LAMMPS 29Aug2024 Update 1

Webpage

https://www.lammps.org

Version

29Aug2024 Update 1

Build Environment

- GCC 13.1.1 (gcc-toolset-13)
- Intel MPI 2021.13
- GSL 2.8

Files Required

- lammps-stable_29Aug2024_update1.tar.gz
- (N2P2 and MDI for 29Aug2024 are also used for this build.)
- (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}

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
MDI_ROOT=/apl/lammps/2024-Aug29/mdi-1.4.29
N2P2_ROOT=/apl/lammps/2024-Aug29/n2p2-2.2.0

if [ ! -f ${INSTALL_PREFIX}/mdi-1.4.29 ]; then
 ln -s ${MDI_ROOT} ${INSTALL_PREFIX}/mdi-1.4.29
fi
if [ ! -f ${INSTALL_PREFIX}/n2p2-2.2.0 ]; then
 ln -s ${N2P2_ROOT} ${INSTALL_PREFIX}/n2p2-2.2.0
fi

PARALLEL=12

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

module -s purge
module -s load gcc-toolset/13
module -s load intelmpi/2021.13
module -s load gsl/2.8

PYTHONEXE=/usr/bin/python3.6m
PYTHONINC=/usr/include/python3.6m

export CPATH="${MDI_ROOT}/include/mdi:${CPATH}"
```

```
export LIBRARY_PATH="${MDI_ROOT}/lib64/mdi:${LIBRARY_PATH}"
export LD_LIBRARY_PATH="${MDI_ROOT}/lib64/mdi:${LD_LIBRARY_PATH}"

cd ${WORKDIR}
if [ -d ${NAME} ]; then
 mv ${NAME} lammps_erase
 rm -rf lammps_erase &
fi

tar zxf ${LAMMPS_TARBALL}

cd ${NAME}
mkdir build && cd build

# Disabled PKGs:
# ADIOS, VTK: noavail
# GUI: to avoid complicated dependecies
# KIM: CDDL is imcompatible with GPL
# INTEL: not necessary for gcc build
# ML-IAP: compilation error

cmake ../cmake \
 -DLAMMPS_MACHINE=rccs \
 -DENABLE_TESTING=on \
 -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
 -DCMAKE_C_COMPILER=gcc \
 -DCMAKE_CXX_COMPILER=g++ \
 -DCMAKE_Fortran_COMPILER=gfortran \
 -DCMAKE_MPI_C_COMPILER=mpicc \
 -DCMAKE_MPI_CXX_COMPILER=mpicxx \
 -DCMAKE_MPI_Fortran_COMPILER=mpif90 \
 -DCMAKE_C_FLAGS_RELEASE="-O3 -DNDEBUG" \
 -DCMAKE_CXX_FLAGS_RELEASE="-O3 -DNDEBUG" \
 -DCMAKE_Fortran_FLAGS_RELEASE="-O3 -DNDEBUG" \
 -DPython_EXECUTABLE=${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=off \
  -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_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 \
-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=off \
-DPKG_MEAM=on \
-DPKG_MESONT=on \
-DPKG_MGPT=on \
-DPKG_MISC=on \
-DPKG_ML-HDNNP=on \
-DDOWNLOAD_N2P2=off \
-DN2P2_DIR=${N2P2_ROOT} \
-DPKG_ML-IAP=off \
-DMLIAP_ENABLE_PYTHON=off \
-DPKG_ML-PACE=on \
-DPKG_ML-POD=on \
-DPKG_ML-QUIP=on \
-DDOWNLOAD_QUIP=on \
-DPKG_ML-RANN=on \
-DPKG_ML-SNAP=on \
-DPKG_ML-UF3=on \
-DPKG_MOFFF=on \
-DPKG_MOLECULE=on \
-DPKG_MOLFILE=on \
 -DMOLFILE_INCLUDE_DIR=${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 \
 -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.
- Regarding test results, compared to 2024Aug29, "282 - AtomicPairStyle:meam_2nn" passed but "427 - KSpaceStyle:pppm_dielectric" failed. Test log is available in /apl/lammps/2024-Aug29-u1/Testing.
    - "427 - KSpaceStyle:pppm_dielectric" was not verified in case of 2024Aug29 test. The unchecked test was verified and failed in this version.