Gromacs 2018.3 for LX with GPU support (gcc)

ウェブページ

http://www.gromacs.org/

バージョン

2018.3

ビルド環境

- Intel Parallel Studio XE 2017 update 4 (Intel MPIを利用)
- gcc 6.3.1 (devtoolset-6 Software Collections)
- cuda 9.1.85
- cmake 3.8.2

ビルドに必要なファイル

- gromacs-2018.3.tar.gz
- (regressiontests-2018.3.tar.gz; テストセット)

ビルド手順

(テストはインストール後に実行)

```
#!/bin/sh

VERSION=2018.3
INSTALL_PREFIX=/local/apl/lx/gromacs2018.3-gnu-CUDA

BASEDIR=/home/users/${USER}
GROMACS_TARBALL=${BASEDIR}/gromacs-${VERSION}.tar.gz
WORKDIR=/work/users/${USER}

PARALLEL=12

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

module purge
module load scl/devtoolset-6
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}

# single precision, thread MPI
mkdir rccs-s
cd rccs-s
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=ON \
  -DGMX_BUILD_OWN_FFTW=ON \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j${PARALLEL} && 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-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
make -j${PARALLEL} && make install
cd ..
```

テスト用ジョブスクリプト (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 scl/devtoolset-6
module load cuda/9.1

GMXBASE=/local/apl/lx/gromacs2018.3-gnu-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
```