LAMMPS 2Aug23 with GPU support

Webpage

https://www.lammps.org

Version

2Aug23

Build Environment

- GCC 12.1.1 (gcc-toolset-12)
- Intel MPI 2021.10.0
- CUDA 12.1 update 1

Files Required

- lammps-stable_2Aug2023.tar.gz
- (many packages will be downloaded in the procedure below.)

Build Procedure

```
#!/bin/sh

VERSION=2Aug23
NAME=lammps-stable_2Aug2023
INSTALL_PREFIX=/apl/lammps/2023-Aug2-CUDA

BASEDIR=/home/users/${USER}/Software/LAMMPS/${VERSION}
LAMMPS_TARBALL=${BASEDIR}/${NAME}.tar.gz

WORKDIR=/gwork/users/${USER}
LAMMPS_WORKDIR=${WORKDIR}/${NAME}

VMD_MOLFILE_INC=/home/users/${USER}/Software/VMD/1.9.4/vmd-1.9.4a57/plugins/include

GPU_ARCH=sm_80
PARALLEL=12

#------------------------------------------------------------------
umask 0022
export LANG=C
ulimit -s unlimited

module -s purge
module -s load gcc-toolset/12
module -s load intelmpi/2021.10.0
module -s load cuda/12.1u1

PYTHONEXE=/usr/bin/python3.6m
PYTHONINC=/usr/include/python3.6m

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

tar zxf ${LAMMPS_TARBALL}

cd ${NAME}
mkdir build && cd build
```

```
# Disabled PKGs:
# FFMPEG, ADIOS, MDI, VTK: noavail
# AMOEBA: GPU and FFT single version not available
# ML-HDNNP: failed to build
# ML-IAP: failed to build
# KIM: CDDL is imcompatible with GPL
# MPIIO: not maintained?
# INTEL: not necessary for gcc build

cmake ../cmake \
  -DLAMMPS_MACHINE=rccs-cuda \
  -DENABLE_TESTING=on \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_C_COMPILER=gcc \
  -DCMAKE_CXX_COMPILER=g++ \
  -DCMAKE_Fortran_COMPILER=gfortran \
  -DCMAKE_MPI_C_COMPILER=mpicc \
  -DCMAKE_MPI_CXX_COMPILER=mpicxx \
  -DCMAKE_MPI_Fortran_COMPILER=mpif90 \
  -DCMAKE_C_FLAGS_RELEASE="-O3 -DNDEBUG" \
  -DCMAKE_CXX_FLAGS_RELEASE="-O3 -DNDEBUG" \
  -DCMAKE_Fortran_FLAGS_RELEASE="-O3 -DNDEBUG" \
  -DPython_EXECUTABLE=${PYTHONEXE} \
  -DPython_INCLUDE_DIR=${PYTHONINC} \
  -DLAMMPS_EXCEPTIONS=on \
  -DBUILD_SHARED_LIBS=on \
  -DBUILD_TOOLS=on \
  -DBUILD_MPI=on \
  -DBUILD_OMP=on \
  -DBUILD_LAMMPS_GUI=off \
  -DFFT=FFTW3 \
  -DFFT_SINGLE=on \
  -DFFT_FFTW_THREADS=on \
  -DWITH_JPEG=on \
  -DWITH_PNG=on \
  -DWITH_GZIP=on \
  -DPKG_ADIOS=off \
  -DPKG_AMOEBA=off \
  -DPKG_ASPHERE=on \
  -DPKG_ATC=on \
  -DPKG_AWPMD=on \
  -DPKG_BOCS=on \
  -DPKG_BODY=on \
  -DPKG_BPM=on \
  -DPKG_BROWNIAN=on \
  -DPKG_CG-DNA=on \
  -DPKG_CG-SPICA=on \
  -DPKG_CLASS2=on \
  -DPKG_COLLOID=on \
  -DPKG_COLVARS=on \
  -DPKG_COMPRESS=on \
  -DPKG_CORESHELL=on \
  -DPKG_DIELECTRIC=on \
  -DPKG_DIFFRACTION=on \
  -DPKG_DIPOLE=on \
  -DPKG_DPD-BASIC=on \
  -DPKG_DPD-MESO=on \
  -DPKG_DPD-REACT=on \
  -DPKG_DPD-SMOOTH=on \
  -DPKG_DRUDE=on \
  -DPKG_ELECTRODE=on \
  -DPKG_EFF=on \
  -DPKG_EXTRA-COMPUTE=on \
  -DPKG_EXTRA-DUMP=on \
  -DPKG_EXTRA-FIX=on \
```

```
-DPKG_EXTRA-MOLECULE=on \
-DPKG_EXTRA-PAIR=on \
-DPKG_FEP=on \
-DPKG_GPU=on \
-DGPU_API=cuda \
-DGPU_ARCH=${GPU_ARCH} \
-DPKG_GRANULAR=on \
-DPKG_H5MD=on \
-DPKG_INTEL=off \
-DPKG_INTERLAYER=on \
-DPKG_KIM=off \
-DDOWNLOAD_KIM=off \
-DPKG_KOKKOS=off \
-DKokkos_ARCH_ZEN3=off \
-DKokkos_ENABLE_OPENMP=off \
-DPKG_KSPACE=on \
-DPKG_LATBOLTZ=on \
-DPKG_LEPTON=on \
-DPKG_MACHDYN=on \
-DDOWNLOAD_EIGEN3=on \
-DPKG_MANIFOLD=on \
-DPKG_MANYBODY=on \
-DPKG_MC=on \
-DPKG_MDI=on \
-DPKG_MEAM=on \
-DPKG_MESONT=on \
-DPKG_MGPT=on \
-DPKG_MISC=on \
-DPKG_ML-HDNNP=off \
-DDOWNLOAD_N2P2=off \
-DPKG_ML-IAP=off \
-DPKG_ML-PACE=on \
-DPKG_ML-QUIP=on \
-DDOWNLOAD_QUIP=on \
-DPKG_ML-RANN=on \
-DPKG_ML-SNAP=on \
-DPKG_MOFFF=on \
-DPKG_MOLECULE=on \
-DPKG_MOLFILE=on \
-DMOLFILE_INCLUDE_DIR=${VMD_MOLFILE_INC} \
-DPKG_MPIIO=off \
-DPKG_MSCG=on \
-DPKG_NETCDF=on \
-DPKG_OPENMP=on \
-DPKG_OPT=on \
-DPKG_ORIENT=on \
-DPKG_PERI=on \
-DPKG_PHONON=on \
-DPKG_PLUGIN=on \
-DPKG_PLUMED=on \
-DDOWNLOAD_PLUMED=on \
-DPKG_POEMS=on \
-DPKG_PTM=on \
-DPKG_PYTHON=on \
-DPKG_QEQ=on \
-DPKG_QMMM=on \
-DPKG_QTB=on \
-DPKG_REACTION=on \
-DPKG_REAXFF=on \
-DPKG_REPLICA=on \
-DPKG_RIGID=on \
-DPKG_SCAFACOS=on \
-DDOWNLOAD_SCAFACOS=on \
-DPKG_SHOCK=on \
-DPKG_SMTBQ=on \
```

```
  -DPKG_SPH=on \
  -DPKG_SPIN=on \
  -DPKG_SRD=on \
  -DPKG_TALLY=on \
  -DPKG_UEF=on \
  -DPKG_VORONOI=on \
  -DDOWNLOAD_VORO=on \
  -DPKG_VTK=off \
  -DPKG_YAFF=on \
  -DBLA_VENDOR=OpenBLAS \
  -DCMAKE_BUILD_TYPE=Release

make VERBOSE=1 -j ${PARALLEL}

export OMP_NUM_THREADS=2

#make test # need to do it separately...
make install

cp -a ../examples ${INSTALL_PREFIX}

cd ${INSTALL_PREFIX}
for f in etc/profile.d/*; do
  if [ -f $f ]; then
    ln -s $f .
  fi
done

cd lib64
if [ -f liblammps_rccs-cuda.so ]; then
  ln -s liblammps_rccs-cuda.so liblammps.so
fi
if [ -f liblammps_rccs-cuda.so.0 ]; then
  ln -s liblammps_rccs-cuda.so.0 liblammps.so.0
fi
```

List of Packages

```
ASPHERE ATC AWPMD BOCS BODY BPM BROWNIAN CG-DNA CG-SPICA CLASS2 COLLOID COLVARS COMPRESS CORESHELL DIELECTRIC DIFFRACTION DIPOLE DPD-BASIC DPD-MESO DPD-REACT DPD-SMOOTH DRUDE EFF ELECTRODE EXTRA-COMPUTE EXTRA-DUMP EXTRA-FIX EXTRA-MOLECULE EXTRA-PAIR FEP GPU GRANULAR H5MD INTERLAYER KSPACE LATBOLTZ LEPTON MACHDYN MANIFOLD MANYBODY MC MDI MEAM MESONT MGPT MISC ML-PACE ML-QUIP ML-RANN ML-SNAP MOFFF MOLECULE MOLFILE MSCG NETCDF OPENMP OPT ORIENT PERI PHONON PLUGIN PLUMED POEMS PTM PYTHON QEQ QMMM QTB REACTION REAXFF REPLICA RIGID SCAFACOS SHOCK SMTBQ SPH SPIN SRD TALLY UEF VORONOI YAFF
```

Tests

Tests were done with the following job script.

```
#!/bin/sh
#PBS -l select=1:ncpus=16:mpiprocs=8:ompthreads=1:ngpus=2
#PBS -l walltime=24:00:00

VERSION=2Aug23
NAME=lammps-stable_2Aug2023
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GPU_ARCH=sm_80
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```
PARALLEL=12

#------------------------------------------------------------------
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PYTHONEXE=/usr/bin/python3.6m
PYTHONINC=/usr/include/python3.6m

cd ${WORKDIR}
cd ${NAME}
cd build
make test # need to do it separately...
```

Copy of test logs is available at /apl/lammps/2023-Aug2-CUDA/Testing/.
Only one of the tests failed. This maybe negligible.

```
    37 - SimpleCommands (SEGFAULT)
```

Notes

- Please also check notes for CPU version.