

## LAMMPS 29Aug2024 Update 1 - Intel

### Webpage

<https://www.lammps.org>

### Version

29Aug2024 Update 1

### Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- Intel oneAPI Compiler 2023.2.0
- Intel MKL 2023.2.0
- Intel MPI 2021.10.0
- GSL 2.8

### Files Required

- lammps-stable\_29Aug2024\_update1.tar.gz
- (some of files are downloaded during the installation)

### Build Procedure

```
#!/bin/sh

VERSION=2024-Aug29-u1
NAME=lammps-stable_29Aug2024_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 # intel 2023.2.0
module -s load gcc-toolset/10
module -s load compiler-rt/2023.2.0
module -s load intelmpi/2021.10.0
module -s load mkl/2023.2.0
module -s load gsl/2.8

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/" cmake/CMakeLists.txt
mkdir build && cd build

cmake ../cmake \
-DLAMMPS_MACHINE=rccs \
-DENABLE_TESTING=on \
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
-DCMAKE_C_COMPILER=icx \
-DCMAKE_CXX_COMPILER=icpx \
-DCMAKE_Fortran_COMPILER=ifx \
-DCMAKE_MPI_C_COMPILER=mpiicx \
-DCMAKE_MPI_CXX_COMPILER=mpicpx \
-DCMAKE_MPI_Fortran_COMPILER=mpiifx \
-DCMAKE_C_FLAGS_RELEASE="-O3 -DNDEBUG -march=core-avx2" \
-DCMAKE_CXX_FLAGS_RELEASE="-O3 -DNDEBUG -march=core-avx2" \
-DCMAKE_Fortran_FLAGS_RELEASE="-O3 -DNDEBUG -march=core-avx2" \
-DPython_EXECUTABLE=${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=off \
-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_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=off \  
-DPKG\_GRANULAR=on \  
-DPKG\_H5MD=on \  
-DPKG\_INTEL=on \  
-DPKG\_INTERLAYER=on \  
-DPKG\_KIM=off \  
-DDOWNLOAD\_KIM=off \  
-DPKG\_KOKKOS=off \  
-DKokkos\_ARCH\_ZEN3=off \  
-DKokkos\_ENABLE\_OPENMP=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=off \  
-DDOWNLOAD\_MDI=off \  
-DPKG\_MEAM=on \  
-DPKG\_MESONT=on \  
-DPKG\_MGPT=on \  
-DPKG\_MISC=on \  
-DPKG\_ML-HDNNP=off \  
-DDOWNLOAD\_N2P2=off \  
-DPKG\_ML-IAP=off \  
-DMLIAP\_ENABLE\_PYTHON=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=off \  
-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=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 \  
-DBLAS_LIBRARIES="-qmk!" \  
-DCMAKE_BUILD_TYPE=Release  
  
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
```

## Notes

- [Please check installation details about 2024Aug29](#). The procedure and the results are almost the same as that version.
- Test "282 - AtomicPairStyle:meam\_2nn" passed in this version.