Gromacs 2020.4 with GPU support (gnu)

Webpage

http://www.gromacs.org/

Version

2020.4

Build Environment

- Intel Parallel Studio XE 2018 update 4 (MPI)
- GCC 8.3.1 (Software Collections devtoolset-8)
- CUDA 10.1
- cmake 3.16.3

Files Required

- gromacs-2020.4.tar.gz
- regressiontests-2020.4.tar.gz
- tests_CMakelists.patch

```
--- tests/CMakeLists.txt.org    2019-10-07 19:24:40.524863424 +0900
+++ tests/CMakeLists.txt        2019-10-07 19:25:13.736715189 +0900
@@ -125,6 +125,11 @@
         endif()
         #We should use MPIEXEC_NUMPROC_FLAG but gmxtest.pl doesn't let us pass it
     endif()
+    if(GMX_THREAD_MPI)
+        set(GMX_TEST_NUMBER_PROCS 8 CACHE STRING "Number of processors used for testing")
+        mark_as_advanced(GMX_TEST_NUMBER_PROCS)
+        list(APPEND ARGS -nt ${GMX_TEST_NUMBER_PROCS})
+    endif()
     if(GMX_BINARY_SUFFIX)
         list(APPEND ARGS -suffix ${GMX_BINARY_SUFFIX})
     endif()
```

(This patch was used upon building 2019.4 on ccgpup. We didn't do build test without this patch.)

- fftw-3.3.8.tar.gz (build host ccgpup cannot access internet)

Build Procedure

```
#!/bin/sh

VERSION=2020.4
INSTALL_PREFIX=/local/apl/lx/gromacs${VERSION}-gnu-CUDA

BASEDIR=/home/users/${USER}/Software/Gromacs/${VERSION}/
GROMACS_TARBALL=${BASEDIR}/gromacs-${VERSION}.tar.gz
REGRESSION_TARBALL=${BASEDIR}/regressiontests-${VERSION}.tar.gz
WORKDIR=/work/users/${USER}
REGRESSION_PATH=${WORKDIR}/regressiontests-${VERSION}

FFTW_VER=3.3.8
FFTW_PATH=${BASEDIR}/fftw-${FFTW_VER}.tar.gz

PATCH_TEST=${BASEDIR}/tests_CMakelists.patch

PARALLEL=12

#------------------------------------------------------------------------
umask 0022
```

```
module purge
module load scl/devtoolset-8
module load intel_parallelstudio/2018update4
module load cuda/10.1
module load cmake/3.16.3

cd ${WORKDIR}
if [ -d gromacs-${VERSION} ]; then
  mv gromacs-${VERSION} gromacs_erase
  rm -rf gromacs_erase &
fi

if [ -d regressiontests-${VERSION} ]; then
  mv regressiontests-${VERSION} regressiontests_erase
  rm -rf regressiontests_erase &
fi

tar xzf ${GROMACS_TARBALL}
tar xzf ${REGRESSION_TARBALL}
cd gromacs-${VERSION}
patch -p0 < ${PATCH_TEST}

# single precision, no MPI
mkdir rccs-s
cd rccs-s
cmake .. \
   -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
   -DCMAKE_VERBOSE_MAKEFILE=ON \
   -DGMX_MPI=OFF \
   -DGMX_GPU=ON \
   -DGMX_DOUBLE=OFF \
   -DGMX_THREAD_MPI=ON \
   -DGMX_BUILD_OWN_FFTW=ON \
   -DGMX_BUILD_OWN_FFTW_URL=${FFTW_PATH} \
   -DREGRESSIONTEST_DOWNLOAD=OFF \
   -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && 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-mpi-s
cd rccs-mpi-s
cmake .. \
   -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
   -DCMAKE_VERBOSE_MAKEFILE=ON \
   -DGMX_MPI=ON \
   -DGMX_GPU=ON \
   -DGMX_DOUBLE=OFF \
   -DGMX_THREAD_MPI=OFF \
   -DGMX_BUILD_OWN_FFTW=ON \
   -DGMX_BUILD_OWN_FFTW_URL=${FFTW_PATH} \
   -DREGRESSIONTEST_DOWNLOAD=OFF \
   -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..
```

Notes

- Built and tested on ccgpup. The procedure is exactly the same as that for 2020.2.