

LAMMPS 22Jul2025 - CUDA

Webpage

<https://www.lammps.org>

Version

22Jul2025

Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- Open MPI 4.1.8 (CUDA-aware)
- GSL 2.8
- OpenBLAS 0.3.29
- CUDA 12.8 Update 1

Files Required

- lammps-stable_22Jul2025.tar.gz
- (some files will be downloaded during building process.)

Build Procedure

```
#!/bin/sh

VERSION=2025-Jul22
NAME=lammps-stable_22Jul2025
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}

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

GPU_ARCH=sm_80
PARALLEL=12

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

module -s purge
module -s load gcc-toolset/10
module -s load openmpi/4.1.8/gcc13-cuda12.8u1
module -s load gsl/2.8
module -s load openblas/0.3.29-lp64
module -s load cuda/12.8u1

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 xzf ${LAMMPS_TARBALL}

cd ${NAME}

# for FFT_SINGLE=on
sed -i -e '26i#include "force.h"' unittest/force-styles/test_fix_timestep.cpp
sed -i -e '29i#include "kspace.h"' unittest/force-styles/test_pair_style.cpp

# pass python exe path to MDI cmake
sed -i -e "59i\ -DPython_EXECUTABLE=${PYTHONEXE}" cmake/Modules/Packages/MDI.cmake
mkdir build && cd build

# Disabled PKGs:
# ADIOS, VTK: noavail
# GUI: manually disabled
# KIM: to avoid dependence to libkim-api.so.2
# INTEL: not necessary for gcc build

cmake ../cmake \
-DLAMMPS_MACHINE=rccs-cuda \
-DENABLE_TESTING=on \
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
-DCMAKE_C_COMPILER=mpicc \
-DCMAKE_CXX_COMPILER=mpicxx \
-DCMAKE_Fortran_COMPILER=mpif90 \
-DCMAKE_C_FLAGS_RELEASE="-O3 -DNDEBUG" \
-DCMAKE_CXX_FLAGS_RELEASE="-O3 -DNDEBUG" \
-DCMAKE_Fortran_FLAGS_RELEASE="-O3 -DNDEBUG" \
-DPython_EXECUTABLE=${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 \
-DBUILD_WHAM=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_APIP=on \
-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 \
-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 \
-DDOWNLOAD_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-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 \
-DBLA_PREFER_PKGCONFIG=on \
-DCMAKE_BUILD_TYPE=Release

```

```

#make -j ${PARALLEL}
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

```

Tests

Tests were performed on ccgpu (equipped with A30) using this script.

```

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```

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/10
module -s load openmpi/4.1.8/gcc13-cuda12.8u1
module -s load gsl/2.8
module -s load openblas/0.3.29-lp64
module -s load cuda/12.8u1

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

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

```

Test Results

- 38 SimpleCommands failed.
 - [FATAL] /gwork/.../gtest-port.cc:1155:: Only one stdout capturer can exist at a time.
 - There were no errors other than this. However, many tests were skipped.

Installed packages

```

AMOEBA APIP 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-COMMAND EXTRA-COMPUTE
EXTRA-DUMP EXTRA-FIX EXTRA-MOLECULE EXTRA-PAIR FEP GRANULAR H5MD INTERLAYER
KOKKOS KSPACE LATBOLTZ LEPTON MACHDYN MANIFOLD MANYBODY MC MDI MEAM MESONT
MGPT MISC ML-HDNNP ML-PACE ML-POD ML-QUIP ML-RANN ML-SNAP ML-UF3 MOFFF
MOLECULE MOLFILE NETCDF OPENMP OPT ORIENT PERI PHONON PLUGIN PLUMED POEMS PTM
PYTHON QEQ QMMM QTB REACTION REAXFF REPLICAS RHEO RIGID SCAFACOS SHOCK SMTBQ
SPH SPIN SRD TALLY UEF VORONOI YAFF

```

Notes

- Except for GPU related points, it is basically the same as [the GCC version](#).