

NWChem-7.2.2 with CUDA

Webpage

<https://nwchemgit.github.io/>

Version

7.2.2

Build Environment

- GCC 12.1.1 (gcc-toolset-12)
- Intel MKL 2023.2.0
- Open MPI 4.1.6

Files Required

- nwchem-7.2.2-release.revision-74936fb9-src.2023-11-03.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=7.2.2
INSTALL_PREFIX=/apl/nwchem/7.2.2-CUDA

BASEDIR=/home/users/${USER}/Software/NWChem/${VERSION}
TARBALL=${BASEDIR}/nwchem-7.2.2-release.revision-74936fb9-src.2023-11-03.tar.bz2

WORKDIR=/gwork/users/${USER}

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

module -s purge
module -s load gcc-toolset/12
module -s load mkl/2023.2.0
module -s load openmpi/4.1.6/gcc12
module -s load cuda/12.1u1

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 TCE_CUDA=y

export CUDA_FLAGS="-arch sm_80"
export CUDA_LIBS="-lcudart"

export USE_NOFSCHECK=TRUE
export USE_NOIO=TRUE
export MRCC_METHODS=TRUE
export CCSDTQ=TRUE
export LIB_DEFINES=-DDFLT_TOT_MEM=180000000 # 1.8 GB/process

export PYTHONVERSION=3.6

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

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; 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/basis/libraries.bse ${INSTALL_PREFIX}/data
cp -fr ${NWCHEM_TOP}/src/nwppw/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/libraryyps/
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

```

Tests

Serial and parallel tests were performed with the job scripts below. (Only the "tce_cuda" test uses GPU.)

```

#!/bin/sh
#PBS -l select=1:ncpus=16:mpiprocs=16:ompthreads=1:ngpus=1
#PBS -l walltime=24:00:00

VERSION=7.2.2
INSTALL_PREFIX=/apl/nwchem/7.2.2-CUDA

BASEDIR=/home/users/${USER}/Software/NWChem/${VERSION}
TARBALL=${BASEDIR}/nwchem-7.2.2-release.revision-74936fb9-src.2023-11-03.tar.bz2

WORKDIR=/gwork/users/${USER}

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

module -s purge
module -s load gcc-toolset/12
module -s load mkl/2023.2.0
module -s load openmpi/4.1.6/gcc12
module -s load cuda/12.1u1

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

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

```

```

#!/bin/sh
#PBS -l select=1:ncpus=32:mpiprocs=32:ompthreads=1:ngpus=2
#PBS -l walltime=24:00:00

VERSION=7.2.2
INSTALL_PREFIX=/apl/nwchem/7.2.2-CUDA

```

```

BASEDIR=/home/users/${USER}/Software/NWChem/${VERSION}
TARBALL=${BASEDIR}/nwchem-7.2.2-release.revision-74936fb9-src.2023-11-03.tar.bz2

WORKDIR=/gwork/users/${USER}

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

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

module -s purge
module -s load gcc-toolset/12
module -s load mkl/2023.2.0
module -s load openmpi/4.1.6/gcc12
module -s load cuda/12.1u1

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

cd ${NWCHEM_TOP}/QA
./doqmtests.mpi 32 >& doqmtests.mpi.log
sed -e "s/48/32/" ${RUNTESTMD_PATH} > ${RUNTESTMD}
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

Test results were copied to `/apl/nwchem/7.2.2-CUDA/testlog`.

Failed tests for serial version.

- tests/h2o-b3lyp-disp/h2o-b3lyp-disp: insufficient memory
- (tests/oh2/oh2: to be failed)
- tests/dft_siosi3/dft_siosi3: insufficient memory
- tests/pspw_md/pspw_md: minor numerical error (-14.38970 vs -14.38971)
- tests/tce_cr_eom_t_ozone/tce_cr_eom_t_ozone: createfile: failed ga_create size/nproc bytes:
- tests/qmmm_grad0/qmmm_grad0: insufficient memory
- tests/lys_qmmm/lys_qmmm: insufficient memory
- tests/ethane_qmmm/ethane_qmmm: insufficient memory
- tests/qmmm_freq/qmmm_freq: insufficient memory
- tests/h2o-b3lyp-disp/h2o-b3lyp-disp: insufficient memory
- tests/o2_ccca/o2_ccca: createfile: failed ga_create size/nproc bytes:

Failed tests for parallel version.

- tests/h2o-b3lyp-disp/h2o-b3lyp-disp: insufficient memory
- (tests/oh2/oh2: to be failed)
- tests/qmmm_grad0/qmmm_grad0: insufficient memory
- tests/lys_qmmm/lys_qmmm: insufficient memory
- tests/ethane_qmmm/ethane_qmmm: insufficient memory
- tests/qmmm_freq/qmmm_freq: insufficient memory
- tests/h2o-b3lyp-disp/h2o-b3lyp-disp: insufficient memory

MD tests

- tests/na_k/nak_md: ?
- tests/crown/crown_md: Unable to read previous box pair list
- tests/ethanol/ethanol_md: ethanol_md.err: No such file or directory
- tests/ethanol/ethanol_ti: Unable to read previous box pair list
- tests/had/had_em: 0: Dimension mwm too small 0
- tests/had/had_md: Unresolved atom types in fragment HEM
- tests/prep/a3n: Unresolved atom types in fragment HEM

Notes

- [Please check article of CPU version.](#)
- Note: GPU is available only in TCE module.
- (This version was built as a separated binary from CPU version.)