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 ..
```