Gromacs 2016.6-CUDA (GCC)

Webpage

http://www.gromacs.org/

Version

2016.6

Build Environment

- GCC 5.3.1 (via Software Collections devtoolset-4)
- Intel Parallel Studio 2017 Update8 (MKL & MPI)
- FFTW 3.3.2 (sse enabled)
- cmake 2.8.12.2
- CUDA 9.1.85

Files Required

- gromacs-2016.6.tar.gz
- (regressiontests-2016.6.tar.gz; testset)

Build Procedure

```
#!/bin/sh

VERSION=2016.6
SCL_TOOLSET=devtoolset-4
INSTALL_PREFIX=/local/apl/lx/gromacs2016.6-gnu-CUDA

BASEDIR=/home/users/${USER}/Software/Gromacs/${VERSION}/
GROMACS_TARBALL=${BASEDIR}/gromacs-${VERSION}.tar.gz

WORKDIR=/work/users/${USER}
REGRESSION=${WORKDIR}/regressiontests-${VERSION} # unpacked

PARALLEL=12

module purge
module load scl/${SCL_TOOLSET}
module load intel_parallelstudio/2017update8
module load cuda/9.1

export LANG=C
export LC_ALL=C

#------------------------------------------------------------------------
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
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 -j${PARALLEL} && 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=${INSTALL_PREFIX} \
      -DCMAKE_VERBOSE_MAKEFILE=ON \
      -DGMX_MPI=ON \
      -DGMX_GPU=ON \
      -DGMX_DOUBLE=OFF \
      -DGMX_USE_NVML=OFF \
      -DGMX_THREAD_MPI=OFF \
      -DGMX_FFT_LIBRARY=fftw3 \
      -DREGRESSIONTEST_DOWNLOAD=OFF
make -j${PARALLEL} && make install
cd ..
```

Notes

- Regression tests were performed at one of P100 nodes.
- Gcc 6 is not employed since binaries could not pass the regression tests.