

Gromacs 2018.7 with GPU for LX (intel)

Webpage

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

Version

2018.7

Build Environment

- Intel Parallel Studio XE 2017 update 8
- cmake 3.8.2
- cuda 9.1.85

Files Required

- gromacs-2018.7.tar.gz
- (regressiontests-2018.7.tar.gz; testset)

Build Procedure

```
#!/bin/sh

VERSION=2018.7
INSTALL_PREFIX=/local/apl/lx/gromacs2018.7-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 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=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
#-DREGRESSIONTEST_PATH=${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=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
#-DREGRESSIONTEST_PATH=${REGRESSION_PATH}
make -j${PARALLEL} && make install
cd ..

```

Regression Test

12CPU + 1GPU, MPI version only

```

#!/bin/sh
#PBS -l select=ncpus=12:mpiprocs=12: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 cuda/9.1

GMXBASE=/local/apl/lx/gromacs2018.7-CUDA
REGRESSIONS=/home/users/${USER}/Software/Gromacs/2018.7/regressiontests-2018.7
MPIRUN=`which mpirun`

cd $REGRESSIONS
. ${GMXBASE}/bin/GMXRC.bash

PARALLEL="-np 12"
./gmxtest.pl ${PARALLEL} \
  -ntomp 1 \
  -mpirun ${MPIRUN} \

```

