Gromacs 2020.2 (gnu)

Webpage

http://www.gromacs.org/

Version

2020.2

Build Environment

- Intel Parallel Studio XE 2018 update 4 (for MKL and MPI)
- GCC 8.3.1 (Software Collections devtoolset-8)
- cmake 3.16.3

Files Required

- gromacs-2020.2.tar.gz
- regressiontests-2020.2.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=2020.2
INSTALL_PREFIX=/local/apl/lx/gromacs${VERSION}-gnu

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

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

module purge
module load scl/devtoolset-8
module load intel_parallelstudio/2018update4
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=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=ON \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..

# double precision, no MPI
mkdir rccs-d
cd rccs-d
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
```

```
  -DGMX_DOUBLE=ON \
  -DGMX_THREAD_MPI=ON \
  -DGMX_BUILD_OWN_FFTW=mkl \
  -DMKL_LIBRARIES="-L${MKLROOT}/lib/intel64 -Wl,--no-as-needed -lmkl_intel_lp64 -lmkl_sequential -lmkl_core -
lpthread -lm -ldl" \
  -DMKL_INCLUDE_DIR="-m64 -I${MKLROOT}/include" \
  -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=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..

# double precision, with MPI
mkdir rccs-mpi-d
cd rccs-mpi-d
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_BUILD_OWN_FFTW=mkl \
  -DMKL_LIBRARIES="-L${MKLROOT}/lib/intel64 -Wl,--no-as-needed -lmkl_intel_lp64 -lmkl_sequential -lmkl_core -
lpthread -lm -ldl" \
  -DMKL_INCLUDE_DIR="-m64 -I${MKLROOT}/include" \
  -DREGRESSIONTEST_DOWNLOAD=OFF \
  -DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make check && make install
cd ..
```

Notes

- Built on ccfep.
- old lapack (i don't know where it is invoked) causes error on MdrunNonIntegratorTests for double precison version. To avoid this, mkl is used only for double version.
  - https://redmine.gromacs.org/issues/2844
  - gcc version does not concern with this issue.
  - Intel version is free from this issue. It silently employs mkl?