NWChem-7.2.3 (Intel Classic)

Webpage

https://nwchemgit.github.io/

Version

7.2.3

Build Environment

- Intel Compiler Classic 2023.2.0 (oneAPI 2023.2.0)
- Intel MKL 2025.0.0.1 (oneAPI 2025.0.1)
- Open MPI 4.1.8

Files Required

- nwchem-7.2.3-release.revision-d690e065-src.2024-08-27.tar.bz2
- runtest.md.mpi

```
#!/bin/sh
./runtests.mpi.unix procs 48 \
 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=7.2.3
INSTALL_PREFIX=/apl/nwchem/7.2.3-intel

BASEDIR=/home/users/${USER}/Software/NWChem/${VERSION}
TARBALL=${BASEDIR}/nwchem-7.2.3-release.revision-d690e065-src.2024-08-27.tar.bz2

WORKDIR=/gwork/users/${USER}/nwchem-release-intel

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

module -s purge
. ~/intel/oneapi/compiler/latest/env/vars.sh # 2023.2.0
module -s load compiler-rt/2023.2.0
module -s load mkl/2025.0.0.1
module -s load openmpi/4.1.8/intelclassic2023

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=268435456 # 2 GiB/process
export LIB_DEFINES=-DDFLT_TOT_MEM=180000000 # 1.8 GB/process

export PYTHONVERSION=3.6

export BLAS_SIZE=8
export BLASOPT="-m64 -L${MKLROOT}/lib -lmkl_intel_ilp64 -lmkl_intel_thread -lmkl_core -liomp5 -lpthread -lm -ldl"
export LAPACK_SIZE=8
export LAPACK_LIB="${BLASOPT}"
export USE_SCALAPACK=y
export SCALAPACK_SIZE=8
export SCALAPACK="-m64 -L${MKLROOT}/lib -lmkl_scalapack_ilp64 -lmkl_intel_ilp64 -lmkl_intel_thread -lmkl_core -lmkl_blacs_openmpi_ilp64 -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:${NWCHEM_TOP}/QA"

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
mkdir -p ${INSTALL_PREFIX}
cp -fr LICENSE.TXT README.md release.notes.* examples ${INSTALL_PREFIX}

mkdir -p ${INSTALL_PREFIX}/bin

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/basis/libraries.bse ${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_x/
#amber_3 ${INSTALL_PREFIX}/data/amber_q/
#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

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

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

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

mv testoutputs testoutputs-serial

mkdir -p ${INSTALL_PREFIX}/testlog
cp -fr doqmtests.mpi.fast.log \
      testoutputs-serial \
   ${INSTALL_PREFIX}/testlog
```

Tests

Parallel test was submitted as a job with the script below.

```
#!/bin/sh
#PBS -l select=1:ncpus=48:mpiprocs=48:ompthreads=1
#PBS -l walltime=24:00:00

VERSION=7.2.3
INSTALL_PREFIX=/apl/nwchem/7.2.3-intel

BASEDIR=/home/users/${USER}/Software/NWChem/${VERSION}

WORKDIR=/gwork/users/${USER}/nwchem-release-intel

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

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

module -s purge
module -s load compiler-rt/2023.2.0
module -s load mkl/2025.0.0.1
module -s load openmpi/4.1.8/intelclassic2023

export NWCHEM_TOP=${WORKDIR}/nwchem-${VERSION}
# run test
export NWCHEM_EXECUTABLE=${INSTALL_PREFIX}/bin/nwchem
export PATH="$PATH:$NWCHEM_TOP/QA"

cd ${NWCHEM_TOP}/QA

./doqmtests.mpi 48 >& doqmtests.mpi.log
cp -f ${RUNTESTMD_PATH} .
sh ${RUNTESTMD} >& runtest.md.mpi.log
```

```
mv testoutputs testoutputs-mpi

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

Test Results

Copies of the log files are available in /apl/nwchem/7.2.3-intel/testlog.

List of failed tests: serial version (doqmtests.mpi.fast.log)

- h2o-b3lyp-disp/h2o-b3lyp-disp => insufficient memory specification in the input file
- (oh2/oh2 => to be failed)
- dft_siosi3/dft_siosi3 => insufficient memory specification in the input file
- paw/paw => Total PAW energy : NaN
- tce_cr_eom_t_ozone/tce_cr_eom_t_ozone => 0:createfile: failed ga_create size/nproc bytes:
- tce_mrcc_bwcc/tce_mrcc_bwcc => minor numerical error (-76.0643135404 vs -76.0643135403 & -76.0717057877 vs -76.0717057876)
- tce_mrcc_mkcc/tce_mrcc_mkcc => minor numerical error (-76.0630229504 vs -76.0630229503 & -76.0702306002 vs -76.0702306001)
- tce_mrcc_bwcc_subgroups/tce_mrcc_bwcc_subgroups => Caught signal 8 (Floating point exception: integer divide by zero)
- qmmm_grad0/qmmm_grad0 => insufficient memory specification in the input file
- lys_qmmm/lys_qmmm => same as above
- ethane_qmmm/ethane_qmmm => same as above
- qmmm_freq/qmmm_freq => same as above
- h2o-b3lyp-disp/h2o-b3lyp-disp => same as above
- o2_ccca/o2_ccca => 0:createfile: failed ga_create size/nproc bytes:

List of failed tests: parallel version (doqmtests.mpi.log)

- h2o-b3lyp-disp/h2o-b3lyp-disp, oh2/oh2, paw/paw, qmmm_grad0/qmmm_grad0, lys_qmmm/lys_qmmm, ethane_qmmm/ethane_qmmm, qmmm_freq/qmmm_freq, h2o-b3lyp-disp/h2o-b3lyp-disp => same as serial version
- tce_cc2_c2/tce_cc2_c2 => not enough memory on node?
- k6h2o/k6h2o => k6h2o.err: No such file or directory (not enough memory on node?)
- rt_tddft_mocap/rt_tddft_mocap => not enough memory on node?
- rt_tddft_water_abs_spec/rt_tddft_water_abs_spec => same as above
- uoverlap/uoverlap => numerical error (-21866.75356 vs -21862.15661 and -25657.18789 vs -25647.50658)
- p2ta-vem/p2ta-vem => insufficient memory specification in the input file

List of failed tests: MD (runtest.md.mpi.log)

- na_k/nak_md => (not enough memory on node?)
- crown/crown_md => ethanol_md.err: No such file or directory (not enough memory on node?)
- ethanol/ethanol_md => ethanol_md.err: No such file or directory (not enough memory on node?)
- ethanol/ethanol_ti => ethanol_ti.err: No such file or directory (not enough memory on node?)
- had/had_em => 0: Dimension mwm too small 0
- had/had_md => ?
- prep/a3n => Unresolved atom types in fragment HEM

Notes

- Please check gcc version's notes.