Gromacs 2018.1 for LX (gcc)

Webpage

http://www.gromacs.org/

Version

2018.1

Build Environment

- GCC 6.3.1
- Intel MKL 2018 Update 2
- Intel MPI 2017.3.196
- FFTW 3.3.2 (SSE enabled)
- cmake 3.8.2

Files Required

- gromacs-2018.1.tar.gz
- (regressiontests-2018.1.tar.gz; testset)

Build Procedure

(Leading tabs in a block enclosed with "EOF" are replaced with spaces. Please beware when you use this script.)

```
#!/bin/sh

VERSION=2018.1
SCL_TOOLSET=devtoolset-6
INSTALL_PREFIX=/local/apl/lx/gromacs2018.1-gnu

BASEDIR=/home/users/${USER}
GROMACS_TARBALL=${BASEDIR}/gromacs-${VERSION}.tar.gz
WORKDIR=/work/users/${USER}
CMAKE=/local/apl/lx/cmake3.8.2/bin/cmake

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

cd ${WORKDIR}
if [ -d gromacs-${VERSION} ]; then
  mv gromacs-${VERSION} gromacs_erase
  rm -rf gromacs_erase &
fi

tar xzf ${GROMACS_TARBALL}
cd gromacs-${VERSION}

# single precision, no MPI
scl enable ${SCL_TOOLSET} bash <<-EOF
        mkdir rccs-gnu-s
        cd rccs-gnu-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_FFT_LIBRARY=fftw3 \
                -DREGRESSIONTEST_DOWNLOAD=OFF
        make -j12 && make install
        cd ..
```

```
    # double precision, no MPI
    mkdir rccs-gnu-d
    cd rccs-gnu-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_FFT_LIBRARY=fftw3 \
        -DREGRESSIONTEST_DOWNLOAD=OFF
    make -j12 && 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-gnu-mpi-s
    cd rccs-gnu-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_FFT_LIBRARY=fftw3 \
        -DREGRESSIONTEST_DOWNLOAD=OFF
    make -j12 && make install
    cd ..

    # double precision, with MPI
    mkdir rccs-gnu-mpi-d
    cd rccs-gnu-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_FFT_LIBRARY=fftw3 \
        -DREGRESSIONTEST_DOWNLOAD=OFF
    make -j12 && make install
    cd ..
EOF
```

Notice

GPU version (gcc 5.3.1 + CUDA 8.0) is not installed, since it failed on LJ PME related tests (numerical errors in potential energy and forces) in complex test section of regression tests.