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${PATH:+:${PATH}}
export LD_LIBRARY_PATH=/local/apl/lx/cuda-9.1/lib64${LD_LIBRARY_PATH:+:${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.