

Gromacs 2019.2 for LX with GPU support (Intel)

Webpage

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

Version

2019.2

Build Environment

- Intel Parallel Studio XE 2017 update 8
- gcc 6.3.1 (devtoolset-6 Software Collections)
- CUDA 9.1
- cmake 3.8.2

Files Required

- gromacs-2019.2.tar.gz
- regressiontests-2019.2.tar.gz

Build Procedure

```
#!/bin/sh

VERSION=2019.2
INSTALL_PREFIX=/local/apl/lx/gromacs${VERSION}-CUDA

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-6
module load intel_parallelstudio/2017update8
module load cuda/9.1
module load cmake/3.8.2

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}

# 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=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=ON \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DREGRESSIONTEST_DOWNLOAD=OFF
  #-DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && 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=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DREGRESSIONTEST_DOWNLOAD=OFF
  #-DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make install
cd ..

```

Test (MPI version only)

```

#!/bin/sh
#PBS -l select=ncpus=6:mpiprocs=6:ompthreads=1:jobtype=gpu:ngpus=1
#PBS -l walltime=00:30:00

if [ -d "${PBS_O_WORKDIR}" ]; then
  cd ${PBS_O_WORKDIR}
fi

module purge
module load intel_parallelstudio/2017update8
module load scl/devtoolset-6
module load cuda/9.1

VERSION=2019.2
GMXBASE=/local/apl/lx/gromacs${VERSION}-CUDA
#GMXBASE=/local/apl/lx/gromacs${VERSION}-gnu-CUDA
REGRESSIONS=/home/users/${USER}/Software/Gromacs/${VERSION}/regressiontests-${VERSION}
MPIRUN=`which mpirun`

cd $REGRESSIONS

```

```
.$ {GMXBASE}/bin/GMXRC.bash
```

```
PARALLEL="-np 6"
```

```
./gmxtest.pl $ {PARALLEL} \
```

```
  -ntomp 1 \
```

```
  -mpirun $ {MPIRUN} \
```

```
  all
```