

Gromacs 2021.6

Webpage

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

Version

2021.6

Build Environment

- GCC 11.2.1 (gcc-toolset-11)
- HPC-X 2.11 (Open MPI 4.1.4)

Files Required

- gromacs-2021.6.tar.gz
- regressiontests-2021.6.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=2021.6
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 purge
module load gcc-toolset/11
module load openmpi/4.1.4-hpcx/gcc11

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 ..
```

double precision, with MPI

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

Notes

- If HPC-X 2.13.1 (Open MPI 4.1.5) is employed, the `gmx_mpi` processes sometimes don't terminate properly (although computation is finished).