

## LAMMPS 23Jun22 (Intel MPI)

### Webpage

<https://www.lammps.org>

### Version

23Jun22 Update 2

### Build Environment

- Intel oneAPI Compiler Classic 2023.1.0
- Intel MKL 2023.1.0
- Intel MPI 2021.9.0

### Files Required

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

### Build Procedure

```
#!/bin/sh

VERSION=23Jun22
NAME=lammps-23Jun2022
INSTALL_PREFIX=/apl/lammps/2022-Jun23-impi

BASEDIR=/home/users/${USER}/Software/LAMMPS/${VERSION}
LAMMPS_TARBALL=${BASEDIR}/lammps-stable.tar.gz

WORKDIR=/gwork/users/${USER}
LAMMPS_WORKDIR=${WORKDIR}/${NAME}

VMD_MOLFILE_INC=/home/users/${USER}/Software/VMD/1.9.4/vmd-1.9.4a57/plugins/include

PARALLEL=12

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

# load intel env (2023.1.0)
. ~/intel/oneapi/compiler/latest/env/vars.sh

module -s purge
module -s load intelmpi/2021.9.0
module -s load mkl/2023.1.0

export CC=mpiicc
export CXX=mpiicpc
export FC=mpiifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export MPIFC=mpiifort

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

cd ${WORKDIR}
if [ -d ${NAME} ]; then
  mv ${NAME} lammps_erase
```

```
rm -rf lammmps_erase &
fi

tar zxf ${LAMMPS_TARBALL}

cd ${NAME}
sed -i -e "s/xHost/march=core-avx2/" cmake/CMakeLists.txt
mkdir build && cd build

# Disabled PKGs:
# FFMPEG, ADIOS, MDI, VTK: noavail
# MSCG: gsl too old
# MESSAGE: ZeroMQ support not enabled
# QUIP: failed to build
# ML-HDNNP: failed to build
# ML-IAP: failed to build
# KIM: CDDL is imcompatible with GPL
# LATTE: technical problem of cmake? (LAPACK and BLAS)
# MPIIO: not maintained?

cmake ../cmake \
-DLAMMPS_MACHINE=rccs \
-DENABLE_TESTING=on \
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
-DCMAKE_C_COMPILER=mpiicc \
-DCMAKE_CXX_COMPILER=mpiicpc \
-DCMAKE_Fortran_COMPILER=mpiifort \
-DCMAKE_MPI_C_COMPILER=mpiicc \
-DCMAKE_MPI_CXX_COMPILER=mpiicpc \
-DCMAKE_MPI_Fortran_COMPILER=mpiifort \
-DPython_EXECUTABLE=${PYTHONEXE} \
-DPython_INCLUDE_DIR=${PYTHONINC} \
-DLAMMPS_EXCEPTIONS=on \
-DBUILD_SHARED_LIBS=on \
-DBUILD_TOOLS=on \
-DBUILD_MPI=on \
-DBUILD_OMP=on \
-DFFT=MKL \
-DFFT_SINGLE=on \
-DFFT_MKL_THREADS=on \
-DWITH_JPEG=yes \
-DWITH_PNG=yes \
-DWITH_GZIP=yes \
-DPKG_ASPHERE=on \
-DPKG_ATC=on \
-DPKG_AWPMO=on \
-DPKG_BOCS=on \
-DPKG_BODY=on \
-DPKG_BROWNIAN=on \
-DPKG_CG-DNA=on \
-DPKG_CG-SDK=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\_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=no \  
-DPKG\_KOKKOS=on \  
-DKokkos\_ARCH\_ZEN3=yes \  
-DKokkos\_ENABLE\_OPENMP=yes \  
-DPKG\_KSPACE=on \  
-DPKG\_LATBOLTZ=on \  
-DPKG\_MACHDYN=on \  
-DDOWNLOAD\_EIGEN3=on \  
-DPKG\_MANIFOLD=on \  
-DPKG\_MANYBODY=on \  
-DPKG\_MC=on \  
-DPKG\_MDI=off \  
-DPKG\_MEAM=on \  
-DPKG\_MESONT=on \  
-DPKG\_MESSAGE=on \  
-DPKG\_MGPT=on \  
-DPKG\_MISC=on \  
-DPKG\_ML-HDNNP=off \  
-DDOWNLOAD\_N2P2=no \  
-DPKG\_ML-IAP=off \  
-DPKG\_ML-PACE=on \  
-DPKG\_ML-QUIP=off \  
-DDOWNLOAD\_QUIP=no \  
-DPKG\_ML-RANN=on \  
-DPKG\_ML-SNAP=on \  
-DPKG\_MOFFF=on \  
-DPKG\_MOLECULE=on \  
-DPKG\_MOLFILE=on \  
-DMOLFILE\_INCLUDE\_DIR=\${VMD\_MOLFILE\_INC} \  
-DPKG\_MPIIO=off \  
-DPKG\_MSCG=off \  
-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=yes \  
-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\_RIGID=on \  
-DPKG\_SCAFACOS=on \  
-DDOWNLOAD\_SCAFACOS=yes \  
-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=yes \  
-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 # will put error...  
make install  
  
cp -a ../examples ${INSTALL_PREFIX}  
  
cd ${INSTALL_PREFIX}  
for f in etc/profile.d/*; do  
  ln -s $f .  
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
```

## Test Result

### List of failed tests:

```
The following tests FAILED:  
 11 - AtomStyles (Failed)  
 35 - SimpleCommands (SEGFAULT)  
 38 - Regions (Subprocess aborted)  
 43 - ComputeGlobal (Failed)  
 95 - MolPairStyle:coul_diel (Failed)  
101 - MolPairStyle:coul_shield (Failed)  
103 - MolPairStyle:coul_slater_long (Failed)  
138 - MolPairStyle:lj_class2_soft (Failed)  
153 - MolPairStyle:lj_cut_soft (Failed)  
159 - MolPairStyle:lj_expand_coul_long (Failed)  
172 - MolPairStyle:lj_sdk_coul_long (Failed)  
173 - MolPairStyle:lj_sdk_coul_table (Failed)  
177 - MolPairStyle:lj_switch3_coulgauss_long (Failed)  
201 - MolPairStyle:tip4p_long_soft (Failed)  
204 - MolPairStyle:wf_cut (Failed)  
212 - AtomicPairStyle:buck_coul_cut_qeq_point (Failed)  
213 - AtomicPairStyle:buck_coul_cut_qeq_shielded (Failed)  
230 - AtomicPairStyle:edip (Failed)  
237 - AtomicPairStyle:meam (Failed)  
238 - AtomicPairStyle:meam_spline (Failed)  
239 - AtomicPairStyle:meam_sw_spline (Failed)  
242 - AtomicPairStyle:reaxff-acks2 (Failed)  
243 - AtomicPairStyle:reaxff-acks2_efield (Failed)  
244 - AtomicPairStyle:reaxff (Failed)  
245 - AtomicPairStyle:reaxff_lgvdw (Failed)  
246 - AtomicPairStyle:reaxff_noqeq (Failed)
```

247 - AtomicPairStyle:reaxff\_tabulate (Failed)  
248 - AtomicPairStyle:reaxff\_tabulate\_flag (Failed)  
265 - ManybodyPairStyle:comb (Failed)  
273 - ManybodyPairStyle:ilp-graphene-hbn (Failed)  
274 - ManybodyPairStyle:ilp-graphene-hbn\_notaper (Failed)  
278 - ManybodyPairStyle:lcbop (Failed)  
287 - ManybodyPairStyle:pace\_product (Failed)  
288 - ManybodyPairStyle:pace\_recursive (Failed)  
300 - ManybodyPairStyle:tersoff (Failed)  
305 - ManybodyPairStyle:tersoff\_shift (Failed)  
315 - BondStyle:gaussian (Failed)  
358 - KSpaceStyle:ewald\_tri (Failed)  
360 - KSpaceStyle:pppm\_ad (Failed)  
361 - KSpaceStyle:pppm\_cg (Failed)  
363 - KSpaceStyle:pppm\_cg\_tiled (Failed)  
370 - KSpaceStyle:pppm\_disp\_tip4p (Failed)  
378 - KSpaceStyle:pppm\_tip4p (Failed)  
383 - KSpaceStyle:scafacos\_direct (Failed)  
384 - KSpaceStyle:scafacos\_ewald (Failed)  
385 - KSpaceStyle:scafacos\_fmm (Failed)  
386 - KSpaceStyle:scafacos\_fmm\_tuned (Failed)  
387 - KSpaceStyle:scafacos\_p2nfft (Failed)  
388 - FixTimestep:adapt\_coul (Failed)  
391 - FixTimestep:addforce\_const (Failed)  
393 - FixTimestep:addtorque\_const (Failed)  
412 - FixTimestep:nph (Failed)  
413 - FixTimestep:nph\_sphere (Failed)  
415 - FixTimestep:npt\_iso (Failed)  
416 - FixTimestep:npt\_sphere\_aniso (Failed)  
417 - FixTimestep:npt\_sphere\_iso (Failed)  
441 - FixTimestep:rigid\_npt\_small (Failed)  
455 - FixTimestep:smd\_couple (Failed)  
463 - FixTimestep:temp\_csld (Failed)  
484 - DihedralStyle:table\_cut\_linear (Failed)  
486 - DihedralStyle:table\_linear (Failed)  
487 - DihedralStyle:table\_spline (Failed)  
497 - ImproperStyle:inversion\_harmonic (Failed)

## Notes

- Python 3.6 is employed instead of python 3.9. NETCDF is enabled in this version, while ML-IAP is disabled to avoid compilation error.
- In case of OpenMPI build, there is significant performance degradation in LJ system. This version is free from that issue.
  - In the problematic case, "Comm" spends 10 or more times than "Pair" according to timing statistics.
  - "intel" package seems bit unstable, while Intel MPI is employed...