

LAMMPS 29Aug2024 Update 2 - CUDA

Webpage

<https://www.lammps.org>

Version

29Aug2024 Update 2

Build Environment

- GCC 13.3.1 (gcc-toolset-13)
- Open MPI 4.1.6 (CUDA-aware)
- CUDA 12.4 Update 1
- GSL 2.8

Files Required

- lammps-stable_29Aug2024_update2.tar.gz
- (some of files are downloaded during installation)

Build Procedure

```
#!/bin/sh

VERSION=2024-Aug29-u2
NAME=lammps-stable_29Aug2024_update2
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 test
```

```
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

Performed with this script on ccgpu.

```
#!/bin/sh
```

```
VERSION=2024-Aug29-u2
```

```
NAME=lammps-stable_29Aug2024_update2
```

```
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  
export OMP_NUM_THREADS=1  
  
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

- The procedure is the same as that for 29Aug2024 Update 1 (CUDA).
 - (Slightly newer GCC was used, though. 13.1.1 => 13.3.1)
- Test script and results are the same as those for 29Aug2024 Update 1 (CUDA). Please check following links for details.
 - [29Aug2024 CUDA version installation details and notes](#)
 - [29Aug2024 Update 1 CUDA version installation details and notes](#)