

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 gmxtst.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 ccgpus. We didn't do build test without this patch.)

- ▶ fftw-3.3.8.tar.gz (build host ccgpus 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 cccgpp. The procedure is exactly the same as that for 2020.2.