

Gromacs 2016.6 (GCC)

Webpage

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

Version

2016.6

Build Environment

- Intel Parallel Studio 2017 Update 8 (MPI and MKL)
- GCC 5.3.1 (via Software Collections devtoolset-4)

Files Required

- gromacs-2016.6.tar.gz
- (regressiontests-2016.6.tar.gz; testset)

Build Procedure

```
#!/bin/sh

VERSION=2016.6
SCL_TOOLSET=devtoolset-4
INSTALL_PREFIX=/local/apl/ix/gromacs2016.6-gnu

BASEDIR=/home/users/${USER}/Software/Gromacs/${VERSION}/
GROMACS_TARBALL=${BASEDIR}/gromacs-${VERSION}.tar.gz
REGRESSION=${BASEDIR}/regressiontests-${VERSION} # unpacked

WORKDIR=/work/users/${USER}

MPIRUN=`which mpirun`
MPI_NPROCS=8
PARALLEL=12

module purge
module load scl/${SCL_TOOLSET}
module load intel_parallelstudio/2017update8

export LC_ALL=C
export LANG=C
export OMP_NUM_THREADS=1

#-----
umask 0022

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

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

# single precision, no MPI
mkdir rccs-gnu-s
cd rccs-gnu-s
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
```

```
-DGMX_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=OFF \  
-DGMX_THREAD_MPI=ON \  
-DGMX_FFT_LIBRARY=fftw3 \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION}  
make -j${PARALLEL} && make check && make install  
cd ..
```

```
# double precision, no MPI  
mkdir rccs-gnu-d  
cd rccs-gnu-d  
cmake .. \  
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=ON \  
-DGMX_SIMD=AVX2_256 \  
-DGMX_THREAD_MPI=ON \  
-DGMX_FFT_LIBRARY=fftw3 \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION}  
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-gnu-mpi-s  
cd rccs-gnu-mpi-s  
cmake .. \  
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=ON \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=OFF \  
-DGMX_THREAD_MPI=OFF \  
-DGMX_FFT_LIBRARY=fftw3 \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION} \  
-DMPIEXEC=${MPIRUN} \  
-DMPIEXEC_NUMPROC_FLAG="-np" \  
-DNUMPROC=${MPI_NPROCS} \  
-DMPIEXEC_PREFLAGS="" \  
-DMPIEXEC_POSTFLAGS=""  
make -j${PARALLEL} && make check && make install  
cd ..
```

```
# double precision, with MPI  
mkdir rccs-gnu-mpi-d  
cd rccs-gnu-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_FFT_LIBRARY=fftw3 \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION} \  
-DMPIEXEC=${MPIRUN} \  
-DMPIEXEC_NUMPROC_FLAG="-np" \  
-DNUMPROC=${MPI_NPROCS} \  
-DMPIEXEC_PREFLAGS="" \  
-DMPIEXEC_POSTFLAGS=""
```

```
make -j${PARALLEL} && make check && make install
```

```
cd ..
```