

Gromacs 2018.3 for LX with GPU support (intel)

Webpage

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

Version

2018.3

Build Environment

- ▶ Intel Parallel Studio XE 2017 update 4
- ▶ cmake 3.8.2
- ▶ cuda 9.1.85

Files Required

- ▶ gromacs-2018.3.tar.gz
- ▶ (regressiontests-2018.3.tar.gz; testset)

Build Procedure

(Tests are performed after the installation, see below.)

```
#!/bin/sh
VERSION=2018.3
INSTALL_PREFIX=/local/apl/lx/gromacs2018.3-CUDA
BASEDIR=/home/users/${USER}
GROMACS_TARBALL=${BASEDIR}/gromacs-${VERSION}.tar.gz
WORKDIR=/work/users/${USER}
PARALLEL=12
#-----
umask 0022
module purge
module load intel_parallelstudio/2017update4
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
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=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j${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 rocs-mpi-s
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j${PARALLEL} && make install
cd ..

```

Job script to run tests (12 CPUs + 1 GPU)

```

#!/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/2017update4
module load cuda/9.1

GMXBASE=/local/apl/lx/gromacs2018.3-CUDA
REGRESSIONS=/work/users/${USER}/regressiontests-2018.3
MPIRUN=`which mpirun`

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

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

# thread MPI test
PARALLEL="-nt 12"
./gmxtest.pl ${PARALLEL} \
  -ntomp 1 \
  all

```

Misc

- ▶ [Bug of parallel run with GPU in former Gromacs 2018 releases](#) is finally fixed in this version.
 - ▶ Tests successfully passed.