

LAMMPS 22Jul2025 Update 1 - Intel

Webpage

<https://www.lammps.org>

Version

22Jul2025 Update 1

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_update1.tar.gz
- (some of files will be downloaded in the procedure below)

Build Procedure

```
#!/bin/sh

VERSION=2025-Jul22-u1
NAME=lammps-stable_22Jul2025_update1
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 xzf ${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: compilation 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_AWPMMD=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="-qmkI" \
-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 Result

Copy of test log can be found in /apl/lammps/2025-Jul22-u1-intel/Testing.

✕

- [Same build procedure as 22Jul2025\(intel\)](#). No particular changes were observed in the test results.

