Gromacs 2016.5 for LX with GPU support (gcc)

Webpage

http://www.gromacs.org/

Version

2016.5

Build Environment

- GCC 5.3.1
- Intel MKL 2018 Update 2
- Intel MPI 2017.3.196
- FFTW 3.3.2 (sse enabled)
- cmake 2.8.12.2
- CUDA 8.0.61

Files Required

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

Build Procedure

(Leading tabs in a block enclosed with "EOF" are replaced with spaces. Please beware when you use this script.)

```
#!/bin/sh

VERSION=2016.5
SCL_TOOLSET=devtoolset-4
INSTALL_PREFIX=/local/apl/lx/gromacs2016.5-gnu-CUDA

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

WORKDIR=/work/users/${USER}
#export OMP_NUM_THREADS=1

#-----------------------------------------------------------------------
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}

# single precision, no MPI
scl enable ${SCL_TOOLSET} bash <<-EOF
        mkdir rccs-gnu-s
        cd rccs-gnu-s
        cmake .. \
              -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
              -DCMAKE_VERBOSE_MAKEFILE=ON \
              -DGMX_MPI=OFF \
              -DGMX_GPU=ON \
              -DGMX_DOUBLE=OFF \
              -DGMX_THREAD_MPI=ON \
              -DGMX_FFT_LIBRARY=fftw3 \
              -DGMX_USE_NVML=OFF \
```

```
        -DREGRESSIONTEST_DOWNLOAD=OFF
    make -j12 && make install
    cd ..

    # compiler setting for MPI versions
    export CC=mpicc
    export CXX=mpicxx
    export F77=mpif90
    export F90=mpif90
    export FC=mpif90

    # single precision, with MPI
    mkdir rccs-gnu-mpi-s
    cd rccs-gnu-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=fftw3 \
        -DREGRESSIONTEST_DOWNLOAD=OFF
    make -j12 && make install
    cd ..
EOF
```

Notice

To avoid libnvidia-ml.so error, -DGMX_USE_NVML=OFF is required. (This happens only in this version.)