

Gromacs 2016.6 (Intel)

Webpage

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

Version

2016.6

Build Environment

- Intel Parallel Studio 2018 Update 4

Files Required

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

Build Procedure

```
#!/bin/sh

VERSION=2016.6
INSTALL_PREFIX=/local/apl/lx/gromacs2016.6

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

WORKDIR=/work/users/${USER}
PARALLEL=12

MPIRUN=`which mpirun`
MPI_NPROCS=8

module purge
module load intel_parallelstudio/2018update4

export LANG=C
export LC_ALL=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}

# compiler setting
export CC=icc
export CXX=icpc
export F77=ifort
export F90=ifort
export FC=ifort

# single precision, no MPI
mkdir rccs-s
```

```
cd rccs-s
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION}
make -j${PARALLEL} && make check && make install
cd ..
```

double precision, no MPI

```
mkdir rccs-d
cd rccs-d
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_THREAD_MPI=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION}
make -j${PARALLEL} && make check && make install
cd ..
```

compiler setting for MPI versions

```
export CC=mpiicc
export CXX=mpiicpc
export F77=mpiifort
export F90=mpiifort
export FC=mpiifort
```

single precision, with MPI

```
mkdir rccs-mpi-s
cd rccs-mpi-s
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${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-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_THREAD_MPI=OFF \  
-DGMX_FFT_LIBRARY=mkl \  
-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 ..
```

Notes

- Gcc version is sometimes more efficient than this Intel version. We recommend you to compare the efficiency using your own input files.