

Gromacs 2024.5

Webpage

<http://www.gromacs.org/>

Version

2024.5

Build Environment

- GCC 13.1.1 (gcc-toolset-13)
- HPC-X 2.16 (Open MPI 4.1.5)
- [CP2K 2024.3](#) (only for double precision MPI version)

Files Required

- gromacs-2024.5.tar.gz
- regressiontests-2024.5.tar.gz
- installed [CP2K 2024.3](#) (only for double precision MPI version)

Build Procedure

```
#!/bin/sh

VERSION=2024.5
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}

PARALLEL=12
export LANG=C

#-----
umask 0022

module -s purge
module -s load gcc-toolset/13
module -s load openmpi/4.1.5-hpcx2.16/gcc13

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_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 \  
-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_INSTALL_PREFIX=${INSTALL_PREFIX} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DCMAKE_C_COMPILER=gcc \  
-DCMAKE_CXX_COMPILER=g++ \  
-DGMX_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=ON \  
-DGMX_THREAD_MPI=ON \  
-DGMX_BUILD_OWN_FFTW=ON \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION_PATH}  
make -j${PARALLEL} && make check  
make install  
cd ..
```

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

```
CP2KROOT=/apl/cp2k/2024.3  
CP2KROOT_TC=${CP2KROOT}/tools/toolchain
```

```
# double precision, with MPI  
mkdir rccs-mpi-d  
cd rccs-mpi-d  
cmake .. \  
-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=${CP2KROOT}/lib/rccs/psmp \  
-DGMX_FFT_LIBRARY=fftw3 \  
-DCMAKE_PREFIX_PATH=${CP2KROOT_TC}/install/fftw-3.3.10 \  
-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 \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION_PATH} \  
make -j${PARALLEL} && make check \  
make install \  
cd ..
```

Tests

All the tests have passed successfully.

Notes

- same procedure as [2024.2](#)