

Gromacs 2021.4 Intel20

Webpage

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

Version

2021.4

Build Environment

- Intel Parallel Studio 2020 update 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}-intel

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 intel_parallelstudio/2020update2
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=${INSTALL_PREFIX} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DCMAKE_C_COMPILER=icc \  
-DCMAKE_CXX_COMPILER=icpc \  
-DGMX_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=OFF \  
-DGMX_THREAD_MPI=ON \  
-DGMX_BUILD_OWN_FFTW=ON \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION_PATH}  
make -j${PARALLEL} && make check && make install  
cd ..
```

```
# double precision, no MPI
```

```
mkdir rccs-d
```

```
cd rccs-d
```

```
cmake .. \  

```

```
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DCMAKE_C_COMPILER=icc \  
-DCMAKE_CXX_COMPILER=icpc \  
-DGMX_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=ON \  
-DGMX_THREAD_MPI=ON \  
-DGMX_BUILD_OWN_FFTW=ON \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${REGRESSION_PATH}
```

```
make -j${PARALLEL} && make check
```

```
# ignore errors
```

```
make install
```

```
cd ..
```

```
# single precision, with MPI
```

```
mkdir rccs-mpi-s
```

```
cd rccs-mpi-s
```

```
cmake .. \  

```

```
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DCMAKE_C_COMPILER=mpiicc \  
-DCMAKE_CXX_COMPILER=mpiicpc \  
-DGMX_MPI=ON \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=OFF \  
-DGMX_THREAD_MPI=OFF \  
-DGMX_BUILD_OWN_FFTW=ON \  
-DREGRESSIONTEST_DOWNLOAD=OFF \  
-DREGRESSIONTEST_PATH=${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=mpiicc \  
-DCMAKE_CXX_COMPILER=mpiicpc \  
-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

- Almost the same procedure [as in the case of 2021.2](#).
- 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.