Gromacs 2023.2

Webpage

http://www.gromacs.org/

Version

2023.2

Build Environment

- GCC 9.2.1 (gcc-toolset-9)
- HPC-X 2.11 (Open MPI 4.1.4)

Files Required

- gromacs-2023.2.tar.gz
- regressiontests-2023.2.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=2023.2
INSTALL_PREFIX=/apl/gromacs/${VERSION}

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

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

module -s purge
module -s load gcc-toolset/9
module -s load openmpi/4.1.4-hpcx/gcc9

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
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
make install
cd ..

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

```
make install
cd ..
```

Tests

Double precision versions (both of MPI and thread-MPI) failed on ConvertTprTest.generateVelocitiesTest test.

- https://gitlab.com/gromacs/gromacs/-/issues/4824
- According to the issue above, the requested numerical accuracy is just too strict. This error can be ignored. This shall be fixed in the next release.

Notes

- Performance of GCC 10, 11, 12 versions can be terribly low. There seems to be a problem in nonbonding pairwise interaction (according to the "Force" component in the time accounting section of the logfile).
    - GCC 9 version shows comparable performance as the previous version. GCC 8 or before couldn't build the executable.
        - Gromacs 2022 version might be faster than this one in some cases.
    - Reference: https://gitlab.com/gromacs/gromacs/-/issues/4752
        - In our system (AMD EPYC 7763 64 Cores 2.45 GHz (Zen3)), the overall performance is degraded by more than 30% in some runs.
            - in the STMV system in the following benchmark set for example. AVX2_256 was automatically chosen for SIMD instruction regardless of GCC version.
            - https://aip.scitation.org/doi/10.1063/5.0018516
            - https://zenodo.org/record/3893789
        - AVX512 system may not be seriously affected?
- Intel compiler (icx, icpx) version shows slightly worse performance than gcc9 version.
- AOCC also show slightly worse performance than gcc9 version.
- VMD molfile plugin is not embedded due to the following bug: (will be fixed in the next release)
    - https://gitlab.com/gromacs/gromacs/-/issues/4832