

Gromacs 2016.5 for LX (gcc)

Webpage

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

Version

2016.5

Build Environment

- GCC 5.3.1
- Intel MKL 2018 Update 2
- Intel MPI 2017.3.196
- FFTW 3.3.2 (sse enabled)
- cmake 2.8.12.2

Files Required

- gromacs-2016.5.tar.gz
- (regressiontests-2016.5.tar.gz; testset)

Build Procedure

(Leading tabs in the block enclosed with "EOF" are replaced with spaces. Please beware when you use this script.)

```
#!/bin/sh

VERSION=2016.5
SCL_TOOLSET=devtoolset-4
INSTALL_PREFIX=/local/apl/lx/gromacs2016.5-gnu

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

WORKDIR=/work/users/${USER}
#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
scl enable ${SCL_TOOLSET} bash <<-EOF
  mkdir rccs-gnu-s
  cd rccs-gnu-s
  cmake .. \
    -DCMAKE_INSTALL_PREFIX=${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
make -j12 && 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
make -j12 && 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
make -j12 && 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
make -j12 && make install
cd ..

EOF
```

Notice

Double precision version is compiled with AVX2_256 level, which is the same as the default setting in gromacs 5.1.5, due to a compilation error in AVX_512 setting.