

## Gromacs 2016.5 for LX with GPU support (intel compiler)

### Webpage

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

### Version

2016.5

### Build Environment

- ▶ Intel Compiler 17.0.4.196
- ▶ Intel MKL 2017 update 3
- ▶ Intel MPI 2017.0.3
- ▶ CUDA 9.1.85
- ▶ cmake 2.8.12

### Files Required

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

### Build Procedure

```
#!/bin/sh
VERSION=2016.5
INSTALL_PREFIX=/local/apl/lx/gromacs2016.5-CUDA9
BASEDIR=/home/users/${USER}
GROMACS_TARBALL=${BASEDIR}/gromacs-${VERSION}.tar.gz
WORKDIR=/work/users/${USER}
#REGRESSION=${WORKDIR}/regressiontests-${VERSION} # unpacked
PARALLEL=8
# intel17+cuda-9.1
. /local/apl/lx/intel2017update4/bin/compilervars.sh intel64
export PATH=/local/apl/lx/cuda-9.1/bin:${PATH}
export LD_LIBRARY_PATH=/local/apl/lx/cuda-9.1/lib64:${LD_LIBRARY_PATH}
#-----
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=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DGMX_USE_NVML=OFF \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j${PARALLEL} && 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=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=OFF \
  -DGMX_USE_NVML=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j${PARALLEL} && make install
cd ..
```

## Notice

- ▶ gcc version can be father than this version. If possible, please check the performance before production runs.