NWChem-7.2.2

ウェブページ

https://nwchemgit.github.io/

バージョン

7.2.2

ビルド環境

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

ビルドに必要なファイル

- 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
```

ビルド手順

```
#!/bin/sh

VERSION=7.2.2
INSTALL_PREFIX=/apl/nwchem/7.2.2

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

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 # 1.8 GB/process

export PYTHONVERSION=3.6

export BLAS_SIZE=8
export BLASOPT="-L${MKLROOT}/lib/intel64 -lmkl_intel_ilp64 -lmkl_gnu_thread -lmkl_core -liomp5 -lpthread -lm -ldl"
export LAPACK_SIZE=8
export LAPACK_LIB="${BLASOPT}"
export USE_SCALAPACK=y
export SCALAPACK_SIZE=8
export SCALAPACK="-L${MKLROOT}/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/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
#./doqmtests.mpi 48 >& doqmtests.mpi.log

mv testoutputs testoutputs-serial

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

テスト

上記のシリアルでの簡易テストに加えて、以下の MPI 並列テストをジョブとして実行

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

VERSION=7.2.2
INSTALL_PREFIX=/apl/nwchem/7.2.2

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

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
```

テスト結果

テスト結果は /apl/nwchem/7.2.2/testlog 以下に格納されています。
失敗したシリアル版テスト

- tests/h2o-b3lyp-disp/h2o-b3lyp-disp: メモリ不足
- (tests/oh2/oh2: 失敗するべきテスト)
- tests/dft_siosi3/dft_siosi3: メモリ不足
- tests/pspw_md/pspw_md: マイナーな数値エラー(-14.38970 vs -14.38971)
- tests/tce_cr_eom_t_ozone/tce_cr_eom_t_ozone: createfile: failed ga_create size/nproc bytes:
- tests/tce_mrcc_bwcc/tce_mrcc_bwcc: マイナーな数値エラー(-76.0643135404 vs -76.0643135403)
- tests/tce_mrcc_mkcc/tce_mrcc_mkcc: マイナーな数値エラー(-76.0630229504 vs -76.0630229503, -76.0702306002 vs -76.0702306001)
- tests/tce_mrcc_bwcc_subgroups/tce_mrcc_bwcc_subgroups: Floating point exception: integer divide by zero
- tests/qmmm_grad0/qmmm_grad0: メモリ不足
- tests/lys_qmmm/lys_qmmm: 同上
- tests/ethane_qmmm/ethane_qmmm: 同上
- tests/qmmm_freq/qmmm_freq: 同上
- tests/h2o-b3lyp-disp/h2o-b3lyp-disp: メモリ不足
- tests/o2_ccca/o2_ccca: createfile: failed ga_create size/nproc bytes:

失敗した並列版テスト

- tests/h2o-b3lyp-disp/h2o-b3lyp-disp: メモリ不足
- (tests/oh2/oh2: 失敗するべきテスト)
- tests/qmmm_grad0/qmmm_grad0: メモリ不足
- tests/lys_qmmm/lys_qmmm: 同上
- tests/ethane_qmmm/ethane_qmmm: 同上
- tests/qmmm_freq/qmmm_freq: 同上
- tests/h2o-b3lyp-disp/h2o-b3lyp-disp: 同上
- tests/dmo_tddft_cd_velocity/dmo_tddft_cd_velocity: マイナーな数値エラー(1.620 vs 1.693; Rotatory Strength)
- tests/k6h2o/k6h2o: k6h2o.err: No such file or directory

MDテスト

- 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

メモ

- 特に大きい計算の場合、インテルコンパイラを使った方が速度が出るケースが多い。一方で、一部の計算が劇的に遅くなるケースがあるため、今回は GCC を使用。
- OpenBLAS+Scalapack を使うよりも MKL を使う方が速度が出る
    - GCC でもインテルコンパイラでも同様
- (CUDA 版については一応別バイナリとして作成)