

## LAMMPS 29Sep21

### Webpage

<https://www.lammps.org>

### Version

29Sep21

### Build Environment

- Intel oneAPI Compiler Classic 2022.2.1
- Intel MKL 2022.2.1
- HPC-X 2.13.1 (Open MPI 4.1.5)

### Files Required

- lammps-stable\_29Sep2021.tar.gz
- (some of files will be downloaded during the installation)

### Build Procedure

#### conda environment

When python 3.9 of the system is used, compilation of lammps failed with strange error.

We thus make conda (miniforge) environment in /apl/lammps/2021-Sep29/.

The detailed installation procedure is lost... yaml, scipy, numpy, pandas, mpi4py, mkl, cython and many other packages are installed.

#### lammps

```
#!/bin/sh

VERSION=29Sep21
NAME=lammps-stable_29Sep2021
INSTALL_PREFIX=/apl/lammps/2021-Sep29

BASEDIR=/home/users/${USER}/Software/LAMMPS/${VERSION}
LAMMPS_TARBALL=${BASEDIR}/${NAME}.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

module purge

# load intel compiler (onapi 2022.3.1, compiler 2022.2.1)
. ~/intel/oneapi/compiler/2022.2.1/env/vars.sh

. /apl/lammps/2021-Sep29/conda_init.sh

module load mkl/2022.2.1
module load openmpi/4.1.5-hpcx/intel2022.2.1

export CC=mpicc
export CXX=mpicxx
```

```

export FC=mpif90
export MPICC=mpicc
export MPICXX=mpicxx
export MPIFC=mpif90

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

tar xzf ${LAMMPS_TARBALL}

cd ${NAME}
# for intel pacakge
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
# KIM: CDDL is imcompatible with GPL
# LATTE: technical problem of cmake? (LAPACK and BLAS)
# NETCDF: to avoid EVP_KDF_ctrl error
# MPIIO: not maintained?

cmake ../cmake \
-DLAMMPS_MACHINE=rccs \
-DENABLE_TESTING=on \
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
-DCMAKE_C_COMPILER=mpicc \
-DCMAKE_CXX_COMPILER=mpicxx \
-DCMAKE_Fortran_COMPILER=mpif90 \
-DCMAKE_MPI_C_COMPILER=mpicc \
-DCMAKE_MPI_CXX_COMPILER=mpicxx \
-DCMAKE_MPI_Fortran_COMPILER=mpif90 \
-DCMAKE_CXX_FLAGS_DEBUG="-Wall -Wextra -g" \
-DCMAKE_CXX_FLAGS_RELWITHDEBINFO="-Wall -Wextra -g -O2 -DNDEBUG" \
-DCMAKE_CXX_FLAGS_RELEASE="-O3 -DNDEBUG" \
-DCMAKE_Fortran_FLAGS_DEBUG="-Wall -Wextra -g" \
-DCMAKE_Fortran_FLAGS_RELWITHDEBINFO="-Wall -Wextra -g -O2 -DNDEBUG" \
-DCMAKE_Fortran_FLAGS_RELEASE="-O3 -DNDEBUG" \
-DCMAKE_C_FLAGS_DEBUG="-Wall -Wextra -g" \
-DCMAKE_C_FLAGS_RELWITHDEBINFO="-Wall -Wextra -g -O2 -DNDEBUG" \
-DCMAKE_C_FLAGS_RELEASE="-O3 -DNDEBUG" \
-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=on \  
-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=off \  
-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="-qmk" \  
-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
```

## Packages

ASPHERE ATC AWPMD BOCS BODY BROWNIAN CG-DNA CG-SDK CLASS2 COLLOID  
COLVARS COMPRESS CORESHELL DIELECTRIC DIFFRACTION DIPOLE DPD-BASIC  
DPD-MESO DPD-REACT DPD-SMOOTH DRUDE EFF EXTRA-COMPUTE EXTRA-DUMP  
EXTRA-FIX EXTRA-MOLECULE EXTRA-PAIR FEP GRANULAR H5MD INTEL  
INTERLAYER KOKKOS KSPACE LATBOLTZ MACHDYN MANIFOLD MANYBODY MC  
MEAM MESONT MESSAGE MGPT MISC ML-IAP ML-PACE ML-RANN ML-SNAP  
MOFFF MOLECULE MOLFILE OPENMP OPT ORIENT PERI PHONON PLUGIN  
PLUMED POEMS PTM PYTHON QEQ QMMM QTB REACTION REAXFF REPLICA RIGID  
SCAFACOS SHOCK SMTBQ SPH SPIN SRD TALLY UEF VORONOI YAFF

## Tests

There are errors in the following tests. Error log is copied to /apl/lammps/2021-Sep29/Testing.

The following tests FAILED:

10 - AtomStyle (Failed)  
88 - MolPairStyle:coul\_diel (Failed)  
94 - MolPairStyle:coul\_shield (Failed)  
117 - MolPairStyle:lj\_charmm\_coul\_long\_soft (Failed)  
130 - MolPairStyle:lj\_class2\_soft (Failed)  
139 - MolPairStyle:lj\_cut\_coul\_long\_soft (Failed)  
145 - MolPairStyle:lj\_cut\_soft (Failed)  
151 - MolPairStyle:lj\_expand\_coul\_long (Failed)  
164 - MolPairStyle:lj\_sdk\_coul\_long (Failed)  
165 - MolPairStyle:lj\_sdk\_coul\_table (Failed)  
169 - MolPairStyle:lj\_switch3\_coulgauss\_long (Failed)  
192 - MolPairStyle:tip4p\_long\_soft (Failed)  
195 - MolPairStyle:wf\_cut (Failed)  
203 - AtomicPairStyle:buck\_coul\_cut\_qeq\_point (Failed)  
204 - AtomicPairStyle:buck\_coul\_cut\_qeq\_shielded (Failed)  
221 - AtomicPairStyle:edip (Failed)  
224 - AtomicPairStyle:hybrid-eam (Failed)  
228 - AtomicPairStyle:meam (Failed)  
229 - AtomicPairStyle:meam\_spline (Failed)  
230 - AtomicPairStyle:meam\_sw\_spline (Failed)  
233 - AtomicPairStyle:reaxff (Failed)  
234 - AtomicPairStyle:reaxff\_lgvdw (Failed)  
235 - AtomicPairStyle:reaxff\_noqeq (Failed)  
236 - AtomicPairStyle:reaxff\_tabulate (Failed)  
246 - ManybodyPairStyle:bop (Failed)  
247 - ManybodyPairStyle:bop\_save (Failed)  
248 - ManybodyPairStyle:comb (Failed)  
250 - ManybodyPairStyle:drip (Failed)  
251 - ManybodyPairStyle:drip\_real (Failed)  
256 - ManybodyPairStyle:ilp-graphene-hbn (Failed)  
257 - ManybodyPairStyle:ilp-graphene-hbn\_notaper (Failed)  
258 - ManybodyPairStyle:kolmogorov\_crespi\_full (Failed)  
261 - ManybodyPairStyle:lcbop (Failed)  
262 - ManybodyPairStyle:lebedeva\_z (Failed)  
263 - ManybodyPairStyle:meam (Failed)  
269 - ManybodyPairStyle:nb3b\_harmonic (Failed)  
270 - ManybodyPairStyle:pace\_product (Failed)  
271 - ManybodyPairStyle:pace\_recursive (Failed)  
272 - ManybodyPairStyle:polymorphic\_sw (Failed)  
273 - ManybodyPairStyle:polymorphic\_tersoff (Failed)  
281 - ManybodyPairStyle:ttersoff (Failed)  
286 - ManybodyPairStyle:ttersoff\_shift (Failed)  
287 - ManybodyPairStyle:ttersoff\_table (Failed)  
295 - BondStyle:gaussian (Failed)  
312 - AngleStyle:cosine\_delta (Failed)  
314 - AngleStyle:cosine\_shift (Failed)  
336 - KSpaceStyle:ewald\_tri (Failed)  
338 - KSpaceStyle:pppm\_ad (Failed)  
339 - KSpaceStyle:pppm\_cg (Failed)  
341 - KSpaceStyle:pppm\_cg\_tiled (Failed)  
347 - KSpaceStyle:pppm\_disp\_tip4p (Failed)  
354 - KSpaceStyle:pppm\_tip4p (Failed)  
359 - KSpaceStyle:scafacos\_direct (Failed)  
360 - KSpaceStyle:scafacos\_ewald (Failed)  
361 - KSpaceStyle:scafacos\_fmm (Failed)  
362 - KSpaceStyle:scafacos\_fmm\_tuned (Failed)  
363 - KSpaceStyle:scafacos\_p2nfft (Failed)  
364 - FixTimestep:adapt\_coul (Failed)  
367 - FixTimestep:addforce\_const (Failed)  
368 - FixTimestep:addforce\_variable (Failed)  
369 - FixTimestep:addtorque\_const (Failed)  
372 - FixTimestep:aveforce\_variable (Failed)

```
374 - FixTimestep:drag (Failed)
378 - FixTimestep:heat (Failed)
381 - FixTimestep:momentum (Failed)
383 - FixTimestep:nph (Failed)
384 - FixTimestep:nph_sphere (Failed)
386 - FixTimestep:npt_iso (Failed)
387 - FixTimestep:npt_sphere_aniso (Failed)
388 - FixTimestep:npt_sphere_iso (Failed)
389 - FixTimestep:npt_sphere_tri (Failed)
397 - FixTimestep:nvt (Failed)
399 - FixTimestep:oneway (Failed)
412 - FixTimestep:rigid_npt_small (Failed)
424 - FixTimestep:shake_angle (Failed)
426 - FixTimestep:smd_couple (Failed)
429 - FixTimestep:spring_couple (Failed)
430 - FixTimestep:spring_rg (Failed)
432 - FixTimestep:spring_tether (Failed)
433 - FixTimestep:temp_berendsen (Failed)
434 - FixTimestep:temp_csld (Failed)
435 - FixTimestep:temp_csvr (Failed)
436 - FixTimestep:temp_rescale (Failed)
455 - DihedralStyle:table_cut_linear (Failed)
457 - DihedralStyle:table_linear (Failed)
458 - DihedralStyle:table_spline (Failed)
466 - ImproperStyle:harmonic (Failed)
468 - ImproperStyle:inversion_harmonic (Failed)
```

Most errors are minor numerical ones or "lattice" command problem when intel compiler is employed. There may not be serious problems.

## Notes

- If NETCDF is set to on, the build failed. We thus disabled NETCDF this time. This may be due to the problem of system library.
- The compilation errors could be avoided if python 3.6 of the system was employed... We will try it in the next time.