Gromacs 2021.4 GCC9

Webpage

http://www.gromacs.org/

Version

2021.4

Build Environment

- Intel MPI 2018.0.4 (2018.4.274)
- Intel MKL 2020.0.2
- GCC 9.3.1 (Software Collections devtoolset-9)
- cmake 3.16.3

Files Required

- gromacs-2021.4.tar.gz
- regressiontests-2021.4.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=2021.4
INSTALL_PREFIX=/local/apl/lx/gromacs${VERSION}

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}

PARALLEL=12
export LANG=C

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

module purge
module load scl/devtoolset-9
module load mpi/intelmpi/2018.4.274
module load mkl/2020.0.2
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}

# single precision, no MPI
mkdir rccs-s
```

```
cd rccs-s
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DCMAKE_C_COMPILER=gcc \
  -DCMAKE_CXX_COMPILER=g++ \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=ON \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..

# double precision, no MPI
module unload mkl
mkdir rccs-d
cd rccs-d
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DCMAKE_C_COMPILER=gcc \
  -DCMAKE_CXX_COMPILER=g++ \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_THREAD_MPI=ON \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check
# ignore errors!
make install
cd ..

# single precision, with MPI
module load mkl/2020.0.2
mkdir rccs-mpi-s
cd rccs-mpi-s
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DCMAKE_C_COMPILER=mpicc \
  -DCMAKE_CXX_COMPILER=mpicxx \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..

# double precision, with MPI
module unload mkl
mkdir rccs-mpi-d
cd rccs-mpi-d
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DCMAKE_C_COMPILER=mpicc \
  -DCMAKE_CXX_COMPILER=mpicxx \
```

```
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check
# ignore errors
make install
cd ..
```

Notes

- Changes from 2021.2 and related notes
  - Intel MPI version was changed to 2018; 2020 version got stuck on a test (there may be other ones).
  - Double precision version with MKL still failed on tests (this does not happen for intel compiler version). We thus don't use MKL for double precision version.
- Double precision version failed on GammaDistributionTest test. (numerical error)
  - This is due to the implementation change.
    - https://gitlab.com/gromacs/gromacs/-/issues/4270
    - https://gitlab.com/gromacs/gromacs/-/merge_requests/2148
    - https://gitlab.com/gromacs/gromacs/-/merge_requests/2172
  - Tolerance is planned to be changed in the next version (see link above). Thus, we can gently ignore this error.