

## LAMMPS 29Aug2024 Update 1 - CUDA

### Webpage

<https://www.lammps.org>

### Version

29Aug2024 Update 1

### Build Environment

- GCC 13.1.1 (gcc-toolset-13)
- Open MPI 4.1.6 (CUDA-aware)
- CUDA 12.4 Update 1
- GSL 2.8

### Files Required

- lammps-stable\_29Aug2024\_update1.tar.gz
- (some of files are downloaded during installation)

### Build Procedure

```
#!/bin/sh

VERSION=2024-Aug29-u1
NAME=lammps-stable_29Aug2024_update1
INSTALL_PREFIX=/apl/lammps/${VERSION}-CUDA

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

WORKDIR=/gwork/users/${USER}/lammps-cuda
LAMMPS_WORKDIR=${WORKDIR}/${NAME}

GPU_ARCH=sm_80

FFMPEG_BIN=/apl/ffmpeg/6.1/bin/ffmpeg
VMD_MOLFILE_INC=/home/users/${USER}/Software/VMD/1.9.4/vmd-1.9.4a57/plugins/include
GSL_ROOT=/apl/gsl/2.8

PARALLEL=12

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

module -s purge
module -s load gcc-toolset/13
module -s load openmpi/4.1.6/gcc13-cuda12.4u1
module -s load gsl/2.8
module -s load cuda/12.4u1

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:
# ADIOS, VTK: noavail
# GUI: to avoid complicated dependencies
# KIM: CDDL is incompatible with GPL
# INTEL: not necessary for gcc build
# ML-IAP: compilation error

cmake ../cmake \
-DLAMMPS_MACHINE=rccs-cuda \
-DENABLE_TESTING=on \
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
-DCMAKE_C_COMPILER=gcc \
-DCMAKE_CXX_COMPILER=g++ \
-DCMAKE_Fortran_COMPILER=gfortran \
-DCMAKE_MPI_C_COMPILER=mpicc \
-DCMAKE_MPI_CXX_COMPILER=mpic++ \
-DCMAKE_MPI_Fortran_COMPILER=mpif90 \
-DCMAKE_C_FLAGS_RELEASE="-O3 -DNDEBUG" \
-DCMAKE_CXX_FLAGS_RELEASE="-O3 -DNDEBUG" \
-DCMAKE_Fortran_FLAGS_RELEASE="-O3 -DNDEBUG" \
-DPython_EXECUTABLE=${PYTHONEXE} \
-DPython_INCLUDE_DIR=${PYTHONINC} \
-DGSL_ROOT_DIR=${GSL_ROOT} \
-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 \
-DWITH_FFmpeg=on \
-DFFMPEG_EXECUTABLE=${FFMPEG_BIN} \
-DPKG_ADIOS=off \
-DPKG_AMOEBA=off \
-DPKG_ASPHERE=on \
-DPKG_ATC=on \
-DPKG_AWPMO=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_EFF=on \
-DPKG_ELECTRODE=on \
```

-DPKG\_EXTRA-COMMAND=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=off \  
-DDOWNLOAD\_MDI=off \  
-DPKG\_MEAM=on \  
-DPKG\_MESONT=on \  
-DPKG\_MGPT=on \  
-DPKG\_MISC=on \  
-DPKG\_ML-HDNNP=off \  
-DDOWNLOAD\_N2P2=off \  
-DPKG\_ML-IAP=off \  
-DMLIAP\_ENABLE\_PYTHON=off \  
-DPKG\_ML-PACE=on \  
-DPKG\_ML-POD=on \  
-DPKG\_ML-QUIP=on \  
-DDOWNLOAD\_QUIP=on \  
-DPKG\_ML-RANN=on \  
-DPKG\_ML-SNAP=on \  
-DPKG\_ML-UF3=on \  
-DPKG\_MOFFF=on \  
-DPKG\_MOLECULE=on \  
-DPKG\_MOLFILE=on \  
-DMOLFILE\_INCLUDE\_DIR=\${VMD\_MOLFILE\_INC} \  
-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_RHEO=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 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
```

## Test

Submitted as a job with the job script below.

```
#!/bin/sh  
#PBS -l select=1:ncpus=16:mpiprocs=8:ompthreads=1:ngpus=2  
#PBS -l walltime=24:00:00  
  
VERSION=2024-Aug29-u1  
NAME=lammps-stable_29Aug2024_update1  
INSTALL_PREFIX=/apl/lammps/${VERSION}-CUDA  
  
BASEDIR=/home/users/${USER}/Software/LAMMPS/${VERSION}  
LAMMPS_TARBALL=${BASEDIR}/${NAME}.tar.gz  
  
WORKDIR=/gwork/users/${USER}/lammps-cuda  
LAMMPS_WORKDIR=${WORKDIR}/${NAME}  
  
GPU_ARCH=sm_80  
  
FFMPEG_BIN=/apl/ffmpeg/6.1/bin/ffmpeg  
VMD_MOLFILE_INC=/home/users/${USER}/Software/VMD/1.9.4/vmd-1.9.4a57/plugins/include  
GSL_ROOT=/apl/gsl/2.8
```

```
PARALLEL=12
```

```
#-----  
umask 0022  
export LANG=C  
ulimit -s unlimited  
  
module -s purge  
module -s load gcc-toolset/13  
module -s load openmpi/4.1.6/gcc13-cuda12.4u1  
module -s load gsl/2.8  
module -s load cuda/12.4u1  
  
PYTHONEXE=/usr/bin/python3.6m  
PYTHONINC=/usr/include/python3.6m  
  
cd ${WORKDIR}  
cd ${NAME}  
cd build  
make test # need to do it separately...
```

## Notes

- [Please check installation details of 2024Aug29](#). The procedure is almost the same. All the tests have passed successfully.