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 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 Result

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

メモ

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