

LAMMPS 22Jul2025 - CUDA

ウェブページ

<https://www.lammps.org>

バージョン

22Jul2025 Update 1

ビルド環境

- 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

ビルドに必要なファイル

- lammps-stable_22Jul2025_update1.tar.gz
- (一部ファイルは以下スクリプト中で取得)

ビルド手順

```
#!/bin/sh

VERSION=2025-Jul22-u1
NAME=lammps-stable_22Jul2025_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}

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 mkl/2023.2.0
module -s load openblas/0.3.29-lp64
module -s load cuda/12.8u1

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

mkdir -p ${WORKDIR}
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_ASPIRE=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
```

テスト

以下のスクリプトでジョブとして実行

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

VERSION=2025-Jul22-u1
NAME=lammps-stable_22Jul2025_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
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...

```

テスト結果

- 38 SimpleCommands でエラー。
 - [FATAL] /gwork/.../gtest-port.cc:1155:: Only one stdout capturer can exist at a time.
 - 他はエラーが無いが、多くは skip されている。
 - (2025-Jul22(CUDA)と同じ結果です)

有効なパッケージ

```

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 GPU GRANULAR H5MD
INTERLAYER KSPACE LATBOLTZ LEPTON MACHDYN MANIFOLD MANYBODY MC MDI MEAM MESONT
MGPT MISC 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 REPLICA RHEO RIGID SCAFACOS SHOCK SMTBQ SPH SPIN SRD TALLY
UEF VORONOI YAFF

```

メモ

- 22Jul2025(CUDA) と同じ手順でビルドしています。テスト結果にも特段の違いは見られません。