Gromacs 2018.1 for LX (intel)

Webpage

http://www.gromacs.org/

Version

2018.1

Build Environment

- Intel Compiler 2018.2.199
- Intel MKL 2018 Update 2
- Intel MPI 2017.3.196
- cmake 3.8.2

Files Required

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

ビルド手順

```
#!/bin/sh

VERSION=2018.1
INSTALL_PREFIX=/local/apl/lx/gromacs2018.1

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}

# compiler setting
export CC=icc
export CXX=icpc
export F77=ifort
export F90=ifort
export FC=ifort

# 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_FFT_LIBRARY=mkl \
```

```
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j12 && 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_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j12 && make install
cd ..

# compiler setting for MPI versions
export CC=mpiicc
export CXX=mpiicpc
export F77=mpiifort
export F90=mpiifort
export FC=mpiifort

# 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_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j12 && 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_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j12 && make install
cd ..
```

Notice

GPU version (with Intel Compiler 2015 and CUDA 8.0) is not installed, since it causes errors in TIP4P related tests (this is the same as gromacs 2016.5).