

Quantum Espresso 7.3 with GPU

Webpage

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

Version

7.3

Build Environment

- NVIDIA HPC SDK 23.5 (nompri version)
- Intel MKL 2023.1.0
- OpenMPI 4.1.6 (CUDA-aware; built with nvhpc 23.5)

Files Required

- qe-7.3-ReleasePack.tar.gz
- [.gitmodules](#)
 - This is missing in release pack but may be necessary to build W90 etc.

Build Procedure

```
#!/bin/sh

QE_VERSION=7.3
BASEDIR=/home/users/${USER}/Software/QE/${QE_VERSION}
TARBALL=${BASEDIR}/qe-${QE_VERSION}-ReleasePack.tar.gz
GITMODULES=${BASEDIR}/.gitmodules

INSTDIR=/apl/qe/7.3-gpu
CUDA_HOME=/apl/nvhpc/23.5/Linux_x86_64/23.5/cuda
PARALLEL=12

# -----
umask 0022

module -s purge
module -s load nvhpc/23.5-nompri
module -s load openmpi/4.1.6/nv23

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

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

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

tar zxf ${TARBALL}
mv qe-${QE_VERSION}/* .
mv qe-${QE_VERSION}/.[a-z]* .
rmdir qe-${QE_VERSION}

sed -i -e "s/wget -O/wget --trust-server-names -O/" \
  -e "s/curl -o/curl -L -o/" test-suite/check_pseudo.sh
```

```

export MPIF90=mpif90
export MPIFC=mpif90
export MPIF77=mpif90
export MPICC=mpicc
export MPICXX=mpicxx

cp ${GITMODULES} .
rm -rf external/wannier90
mkdir -p external/wannier90

sed -i -e '/external/wannier90/s/lib/wannier lib/' install/plugins_makefile

FC=nvfortran F90=nvfortran F77=nvfortran CC=nvc CXX=nvc++ \
./configure --enable-parallel \
--enable-openmp \
--with-scalapack=no \
--with-cuda=${CUDA_HOME} \
--with-cuda-cc=80 \
--with-cuda-runtime=12.1 \
--with-cuda-mpi=yes

for i in w90; do
echo "==== $i ====="
make $i
done

# pwall(pw neb ph pp pwcond acfdt) cp ld1 tddfpt hp xspectra gw1
echo "==== all ====="
make -j${PARALLEL} all

#for i in want; do
# echo "==== $i ====="
# make $i
#done

# gipaw for QE 7.3 doesn't seem to be available
# d3q depends on old version of PH code? (setlocq, setlocq_coul)

for i in all_currents epw couple kcw gw1 gui; do
echo "==== $i ====="
make -j${PARALLEL} $i
done

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

cd test-suite
make pseudo

exit 0

```

Tests

Following script was executed on ccgpu (A30 equipped).

```

#!/bin/sh

QE_VERSION=7.3
BASEDIR=/home/users/${USER}/Software/QE/${QE_VERSION}
TARBALL=${BASEDIR}/qe-${QE_VERSION}-ReleasePack.tar.gz
GITMODULES=${BASEDIR}/.gitmodules

INSTDIR=/apl/qe/7.3-gpu

```

```
CUDA_HOME=/apl/nvhpc/23.5/Linux_x86_64/23.5/cuda
PARALLEL=12
```

```
# -----
```

```
umask 0022
```

```
module -s purge
```

```
module -s load nvhpc/23.5-nompi
```

```
module -s load openmpi/4.1.6/nv23
```

```
export MPIF90=mpif90
```

```
export MPIFC=mpif90
```

```
export MPIF77=mpif90
```

```
export MPICC=mpicc
```

```
export MPICXX=mpicxx
```

```
cd ${INSTDIR}/test-suite
```

```
export OMP_NUM_THREADS=1
```

```
make run-tests-pw NPROCS=1
```

```
make run-tests-cp NPROCS=1
```

```
make run-tests-ph NPROCS=1
```

```
make run-tests-epw NPROCS=1
```

```
make run-tests-hp NPROCS=1
```

```
make run-tests-tddfpt NPROCS=1
```

```
make run-tests-kcw NPROCS=1
```

```
make run-tests-all_currents NPROCS=1
```

```
make run-tests-pp NPROCS=1
```

```
make run-tests-zg NPROCS=1
```

```
#make run-tests-xsd-pw NPROCS=1
```

```
make clean
```

```
export OMP_NUM_THREADS=2
```

```
make run-tests-pw NPROCS=4
```

```
make run-tests-cp NPROCS=4
```

```
make run-tests-ph NPROCS=4
```

```
make run-tests-epw NPROCS=4
```

```
make run-tests-hp NPROCS=4
```

```
make run-tests-tddfpt NPROCS=4
```

```
make run-tests-kcw NPROCS=4
```

```
make run-tests-all_currents NPROCS=4
```

```
make run-tests-pp NPROCS=4
```

```
make run-tests-zg NPROCS=4
```

```
#make run-tests-xsd-pw NPROCS=4
```

```
cd ..
```

Test result (serial)

pw: 243 out of 246 tests passed (1 skipped).

- pw_noncolin - noncolin-rmm.in: ****FAILED****.
- pw_scf - scf-rmm-k.in: ****FAILED****.
- pw_scf - scf-rmm-paro-k.in: ****FAILED****.

cp: 27 out of 27 tests passed (8 skipped).

ph: 37 out of 62 tests passed.

epw: 55 out of 113 tests passed (22 skipped).

hp: 29 out of 41 tests passed.

tddfpt: 9 out of 9 tests passed.

kcw: 5 out of 11 tests passed.

all_currents: 0 out of 10 tests passed.

pp: 2 out of 2 tests passed.

zq: 0 out of 1 test passed.

Test result (parallel)

pw: 241 out of 246 tests passed (1 skipped).

- pw_noncolin - noncolin-rmm.in: ****FAILED****.
- pw_scf - scf-rmm-k.in: ****FAILED****.
- pw_scf - scf-rmm-paro-k.in: ****FAILED****.
- pw_workflow_exx_nscf - uspp-k-restart-1.in (arg(s): 1): ****FAILED****.
- pw_workflow_exx_nscf - uspp-k-restart-2.in (arg(s): 2): ****FAILED****.

cp: 27 out of 27 tests passed (8 skipped).

ph: 37 out of 62 tests passed.

epw: 55 out of 113 tests passed (22 skipped).

hp: 29 out of 41 tests passed.

tddfpt: 8 out of 9 tests passed.

- tddfpt_magnons_fe - Fe.tddfpt_pp_magnons.in (arg(s): 7): ****FAILED****.

kcw: 5 out of 11 tests passed.

all_currents: 0 out of 10 tests passed.

pp: 2 out of 2 tests passed.

zq: 0 out of 1 test passed.

Notes

- [Please also check notes of CPU version.](#)
- There are no remarkable differences in test results and performance (of PW) between nvhpc 23.5 and 23.9.
- WANT and YAMBO can't be built with this setting due to the syntax errors.