

## LAMMPS 7Aug19 with GPU support

### Webpage

<http://lammps.sandia.gov/>

### Version

7Aug19

### Build Environment

- ▶ Intel Parallel Studio XE 2017 update 8
- ▶ CUDA 9.1
- ▶ cmake 3.8.2

### Files Required

- ▶ lammps-stable\_7Aug2019.tar.gz
- ▶ lammps-testing-master.zip (downloaded on Oct. 23, 2019)
- ▶ (Some of packages are installed during the following procedure.)

### Build Procedure

```
#!/bin/sh

NAME=lammps-stable_7Aug2019
VERSION=7Aug19
INSTALL_PREFIX=/local/apl/lx/lammps7Aug19-CUDA

BASEDIR=/home/users/${USER}/Software/LAMMPS/${VERSION}
LAMMPS_TARBALL=${BASEDIR}/${NAME}.tar.gz
TESTS_ARCHIVE=${BASEDIR}/lammps-testing-master.20191023.zip

WORKDIR=/work/users/${USER}
#WORKDIR=/home/users/${USER}/ramdisk
LAMMPS_WORKDIR=${WORKDIR}/${NAME}
TESTS_WORKDIR=${WORKDIR}/lammps-testing-master

VMD_MOLFILE_INC=/local/apl/lx/vmd193/lib/plugins/include

PARALLEL=12

#-----
umask 0022
export LANG=C

module purge
module load intel_parallelstudio/2017update8
module load cuda/9.1
module load cmake/3.8.2

export CC=mpiicc
export CXX=mpiicpc
export FC=mpiifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export MPIFC=mpiifort

cd ${WORKDIR}
if [ -d ${NAME} ]; then
  mv ${NAME} lammps_erase
  rm -rf lammps_erase &
fi

if [ -d lammps-testing-master ]; then
  mv lammps-testing-master lammps-testing-master_erase
  rm -rf lammps-testing-master_erase &
fi

tar zxf ${LAMMPS_TARBALL}
unzip ${TESTS_ARCHIVE}

cd ${NAME}
mkdir build && cd build

# Disabled PKGs:
# ADIOS, QUIP, QMMM, VTK: noavail
# MSCG: gsl too old
# KOKKOS: not sure what this is
# KIM: incompatible with "make install"? Build itself works fine.

cmake ../cmake \
  -DLAMMPS_MACHINE=rccs \
  -DLAMMPS_LIB_SUFFIX=rccs \
  -DENABLE_TESTING=on \
```

-DLAMMPS\_TESTING\_SOURCE\_DIR=\${TESTS\_WORKDIR} \  
-DCMAKE\_INSTALL\_PREFIX=\${INSTALL\_PREFIX} \  
-DCMAKE\_C\_COMPILER=mpiicc \  
-DCMAKE\_CXX\_COMPILER=mpiicpc \  
-DCMAKE\_Fortran\_COMPILER=mpiifort \  
-DCMAKE\_MPI\_C\_COMPILER=mpiicc \  
-DCMAKE\_MPI\_CXX\_COMPILER=mpiicpc \  
-DCMAKE\_MPI\_Fortran\_COMPILER=mpiifort \  
-DBUILD\_LIB=on \  
-DBUILD\_TOOLS=on \  
-DBUILD\_MPI=on \  
-DBUILD\_OMP=on \  
-DFFT=MKL \  
-DFFT\_SINGLE=off \  
-DDOWNLOAD\_LATTE=on \  
-DDOWNLOAD\_SCAFACOS=on \  
-DDOWNLOAD\_VORO=on \  
-DDOWNLOAD\_PLUMED=on \  
-DDOWNLOAD\_EIGEN3=on \  
-DMOLFILE\_INCLUDE\_DIRS=\${VMD\_MOLFILE\_INC} \  
-DWITH\_JPEG=yes \  
-DWITH\_PNG=yes \  
-DWITH\_GZIP=yes \  
-DGPU\_API=cuda \  
-DGPU\_ARCH=sm\_60 \  
-DPKG\_OPT=on \  
-DPKG\_USER-OMP=on \  
-DPKG\_USER-INTEL=on \  
-DPKG\_GPU=on \  
-DPKG\_KOKKOS=off \  
-DPKG ASPHERE=on \  
-DPKG\_BODY=on \  
-DPKG\_CLASS2=on \  
-DPKG\_COLLOID=on \  
-DPKG\_COMPRESS=on \  
-DPKG\_CORESHELL=on \  
-DPKG\_DIPOLE=on \  
-DPKG\_GRANULAR=on \  
-DPKG\_KSPACE=on \  
-DPKG\_LATTE=on \  
-DPKG\_MANYBODY=on \  
-DPKG\_MC=on \  
-DPKG\_MESSAGE=on \  
-DPKG\_MISC=on \  
-DPKG\_MOLECULE=on \  
-DPKG\_MPIIO=on \  
-DPKG\_PERI=on \  
-DPKG\_POEMS=on \  
-DPKG\_PYTHON=on \  
-DPKG\_QEQ=on \  
-DPKG\_REPLICA=on \  
-DPKG\_RIGID=on \  
-DPKG\_SHOCK=on \  
-DPKG\_SNAP=on \  
-DPKG\_SPIN=on \  
-DPKG\_SRD=on \  
-DPKG\_USER-ATC=on \  
-DPKG\_USER-AWPMO=on \  
-DPKG\_USER-BOCS=on \  
-DPKG\_USER-CGDNA=on \  
-DPKG\_USER-CGSDK=on \  
-DPKG\_USER-COLVARS=on \  
-DPKG\_USER-DIFFRACTION=on \  
-DPKG\_USER-DPD=on \  
-DPKG\_USER-DRUDE=on \  
-DPKG\_USER-EFF=on \  
-DPKG\_USER-FEP=on \  
-DPKG\_USER-H5MD=on \  
-DPKG\_USER-LB=on \  
-DPKG\_USER-MANIFOLD=on \  
-DPKG\_USER-MEAMC=on \  
-DPKG\_USER-MESO=on \  
-DPKG\_USER-MGPT=on \  
-DPKG\_USER-MISC=on \  
-DPKG\_USER-MOFFF=on \  
-DPKG\_USER-MOLFILE=on \  
-DPKG\_USER-NETCDF=on

```
-DPKG_USER-PHONON=on \  
-DPKG_USER-PLUMED=on \  
-DPKG_USER-PTM=on \  
-DPKG_USER-QTB=on \  
-DPKG_USER-REAXC=on \  
-DPKG_USER-SCAFACOS=on \  
-DPKG_USER-SDPD=on \  
-DPKG_USER-SMD=on \  
-DPKG_USER-SMTBQ=on \  
-DPKG_USER-SPH=on \  
-DPKG_USER-TALLY=on \  
-DPKG_USER-UEF=on \  
-DPKG_USER-YAFF=on \  
-DPKG_VORONOI=on \  
-DCMAKE_LIBRARY_PATH=/local/apl/lx/cuda-9.1/lib64/stubs \  
-DCMAKE_BUILD_TYPE=Release  
  
make -j ${PARALLEL}  
#make test && make install  
make install
```

## List of Packages

ASPHERE, BODY, CLASS2, COLLOID, COMPRESS, CORESHELL, DIPOLE, GRANULAR, KSPACE, LATTE, MANYBODY, MC, MESSAGE, MISC, MOLECULE, PERI, POEMS, QEQ, REPLICIA, RIGID, SHOCK, SPIN, SNAP, SRD, PYTHON, MPIIO, VORONOI, OPT, GPU

USER-ATC, USER-AWPMD, USER-BOCS, USER-CGDNA, USER-MESO, USER-CGSDK, USER-COLVARS, USER-DIFFRACTION, USER-DPD, USER-DRUDE, USER-EFF, USER-FEP, USER-H5MD, USER-LB, USER-MANIFOLD, USER-MEAMC, USER-MGPT, USER-MISC, USER-MOFFF, USER-MOLFILE, USER-NETCDF, USER-PHONON, USER-PLUMED, USER-PTM, USER-QTB, USER-REAXC, USER-SCAFACOS, USER-SDPD, USER-SMD, USER-SMTBQ, USER-SPH, USER-TALLY, USER-UEF, USER-YAFF, USER-OMP, USER-INTEL

## Notes

- ▶ Built on ccfep, and tested on ccgpup and ccgpuv (only basic tests; make test). All the basic tests were passed successfully.
  - ▶ (Detailed tests were skipped for this version.)
- ▶ Although this version is targeting (or optimizing for) P100 (-DGPU\_ARCH=sm\_60), the compiled binary works not only on P100 nodes but also on V100 nodes.