

Gromacs 2016.6 (HPE)

Webpage

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

Version

2016.6

Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- HPC-X 2.11 (Open MPI 4.1.4)

Files Required

- gromacs-2016.6.tar.gz
- regressiontests-2016.6.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=2016.6
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

#-----
umask 0022

module purge
module load gcc-toolset/10
module load openmpi/4.1.4-hpcx/gcc10

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 \
  -DGMX_MPI=OFF \
```

```
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=OFF \  
-DGMX_SIMD=AVX2_256 \  
-DGMX_THREAD_MPI=ON \  
-DGMX_BUILD_OWN_FFTW=ON \  
-DGMX_HWLOC=off \  
-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=${INSTALL_PREFIX} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=ON \  
-DGMX_SIMD=AVX2_256 \  
-DGMX_THREAD_MPI=ON \  
-DGMX_BUILD_OWN_FFTW=ON \  
-DGMX_HWLOC=off \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION_PATH}  
make -j${PARALLEL} && make check && make install  
cd ..
```

```
# compiler setting for MPI versions  
export CC=mpicc  
export CXX=mpicxx  
export F77=mpif90  
export F90=mpif90  
export FC=mpif90
```

```
# single precision, with MPI  
mkdir rccs-mpi-s  
cd rccs-mpi-s  
cmake .. \  
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=ON \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=OFF \  
-DGMX_SIMD=AVX2_256 \  
-DGMX_THREAD_MPI=OFF \  
-DGMX_BUILD_OWN_FFTW=ON \  
-DGMX_HWLOC=off \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${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 \  
-DGMX_MPI=ON \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=ON \  
-DGMX_SIMD=AVX2_256 \  
-DGMX_THREAD_MPI=OFF \  

```

```
-DGMX_BUILD_OWN_FFTW=ON \  
-DGMX_HWLOC=off \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION_PATH}  
make -j${PARALLEL} && make check && make install  
cd ..
```