Gromacs 2025.4

Webpage

http://www.gromacs.org/

Version

2025.4

Build Environment

- GCC 13.3.1 (gcc-toolset-13)
- Open MPI 4.1.8
- CP2K 2024.3 (for double precision MPI version)
- cmake 3.31.6
- openblas 0.3.29-lp64

Files Required

- gromacs-2025.4.tar.gz
- regressiontests-2025.4.tar.gz
- installed CP2K 2024.3 (for double precision MPI version)
- (some of files will be downloaded during the installation)

Build Procedure

```
#!/bin/sh

VERSION=2025.4
INSTALL_PREFIX=/apl/gromacs/${VERSION}

BASEDIR=/home/users/${USER}/Software/Gromacs/${VERSION}/
GROMACS_TARBALL=${BASEDIR}/gromacs-${VERSION}.tar.gz
REGRESSION_TARBALL=${BASEDIR}/regressiontests-${VERSION}.tar.gz
WORKDIR=/gwork/users/${USER}
REGRESSION_PATH=${WORKDIR}/regressiontests-${VERSION}

TORCH_DIR=/apl/libtorch/2.7.0/cpu

PARALLEL=12
export LANG=C

#------------------------------------------------------------------
umask 0022
```

```
module -s purge
module -s load gcc-toolset/13
module -s load openmpi/4.1.8/gcc13
module -s load cmake/3.31.6

cd ${WORKDIR}
if [ -d gromacs-${VERSION} ]; then
 mv gromacs-${VERSION} gromacs_erase
 rm -rf gromacs_erase &
fi

if [ -d regressiontests-${VERSION} ]; then
 mv regressiontests-${VERSION} regressiontests_erase
 rm -rf regressiontests_erase &
fi

tar xzf ${GROMACS_TARBALL}
tar xzf ${REGRESSION_TARBALL}
cd gromacs-${VERSION}

# single precision, no MPI
mkdir rccs-s
cd rccs-s
cmake .. \
  -DCMAKE_PREFIX_PATH="${TORCH_DIR}" \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DCMAKE_C_COMPILER=gcc \
  -DCMAKE_CXX_COMPILER=g++ \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=ON \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DGMX_NNPOT=TORCH \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..

# double precision, no MPI
mkdir rccs-d
cd rccs-d
cmake .. \
  -DCMAKE_PREFIX_PATH="${TORCH_DIR}" \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DCMAKE_C_COMPILER=gcc \
  -DCMAKE_CXX_COMPILER=g++ \
  -DGMX_MPI=OFF \
```

```
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_THREAD_MPI=ON \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DGMX_NNPOT=TORCH \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check
make install
cd ..

# single precision, with MPI
mkdir rccs-mpi-s
cd rccs-mpi-s
cmake .. \
  -DCMAKE_PREFIX_PATH="${TORCH_DIR}" \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DCMAKE_C_COMPILER=mpicc \
  -DCMAKE_CXX_COMPILER=mpicxx \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DGMX_USE_PLUMED=ON \
  -DGMX_NNPOT=TORCH \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..

# double precision, with MPI
mkdir rccs-mpi-d
cd rccs-mpi-d
cmake .. \
  -DCMAKE_PREFIX_PATH="${TORCH_DIR}" \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DCMAKE_C_COMPILER=mpicc \
  -DCMAKE_CXX_COMPILER=mpicxx \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DGMX_USE_PLUMED=ON \
  -DGMX_NNPOT=TORCH \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
```

```
 -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..

# double precision, with MPI + CP2K
CP2KROOT=/apl/cp2k/2024.3
CP2KROOT_TC=${CP2KROOT}/tools/toolchain

mkdir rccs-mpi-d-cp2k
cd rccs-mpi-d-cp2k
cmake .. \
 -DCMAKE_PREFIX_PATH="${CP2KROOT_TC}/install/fftw-3.3.10" \
 -DGMX_DEFAULT_SUFFIX=OFF \
 -DGMX_BINARY_SUFFIX=_mpi_d_cp2k \
 -DGMX_LIBS_SUFFIX=_mpi_d_cp2k \
 -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
 -DCMAKE_VERBOSE_MAKEFILE=ON \
 -DCMAKE_C_COMPILER=mpicc \
 -DCMAKE_CXX_COMPILER=mpicxx \
 -DGMX_MPI=ON \
 -DGMX_GPU=OFF \
 -DGMX_DOUBLE=ON \
 -DGMX_THREAD_MPI=OFF \
 -DGMX_CP2K=ON \
 -DBUILD_SHARED_LIBS=OFF \
 -DGMXAPI=OFF \
 -DGMX_INSTALL_NBLIB_API=OFF \
 -DCP2K_DIR=${CP2KROOT}/lib/rccs/psmp \
 -DGMX_FFT_LIBRARY=fftw3 \
 -DGMX_EXTERNAL_BLAS=ON \
 -DGMX_BLAS_USER=${CP2KROOT_TC}/install/openblas-0.3.27/lib/libopenblas.so \
 -DGMX_EXTERNAL_LAPACK=ON \
 -DGMX_LAPACK_USER=${CP2KROOT_TC}/install/openblas-0.3.27/lib/libopenblas.so \
 -DGMX_USE_PLUMED=ON \
 -DGMX_NNPOT=OFF \
 -DREGRESSIONTEST_DOWNLOAD=OFF \
 -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check
make install
cd ..
```

Tests

All the tests have passed successfully.

Notes

- This procedure is the same as that for version 2025.2. Please check 2025.2 page for details.