.com/environ-developers/Environ.git"

WORKDIR=/gwork/users/${USER}

INSTDIR=/apl/qe/7.4.1
PARALLEL=24

# ELPA, HDF5, libxc are assumed to be installed in ${INSTDIR}
CMAKE_PREFIX_PATH="${INSTDIR}/hdf5-1.14.5;${INSTDIR}/libxc-6.2.2;/apl/openblas/0.3.29-gcc/lp64"

# ------------------------------------------------------------------------
umask 0022

module -s purge
module -s load gcc-toolset/12
module -s load openmpi/4.1.6/gcc12
module -s load openblas/0.3.29-lp64
module -s load scalapack/2.2.2-ompi416gcc-lp64
## 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
if [ -d Environ ]; then
 mv Environ Environ-erase
 rm -rf Environ-erase &
fi
tar zxf ${TARBALL}
git clone ${ENVIRON_URL} Environ

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

# environ prep
cd ${ENVIRON_WORKDIR}
sed -i -e "s/wget -O/wget --trust-server-names -O/" \
     -e "s/curl -o/curl -L -o/" tests/check_pseudo.sh
FC=mpif90 ./configure \
  --with-qe=${QE_WORKDIR} \
  --enable-openmp
make -j${PARALLEL} compile

# QE
cd ${QE_WORKDIR}
sed -i -e "s/wget -O/wget --trust-server-names -O/" \
     -e "s/curl -o/curl -L -o/" test-suite/check_pseudo.sh
sed -i -e "s/[^ ]* d3q/${D3Q_ID} d3q/" \
     -e "s/[^ ]* qe-gipaw/${GIPAW_ID} qe-gipaw/" \
   external/submodule_commit_hash_records
sed -i -e "s/elpa-20/elpa_openmp-20/" \
     -e "s/NAMES elpa$/NAMES elpa elpa_openmp/" cmake/FindELPA.cmake

mkdir build && cd build
cmake .. \
 -DCMAKE_INSTALL_PREFIX=${INSTDIR} \
 -DCMAKE_Fortran_COMPILER=mpif90 \
 -DCMAKE_Fortran_FLAGS="-ffree-line-length-256" \
 -DCMAKE_C_COMPILER=mpicc \
 -DCMAKE_CXX_COMPILER=mpicxx \
 -DCMAKE_PREFIX_PATH="${CMAKE_PREFIX_PATH}" \
 -DESPRESSO_PSEUDO=${INSTDIR}/pseudo \
 -DBLA_VENDOR=OpenBLAS \
 -DQE_ENABLE_OPENMP=ON \
 -DQE_ENABLE_MPI=ON \
 -DQE_ENABLE_MPI_GPU_AWARE=OFF \
 -DQE_ENABLE_SCALAPACK=ON \
 -DQE_ENABLE_ELPA=ON \
 -DELPA_ROOT=${INSTDIR}/elpa-2024.05.001 \
 -DQE_ENABLE_LIBXC=ON \
 -DQE_ENABLE_HDF5=ON \
 -DQE_ENABLE_PLUGINS="d3q;pw2qmcpack;gipaw" \
 -DQE_ENABLE_FOX=ON \
  -DQE_WANNIER90_INTERNAL=ON \
 -DQE_MBD_INTERNAL=ON \
 -DQE_DEVICEXLIB_INTERNAL=ON \
 -DQE_ENABLE_ENVIRON=ON \
 -DENVIRON_ROOT=${ENVIRON_WORKDIR} \
 -DQE_ENABLE_OSCDFT=ON

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

# environ test
export LD_LIBRARY_PATH="${INSTDIR}/hdf5-1.14.5/lib:${INSTDIR}/elpa-2024.05.001/lib:${LD_LIBRARY_PATH}"
export OMP_NUM_THREADS=4
cd ${ENVIRON_WORKDIR}/tests
make run-tests
```

テスト

- 7.4 の時と同一の結果になっています。

メモ

- 7.4 と同じ手順で導入。
- HDF5, libxc, ELPA については 7.4 のものを再利用。