

Gromacs 2021.4 with GPU support

Webpage

<http://www.gromacs.org/>

Version

2021.4

Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- HPC-X 2.11 (Open MPI 4.1.4)
- CUDA 11.6

Files Required

- gromacs-2021.4.tar.gz
- regressiontests-2021.4.tar.gz
- fftw-3.3.8.tar.gz
 - Computation nodes cannot access fftw download site.

Build Procedure

```
#!/bin/sh

VERSION=2021.4
INSTALL_PREFIX=/apl/gromacs/${VERSION}-CUDA

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

PARALLEL=12
export LANG=C

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

#-----
umask 0022

module purge
module load gcc-toolset/10
module load openmpi/4.1.4-hpcx/gcc10
module load cuda/11.6

export CUDA_VISIBLE_DEVICES=0,1

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}

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

# single precision, with MPI
mkdir rccs-mpi-s
cd rccs-mpi-s
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DCMAKE_C_COMPILER=mpicc \
  -DCMAKE_CXX_COMPILER=mpicxx \
  -DGMX_MPI=ON \
  -DGMX_GPU=CUDA \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DGMX_BUILD_OWN_FFTW_URL=${FFTW_PATH} \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..

```

Notes

- Built and tested on one of GPU nodes.
 - Tests failed if 8 GPUs are visible from gromacs. (avoided by export CUDA_VISIBLE_DEVICES=0,1)
- Failed to build with CUDA 11.8 of NVIDIA HPC SDK.