

LAMMPS 29Sep21

Webpage

<https://www.lammps.org>

Version

29Sep21

Build Environment

- Intel Parallel Studio XE 2018 update 4
- gcc 7.3.1 (devtoolset-7)
- cmake 3.16.3

Files Required

- lammps-stable_29Sep2021.tar.gz
- (some of files are obtained during the installation procedure)

Build Procedure

```
#!/bin/sh

VERSION=29Sep21
NAME=lammps-stable_29Sep2021
INSTALL_PREFIX=/local/apl/lx/lammps${VERSION}

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

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

VMD_MOLFILE_INC=/local/apl/lx/vmd193/lib/plugins/include

PARALLEL=12

#-----
umask 0022
export LANG=C

module purge
module load scl/devtoolset-7
module load intel_parallelstudio/2018update4
module load cmake/3.16.3

export CC=mpiicc
export CXX=mpiicpc
export FC=mpiifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export MPIFC=mpiifort
export PYTHON_EXECUTABLE=/usr/bin/python3

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

tar xzf ${LAMMPS_TARBALL}
```

```
cd ${NAME}
mkdir build && cd build

# Disabled PKGs:
# 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 incompatible with GPL

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 \
-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" \
-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_FFmpeg=yes \
-DFFMPEG_EXECUTABLE=/local/apl/lx/ffmpeg-4.4/bin/ffmpeg \
-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_SKX=yes \
-DKokkos_ENABLE_OPENMP=yes \
-DPKG_KSPACE=on \
-DPKG_LATBOLTZ=on \
-DPKG_LATTE=on \
-DDOWNLOAD_LATTE=yes \
-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=on \
-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="-mkl" \
-DCMAKE_BUILD_TYPE=Release

```

```

#make -j ${PARALLEL}
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

- enabled

```

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 LATTE MACHDYN MANIFOLD MANYBODY MC MEAM MESONT MESSAGE MGPT MISC
ML-IAP ML-PACE ML-RANN ML-SNAP MOFFF MOLECULE MOLFILE MPIIO NETCDF 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

```

- disabled

- ADIOS, MDI, VTK: skipped
- MSCG: system gsl is too old
- MESSAGE: (ZeroMQ support is not active)
- QUIP: failed to auto-build
- ML-HDNNP: failed to auto-build
- KIM: license issue; CDDL is not compatible with GPL
 - it is possible to build KIM-enabled one. But you may need to manually copy library (libkim-api) to the installation directory.

Tests

Following tests failed. (Test log can be found at /local/apl/lx/lammps29Sep21/Testing directory.)

The following tests FAILED:

10 - AtomStyle (Failed)
83 - MolPairStyle:coul_diel (Failed)
89 - MolPairStyle:coul_shield (Failed)
112 - MolPairStyle:lj_charmm_coul_long_soft (Failed)
125 - MolPairStyle:lj_class2_soft (Failed)
134 - MolPairStyle:lj_cut_coul_long_soft (Failed)
140 - MolPairStyle:lj_cut_soft (Failed)
146 - MolPairStyle:lj_expand_coul_long (Failed)
159 - MolPairStyle:lj_sdk_coul_long (Failed)
160 - MolPairStyle:lj_sdk_coul_table (Failed)
164 - MolPairStyle:lj_switch3_coulgauss_long (Failed)
187 - MolPairStyle:tip4p_long_soft (Failed)
190 - MolPairStyle:wf_cut (Failed)
198 - AtomicPairStyle:buck_coul_cut_qeq_point (Failed)
199 - AtomicPairStyle:buck_coul_cut_qeq_shielded (Failed)
216 - AtomicPairStyle:edip (Failed)
219 - AtomicPairStyle:hybrid-eam (Failed)
223 - AtomicPairStyle:meam (Failed)
224 - AtomicPairStyle:meam_spline (Failed)
225 - AtomicPairStyle:meam_sw_spline (Failed)
228 - AtomicPairStyle:reaxff (Failed)
229 - AtomicPairStyle:reaxff_lgvdw (Failed)
230 - AtomicPairStyle:reaxff_noqeq (Failed)
231 - AtomicPairStyle:reaxff_tabulate (Failed)
241 - ManybodyPairStyle:bop (Failed)
242 - ManybodyPairStyle:bop_save (Failed)
243 - ManybodyPairStyle:comb (Failed)
245 - ManybodyPairStyle:drip (Failed)
246 - ManybodyPairStyle:drip_real (Failed)
251 - ManybodyPairStyle:ilp-graphene-hbn (Failed)
252 - ManybodyPairStyle:ilp-graphene-hbn_notaper (Failed)
253 - ManybodyPairStyle:kolmogorov_crespi_full (Failed)
256 - ManybodyPairStyle:lcbop (Failed)
257 - ManybodyPairStyle:lebedeva_z (Failed)
258 - ManybodyPairStyle:meam (Failed)
263 - ManybodyPairStyle:mliap_so3 (Failed)
264 - ManybodyPairStyle:nb3b_harmonic (Failed)
265 - ManybodyPairStyle:pace_product (Failed)
266 - ManybodyPairStyle:pace_recursive (Failed)
267 - ManybodyPairStyle:polymorphic_sw (Failed)
268 - ManybodyPairStyle:polymorphic_tersoff (Failed)
281 - ManybodyPairStyle:tersoff_shift (Failed)
282 - ManybodyPairStyle:tersoff_table (Failed)
290 - BondStyle:gaussian (Failed)
307 - AngleStyle:cosine_delta (Failed)
309 - AngleStyle:cosine_shift (Failed)
333 - KSpaceStyle:pppm_ad (Failed)
334 - KSpaceStyle:pppm_cg (Failed)
336 - KSpaceStyle:pppm_cg_tiled (Failed)
349 - KSpaceStyle:pppm_tip4p (Failed)
354 - KSpaceStyle:scafacos_direct (Failed)
355 - KSpaceStyle:scafacos_ewald (Failed)
356 - KSpaceStyle:scafacos_fmm (SEFAULT)
357 - KSpaceStyle:scafacos_fmm_tuned (Failed)
358 - KSpaceStyle:scafacos_p2nfft (Failed)
359 - FixTimestep:adapt_coul (Failed)
362 - FixTimestep:addforce_const (Failed)
363 - FixTimestep:addforce_variable (Failed)
364 - FixTimestep:addtorque_const (Failed)
367 - FixTimestep:aveforce_variable (Failed)
369 - FixTimestep:drag (Failed)
373 - FixTimestep:heat (Failed)
376 - FixTimestep:momentum (Failed)
378 - FixTimestep:nph (Failed)
379 - FixTimestep:nph_sphere (Failed)

381 - FixTimestep:npt_iso (Failed)
382 - FixTimestep:npt_sphere_aniso (Failed)
383 - FixTimestep:npt_sphere_iso (Failed)
384 - FixTimestep:npt_sphere_tri (Failed)
392 - FixTimestep:nvt (Failed)
394 - FixTimestep:oneway (Failed)
407 - FixTimestep:rigid_npt_small (Failed)
419 - FixTimestep:shake_angle (Failed)
421 - FixTimestep:smd_couple (Failed)
424 - FixTimestep:spring_couple (Failed)
425 - FixTimestep:spring_rg (Failed)
427 - FixTimestep:spring_tether (Failed)
428 - FixTimestep:temp_berendsen (Failed)
429 - FixTimestep:temp_cslid (Failed)
430 - FixTimestep:temp_csvr (Failed)
431 - FixTimestep:temp_rescale (Failed)
450 - DihedralStyle:table_cut_linear (Failed)
452 - DihedralStyle:table_linear (Failed)
453 - DihedralStyle:table_spline (Failed)
461 - ImproperStyle:harmonic (Failed)
463 - ImproperStyle:inversion_harmonic (Failed)

Errors other than minor numerical errors

- probably due to the differences of "lattice" command output between gcc and intel (as is the case [o29Oct20](#))
 - 198 - AtomicPairStyle:buck_coul_cut_qeq_point (Failed)
 - 199 - AtomicPairStyle:buck_coul_cut_qeq_shielded (Failed)
 - 216 - AtomicPairStyle:edip (Failed)
 - 225 - AtomicPairStyle:meam_sw_spline (Failed)
 - 228 - AtomicPairStyle:reaxff (Failed)
 - 229 - AtomicPairStyle:reaxff_lgvdw (Failed)
 - 230 - AtomicPairStyle:reaxff_noeq (Failed)
 - 231 - AtomicPairStyle:reaxff_tabulate (Failed)
 - 354 - KSpaceStyle:scafacos_direct (Failed)
 - 355 - KSpaceStyle:scafacos_ewald (Failed)
 - 357 - KSpaceStyle:scafacos_fmm_tuned (Failed)
 - 358 - KSpaceStyle:scafacos_p2nfft (Failed)
- other non-negligible errors
 - 10 - AtomStyles (Failed): large deviation in quaternion values (same as [29Oct20](#))
 - 356 - KSpaceStyle:scafacos_fmm (SEGFAULT): unknown (not examined)
 - 256 - ManybodyPairStyle:lcbop (Failed): unknown (not examined) (same as [29Oct20](#))
 - 290 - BondStyle:gaussian (Failed): unknown (not examined)

Notes

- Intel20 case: there were a few more errors in tests. no clear performance improvements.
 - other versions are not tested.
- KIM can't be enabled due to its license (CDDL). in the future versions, license of KIM (OpenKIM) might be changed?
- there were build errors for QUIP, ML-HDNNP. we thus simply disable them.