

LAMMPS 29Aug2024 Update 3 - Intel

Webpage

<https://www.lammps.org>

Version

29Aug2024 Update 3

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_update3.tar.gz
- (some of files are downloaded during the installation)

Build Procedure

```
#!/bin/sh

VERSION=2024-Aug29-u3
NAME=lammps-stable_29Aug2024_update3
INSTALL_PREFIX=/apl/lammps/${VERSION}-intel
#INSTALL_PREFIX=/home/users/qf7/Software/LAMMPS/${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 2023.2.0
. ~/intel/oneapi/compiler/latest/env/vars.sh

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_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=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 \

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-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="-qmkl" \
-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

- The procedure is the same as that for 29Aug2024 Update 2 (intel compiler version).
 - [29Aug2024 \(intel\) installation details and notes](#)
 - [29Aug2024 Update 1 \(intel\) installation details and notes](#)
 - [29Aug2024 Update 2 \(intel\) installation details and notes](#)
- Following test failed on Update 2 have passed.
 - 85 - PythonPyLammps
 - Copy of test result is available on [/apl/lammps/2024-Aug29-u3-intel/Testing/](#).