# Gromacs 2016.3 for GPU

## Webpage

http://www.gromacs.org/

## Version

2016.3

## Tools for Compiling

- Intel Compiler 16.0.2
- Intel MPI 5.1.3.181
- cmake 2.8.12
- g++ (GCC) 4.9.2

## Necessary Files for Compiling

- gromacs-2016.3.tar.gz

## Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_gromacs=/home/users/${USER}/build/gromacs2016.3/gromacs-2016.3.tar.gz
set prefix=/local/apl/pg/gromacs2016.3-CUDA
set work=/work/users/${USER}
#------------------------------------------------------------------------------
cat <<EOF | scl enable devtoolset-3 csh
umask 022
source /opt/intel/composer_xe_2015.2.164/bin/compilervars.csh intel64
cd ${work}
if (-d gromacs-2016.3) then
  mv gromacs-2016.3 gromacs-erase
  rm -rf gromacs-erase &
endif
tar xzf ${file_gromacs}
cd gromacs-2016.3
#
setenv CC icc
setenv CXX icpc
setenv F77 ifort
setenv F90 ifort
setenv FC ifort
mkdir rccs-gpu
cd rccs-gpu
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \
    -DCMAKE_VERBOSE_MAKEFILE=ON \
    -DGMX_MPI=OFF \
    -DGMX_GPU=ON \
    -DGMX_DOUBLE=OFF \
    -DGMX_FFT_LIBRARY=mkl \
    -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
EOF
```