NWChem 7.0.2

Webpage

https://nwchemgit.github.io/

Version

7.0.2

Build Environment

- Intel oneAPI Compiler Classic 2022.2.1
- Intel MKL 2022.2.1
- HPC-X 2.11

Files Required

- nwchem-7.0.2-release.revision-b9985dfa-src.2020-10-12.tar.bz2
- runtest.md.mpi

```
#!/bin/sh
./runtests.mpi.unix procs 2 \
 na_k/nak \
 na_k/nak_md \
 crown/crown_md \
 ethanol/ethanol_md \
 ethanol/ethanol_ti \
 had/had_em \
 had/had_md \
 prep/a3n \
 prep/aal \
 prep/fsc \
 water/water_md
```

Build Procedure

```
#!/bin/sh

VERSION=7.0.2
INSTALL_PREFIX=/apl/nwchem/7.0.2

BASEDIR=/home/users/${USER}/Software/NWChem/7.0.2
TARBALL=${BASEDIR}/nwchem-7.0.2-release.revision-b9985dfa-src.2020-10-12.tar.bz2

WORKDIR=/gwork/users/${USER}

RUNTESTMD=runtest.md.mpi
RUNTESTMD_PATH=${BASEDIR}/${RUNTESTMD}

#------------------------------------------------------------------------
umask 0022
export LANG=C
ulimit -s unlimited

module purge

. ~/intel/oneapi/compiler/2022.2.1/env/vars.sh

module load mkl/2022.2.1
module load openmpi/4.1.4-hpcx/intel2022.2.1

cd ${WORKDIR}
if [ -d nwchem-${VERSION} ]; then
```

```
  mv nwchem-${VERSION} nwchem-erase
  rm -rf nwchem-erase &
fi

tar jxf ${TARBALL}

export NWCHEM_TOP=${WORKDIR}/nwchem-${VERSION}
export NWCHEM_MODULES="all python"
export NWCHEM_TARGET=LINUX64
export ARMCI_NETWORK=MPI-PR

export USE_OPENMP=y
export USE_MPI=y
export USE_MPIF=y
export USE_MPIF4=y

export USE_NOFSCHECK=TRUE
export USE_NOIO=TRUE
export MRCC_METHODS=TRUE
export CCSDTQ=TRUE
export LIB_DEFINES=-DDFLT_TOT_MEM=180000000

export PYTHONVERSION=3.6

export BLAS_SIZE=8
export BLASOPT="-L${MKLROOT}/lib/intel64 -lmkl_intel_ilp64 -lmkl_intel_thread -lmkl_core -liomp5 -lpthread -lm -ldl"
export LAPACK_SIZE=8
export LAPACK_LIB="${BLASOPT}"
export USE_SCALAPACK=y
export SCALAPACK_SIZE=8
export SCALAPACK="-L${MKLROOT}/lib/intel64 -lmkl_scalapack_ilp64 -lmkl_blacs_openmpi_ilp64 -lmkl_intel_ilp64 -lmkl_intel_thread -lmkl_core -
liomp5 -lpthread -lm -ldl"

export CC=icc
export FC=ifort

cd ${NWCHEM_TOP}/src

# cheat
mkdir ../bin
ln -s /usr/libexec/platform-python3.6-config ../bin/python3.6-config
export PATH="${PATH}:${NWCHEM_TOP}/bin"

make nwchem_config
make

# involve also version info
cd ${NWCHEM_TOP}/src/util
make version
make
cd ${NWCHEM_TOP}/src
make link
cd ${NWCHEM_TOP}

# installation; assume INSTALL_PREFIX directory already exists
cp -fr LICENSE.TXT README.md release.notes.* examples ${INSTALL_PREFIX}

mkdir ${INSTALL_PREFIX}/bin
mkdir ${INSTALL_PREFIX}/data

cp -f ${NWCHEM_TOP}/bin/${NWCHEM_TARGET}/nwchem ${INSTALL_PREFIX}/bin
chmod 755 ${INSTALL_PREFIX}/bin/nwchem

cp -fr ${NWCHEM_TOP}/src/data           ${INSTALL_PREFIX}
cp -fr ${NWCHEM_TOP}/src/basis/libraries ${INSTALL_PREFIX}/data
```

```
cp -fr ${NWCHEM_TOP}/src/nwpw/libraryps  ${INSTALL_PREFIX}/data

# create default.nwchemrc
cat << EOS > ${INSTALL_PREFIX}/default.nwchemrc
nwchem_basis_library ${INSTALL_PREFIX}/data/libraries/
nwchem_nwpw_library ${INSTALL_PREFIX}/data/libraryps/
ffield amber
amber_1 ${INSTALL_PREFIX}/data/amber_s/
amber_2 ${INSTALL_PREFIX}/data/amber_q/
amber_3 ${INSTALL_PREFIX}/data/amber_x/
amber_4 ${INSTALL_PREFIX}/data/amber_u/
spce    ${INSTALL_PREFIX}/data/solvents/spce.rst
charmm_s ${INSTALL_PREFIX}/data/charmm_s/
charmm_x ${INSTALL_PREFIX}/data/charmm_x/
EOS

# run test
export NWCHEM_EXECUTABLE=${INSTALL_PREFIX}/bin/nwchem
export OMP_NUM_THREADS=1

# some tests need this...
cp -f ${INSTALL_PREFIX}/default.nwchemrc ~/.nwchemrc

cd ${NWCHEM_TOP}/QA
./doqmtests.mpi 2 >& doqmtests.mpi.log

cp -f ${RUNTESTMD_PATH} .
sh ${RUNTESTMD} >& runtest.md.mpi.log

mkdir ${INSTALL_PREFIX}/testlog
cp -fr doqmtests.mpi.log runtest.md.mpi.log testoutputs/ ${INSTALL_PREFIX}/testlog
```

Notes

- In case export ARMCI_NETWORK=OPENIB was used, calculations failed when large number of MPI processes were employed. MPI-PR version is free from this issue.