LAMMPS 22Jul2025 - Intel

Webpage

https://www.lammps.org

Version

22Jul2025

Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- oneAPI Compiler 2025.2.0
- Intel MPI 2021.16
- GSL 2.8
- MKL 2025.2.0

Files Required

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

Build Procedure

```
#!/bin/sh

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

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

PARALLEL=12

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

module -s purge

. ~/intel/oneapi/compiler/latest/env/vars.sh # 2025.2.0

module -s load gcc-toolset/10
module -s load compiler-rt/2025.2.0
module -s load intelmpi/2021.16
module -s load gsl/2.8
module -s load mkl/2025.2.0

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 ${NAME}
sed -i -e "s/xHost/march=core-avx2/" \
     -e "s/-fp-model precise//" cmake/CMakeLists.txt
sed -i -e '26i#include "force.h"' unittest/force-styles/test_fix_timestep.cpp
sed -i -e '29i#include "kspace.h"' unittest/force-styles/test_pair_style.cpp
sed -i -e "59i\    -DPython_EXECUTABLE=${PYTHONEXE}" cmake/Modules/Packages/MDI.cmake
mkdir build && cd build

# Disabled PKGs:
# ADIOS, VTK: noavail
# QUIP: The IntelLLVM Fortran compiler is not (yet) supported for building QUIP
# KIM: to remove dependence on libkim-api.so.2
# KOKKOS: to avoid performance degradation of intel package
# SCAFACOS: comiplation problem regarding gfortran?

cmake ../cmake \
 -DLAMMPS_MACHINE=rccs \
 -DENABLE_TESTING=on \
 -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
 -DCMAKE_C_COMPILER=mpiicx \
 -DCMAKE_CXX_COMPILER=mpiicpx \
 -DCMAKE_Fortran_COMPILER=mpiifx \
 -DCMAKE_C_FLAGS_RELEASE="-O3 -DNDEBUG -march=core-avx2" \
 -DCMAKE_CXX_FLAGS_RELEASE="-O3 -DNDEBUG -march=core-avx2" \
 -DCMAKE_Fortran_FLAGS_RELEASE="-O3 -DNDEBUG -march=core-avx2" \
 -DPython_EXECUTABLE=${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=MKL \
 -DFFT_SINGLE=on \
 -DFFT_MKL_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=on \
-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=off \
-DDOWNLOAD_QUIP=off \
-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=off \
 -DDOWNLOAD_SCAFACOS=off \
 -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 \
 -DBLAS_LIBRARIES="-qmkl" \
 -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 INTEL
INTERLAYER KSPACE LATBOLTZ LEPTON MACHDYN MANIFOLD MANYBODY MC MDI MEAM MESONT
MGPT MISC ML-PACE ML-POD 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 SHOCK SMTBQ SPH SPIN SRD TALLY UEF VORONOI
YAFF
```

Test Results

Following tests have failed. Copy of test log is available in /apl/lammps/2025-Jul22-intel/Testing.
Please also check results of GCC version.

- 14:AtomStyles => body_nparticle: something worng with quarternion?
- 38:SimpleCommands => Quit test failed.
- 40:Groups => VariableFunctions: numerical error

- 54:LibraryProperties => same error as GCC version
- 72:FortranProperties => same error as 54:LibraryProperties. GCC version also failed with the same error.

Following tests failed with "free(): invalid pointer". No further details available now.

- 55:LibraryObjects
- 84:PythonCommands
- 270:AtomicPairStyle:eam_alloy
- 271:AtomicPairStyle:eam_alloy_real
- 275:AtomicPairStyle:eam_fs
- 276:AtomicPairStyle:eam_fs_real

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

Large numerical errors found in following tests. There should be something wrong.

- 337:ManybodyPairStyle:lcbop
- 383:BondStyle:harmonic_restrain

Minor numerical errors found for following tests.

- 130:MolPairStyle:coul_shield
- 219:MolPairStyle:lj_pirani
- 244:MolPairStyle:python_hybrid
- 291:AtomicPairStyle:meam_2nn
- 294:AtomicPairStyle:meam_spline
- 332:ManybodyPairStyle:ilp-graphene-hbn
- 333:ManybodyPairStyle:ilp-graphene-hbn_notaper
- 336:ManybodyPairStyle:kolmogorov_crespi_z
- 350:ManybodyPairStyle:polymorphic_sw
- 353:ManybodyPairStyle:rann
- 380:BondStyle:gaussian
- 384:BondStyle:harmonic_shift
- 397:AngleStyle:charmm
- 434:KSpaceStyle:pppm_ad
- 435:KSpaceStyle:pppm_cg
- 436:KSpaceStyle:pppm_cg_ad
- 437:KSpaceStyle:pppm_cg_tiled
- 454:KSpaceStyle:pppm_tip4p
- 455:KSpaceStyle:pppm_tip4p_ad
- 476:FixTimestep:deform_tri
- 502:FixTimestep:npt_iso
- 513:FixTimestep:nvt-psllod
- 514:FixTimestep:nvt-sllod
- 526:FixTimestep:recenter-init
- 535:FixTimestep:rigid_npt_small
- 565:FixTimestep:wall_lj1043_const
- 569:FixTimestep:wall_reflect
- 570:FixTimestep:wall_region_harmonic
- 571:FixTimestep:wall_region_lj1043
- 572:FixTimestep:wall_region_lj126
- 573:FixTimestep:wall_region_lj93
- 574:FixTimestep:wall_region_morse
- 575:FixTimestep:wall_region_sphere
- 591:DihedralStyle:quadratic
- 593:DihedralStyle:table_cut_linear

Notes

- Please also check test results and notes of GCC version.
- GCC version may be better than this one if you do not plan to use INTEL package.

- To prevent performance degradation of INTEL package, "-fp-model precise" option was removed.
  - "-fp-model precise" is the default setting for clang. However, this is not the default setting for Intel LLVM compilers ("-fp-model fast" is the default).
  - If "-fp-model precise" is employed, the performance improvement by INTEL package is significantly decreased.
    - Kokkos is also disabled, since enabling Kokkos_ARCH_ZEN3 will reduce the performance improvement by INTEL package.
  - NOTE: "-fp-model fast=2" was employed for Intel Classic Compilers.