LAMMPS 22Jul2025

Webpage

https://www.lammps.org

Version

22Jul2025

Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- Intel MPI 2021.16
- GSL 2.8
- OpenBLAS 0.3.29

Files Required

- lammps-stable_22Jul2025.tar.gz
- n2p2-2.2.0.tar.gz
- (some of files downloaded during the build)

Build Procedure

n2p2-2.2.0 (briefly)

```
$ module -s purge
$ module -s load gcc-toolset/10
$ module -s load intelmpi/2021.16
$ module -s load gsl/2.8
$ cd /apl/lammps/2025-Jul22
$ tar xf n2p2-2.2.0.tar.gz
$ cd n2p2-2.2.0/src
$ make INTERFACES=LAMMPS COMP=gnu PROJECT_CC=g++ PROJECT_MPICC=mpicxx PROJECT_CFLAGS="-O3 -march=native -std=c++11 -fPIC"
APP_CORE=nnp-convert APP_TRAIN=nnp-train APP=nnp-convert -j8
```

- automatic build of n2p2 (-DDOWNLOAD_N2P2=on) does not work. It does not work even when editing cmake files, so n2p2 was installed it manually.
- same procedure as 29Aug2024

lammps

```
#!/bin/sh

VERSION=2025-Jul22
NAME=lammps-stable_22Jul2025
INSTALL_PREFIX=/apl/lammps/${VERSION}

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

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

FFMPEG_BIN=/apl/ffmpeg/6.1/bin/ffmpeg
VMD_MOLFILE_INC=/home/users/${USER}/Software/VMD/1.9.4/vmd-1.9.4a57/plugins/include
GSL_ROOT=/apl/gsl/2.8
N2P2_ROOT=${INSTALL_PREFIX}/n2p2-2.2.0

PARALLEL=12

#------------------------------------------------------------------
umask 0022
export LANG=C
```

```
ulimit -s unlimited

module -s purge
module -s load gcc-toolset/10
module -s load intelmpi/2021.16
module -s load gsl/2.8
#module -s load mkl/2023.2.0
module -s load openblas/0.3.29-lp64

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 ${NAME}
# for FFT_SINGLE=on
sed -i -e '26i#include "force.h"' unittest/force-styles/test_fix_timestep.cpp
sed -i -e '29i#include "kspace.h"' unittest/force-styles/test_pair_style.cpp
# pass python exe path to MDI cmake
sed -i -e "59i\    -DPython_EXECUTABLE=${PYTHONEXE}" cmake/Modules/Packages/MDI.cmake
mkdir build && cd build

# Disabled PKGs:
# ADIOS, VTK: noavail
# KIM: to avoid unfavorable dependence to libkim-api.so.2
# ML-IAP: compilation error
# INTEL: not necessary for gcc build

cmake ../cmake \
 -DLAMMPS_MACHINE=rccs \
 -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=on \
 -DBUILD_WHAM=on \
 -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=on \
 -DPKG_APIP=on \
 -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_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=off \
-DPKG_GRANULAR=on \
-DPKG_H5MD=on \
-DPKG_INTEL=off \
-DPKG_INTERLAYER=on \
-DPKG_KIM=off \
-DDOWNLOAD_KIM=off \
-DPKG_KOKKOS=on \
-DKokkos_ARCH_ZEN3=on \
-DKokkos_ENABLE_OPENMP=on \
-DFFT_KOKKOS=FFTW3 \
-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=on \
-DDOWNLOAD_N2P2=off \
-DN2P2_DIR=${N2P2_ROOT} \
-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.so ]; then
 ln -s liblammps_rccs.so liblammps.so
fi
if [ -f liblammps_rccs.so.0 ]; then
 ln -s liblammps_rccs.so.0 liblammps.so.0
fi
```

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 REPLICA RHEO RIGID SCAFACOS SHOCK SMTBQ
SPH SPIN SRD TALLY UEF VORONOI YAFF

Test Results

Following tests of lammps were failed. Copy of test log is available in /apl/lammps/2025-Jul22/Testing.

- 38:SimpleCommands => Quit test failed.
- 54:LibraryProperties => memory_usage test failed.
  - meminfo[1] was used for the failed test. It should be meminfo[2] or some other?
- 72:FortranProperties => same as 54:LibraryProperties

Following tests containing "lattice" command in the input failed with somewhat large numerical error.

- AtomicPairStyle:
  - buck_coul_cut_qeq_point, buck_coul_cut_qeq_shielded, edip, lepton_sphere, lj_cut_sphere, lj_expand_sphere, meam_sw_spline, pedone, reaxff-acks2, reaxff-acks2_efield, reaxff-qtpie, reaxff, reaxff_lgvdw, reaxff_noqeq, reaxff_tabulate, reaxff_tabulate_flag
- KSpaceStyle:
  - scafacos_direct, scafacos_ewald, scafacos_fmm, scafacos_fmm_tuned, scafacos_p2nfft

Minor numerical errors occurred on following tests.

- 333:ManybodyPairStyle:ilp-graphene-hbn
- 334:ManybodyPairStyle:ilp-graphene-hbn_notaper
- 435:KSpaceStyle:pppm_ad
- 436:KSpaceStyle:pppm_cg
- 437:KSpaceStyle:pppm_cg_ad
- 438:KSpaceStyle:pppm_cg_tiled
- 455:KSpaceStyle:pppm_tip4p
- 592:DihedralStyle:quadratic
- 594:DihedralStyle:table_cut_linear
- 596:DihedralStyle:table_linear

Notes

- ADIOS, VTK were not verified. INTEL may not be useful when GCC is employed.
- GUI is enabled for this build.
- To avoid dependence on libkim-api.so.2 at runtime, KIM was disabled.
- Compilation error occurred when ML-IAP was enabled.
- Build of unit tests (test_fix_timestep.cpp & test_pair_style.cpp in force-styles) failed when FFT_SINGLE is enabled.
  - One header file was added for each to pass the build. (Please see "sed" lines in the procedure above.)
- Python of MDI was added to MDI cmake file. (Otherwise, python2 was chosen and the build failed.)
- -DDOWNLOAD_N2P2=on does not work. The reason is not yet identified.。
  - $(shell ...) might be the problem...
- gcc10 version shows slightly better performance then gcc13, gcc14. (The performance was compared using in.rhodo (replicate 2 2 2) test.)