

## Gromacs 5.1.5 for LX with GPU support (intel compiler)

### Webpage

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

### Version

5.1.5

### Build Environment

- Intel Compiler 2015.1.133
- Intel MPI 5.0.2
- Intel MKL 11.2.1
- CUDA 8.0.61

### Files Required

- gromacs 5.1.5.tar.gz
- (regressiontests-5.1.5.tar.gz; testset)

### Build Procedure

```
#!/bin/sh

VERSION=5.1.5

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

INSTALL_PREFIX=/local/apl/lx/gromacs515-CUDA
WORKDIR=/work/users/${USER}

#-----
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}

# intel 15 or 16 is required for cuda-8.0
./local/apl/lx/intel2015update1/bin/compilervars.sh intel64

# compiler setting for single node versions
export CC=icc
export CXX=icpc
export F77=ifort
export F90=ifort
export FC=ifort

# single precision, no MPI
mkdir rccs-cuda
cd rccs-cuda
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 \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j12 && make install  
cd ..  
  
# corresponding version of intel MPI  
./local/apl/lx/intel2015update1/impi/5.0.2.044/intel64/bin/mpivars.sh  
  
# 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-cuda-mpi  
cd rccs-cuda-mpi  
cmake .. \  
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=ON \  
-DGMX_GPU=ON \  
-DGMX_DOUBLE=OFF \  
-DGMX_THREAD_MPI=OFF \  
-DGMX_FFT_LIBRARY=mkl \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j12 && make install  
cd ..
```