

Gromacs 2023.5

Webpage

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

Version

2023.5

Build Environment

- GCC 9.2.1 (gcc-toolset-9)
- Open MPI 4.1.5

Files Required

- gromacs-2023.5.tar.gz
- regressiontests-2023.5.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=2023.5
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/9
module -s load openmpi/4.1.5/gcc9

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

- [Please check procedure and notes of version 2023.2.](#)