

LAMMPS 29Aug2024 - Intel

Webpage

<https://www.lammps.org>

Version

29Aug2024

Build Environment

- GCC 10.3.1 (gcc-toolset-10)
- Intel oneAPI Compiler 2023.2.0
- Intel MKL 2023.2.0
- Intel MPI 2021.10.0
- GSL 2.8

Files Required

- lammps-stable_29Aug2024.tar.gz
- (some of files will be downloaded in the procedure below)

Build Procedure

```
#!/bin/sh

VERSION=2024-Aug29
NAME=lammps-stable_29Aug2024
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.2023.2.0/oneapi/compiler/latest/env/vars.sh

module -s load gcc-toolset/10
module -s load compiler-rt/2023.2.0
module -s load intelmpi/2021.10.0
module -s load mkl/2023.2.0
module -s load gsl/2.8

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 xzf ${LAMMPS_TARBALL}
```

```
cd ${NAME}
```

```
sed -i -e "s/xHost/march=core-avx2/" cmake/CMakeLists.txt
```

```
mkdir build && cd build
```

```
cmake ../cmake \
```

```
-DLAMMPS_MACHINE=rccs \
```

```
-DENABLE_TESTING=on \
```

```
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
```

```
-DCMAKE_C_COMPILER=icx \
```

```
-DCMAKE_CXX_COMPILER=icpx \
```

```
-DCMAKE_Fortran_COMPILER=ifx \
```

```
-DCMAKE_MPI_C_COMPILER=mpiicx \
```

```
-DCMAKE_MPI_CXX_COMPILER=mpicpx \
```

```
-DCMAKE_MPI_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} \
```

```
-D GSL_ROOT_DIR=${GSL_ROOT} \
```

```
-DBUILD_SHARED_LIBS=on \
```

```
-DBUILD_TOOLS=on \
```

```
-DBUILD_MPI=on \
```

```
-DBUILD_OMP=on \
```

```
-DBUILD_LAMMPS_GUI=off \
```

```
-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_ASPHERE=on \
```

```
-DPKG_ATC=on \
```

```
-DPKG_AWPMO=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 \
-DKokkos_ARCH_ZEN3=off \
-DKokkos_ENABLE_OPENMP=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=off \
-DDOWNLOAD_MDI=off \
-DPKG_MEAM=on \
-DPKG_MESONT=on \
-DPKG_MGPT=on \
-DPKG_MISC=on \
-DPKG_ML-HDNNP=off \
-DDOWNLOAD_N2P2=off \
-DPKG_ML-IAP=off \
-DMLIAP_ENABLE_PYTHON=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=off \
-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=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 \
-DBLAS_LIBRARIES="-qmk!" \
-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

```

Enabled Packages

AMOEBA 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 MEAM MESONT MGPT MISC ML-PACE ML-POD ML-RANN ML-SNAP ML-UF3 MOFFF
 MOLECULE MOLFILE NETCDF OPENMP OPT ORIENT PERI PHONON PLUGIN POEMS PTM
 PYTHON QEQ QMMM QTB REACTION REAXFF REPLICIA RHEO RIGID SHOCK SMTBQ SPH
 SPIN SRD TALLY UEF VORONOI YAFF

Tests

Copy of test log is available at </apl/lammps/2024-Aug29-intel/Testing>.

The following tests FAILED:

- 37 - SimpleCommands (SEGFAULT)
- 39 - Groups (Failed)
- 85 - PythonPyLammps (Failed)
- 119 - MolPairStyle:coul_diel (Failed)
- 126 - MolPairStyle:coul_shield (Failed)
- 128 - MolPairStyle:coul_slater_long (Failed)
- 253 - AtomicPairStyle:buck_coul_cut_qeq_point (Failed)
- 254 - AtomicPairStyle:buck_coul_cut_qeq_shielded (Failed)
- 271 - AtomicPairStyle:edip (Failed)
- 277 - AtomicPairStyle:lepton_sphere (Failed)

278 - AtomicPairStyle:lj_cut_sphere (Failed)
279 - AtomicPairStyle:lj_expand_sphere (Failed)
282 - AtomicPairStyle:meam_2nn (Failed)
283 - AtomicPairStyle:meam_ms (Failed)
285 - AtomicPairStyle:meam_spline (Failed)
286 - AtomicPairStyle:meam_sw_spline (Failed)
288 - AtomicPairStyle:pedone (Failed)
290 - AtomicPairStyle:reaxff-acks2 (Failed)
291 - AtomicPairStyle:reaxff-acks2_efield (Failed)
292 - AtomicPairStyle:reaxff (Failed)
293 - AtomicPairStyle:reaxff_lgvdw (Failed)
294 - AtomicPairStyle:reaxff_noqueq (Failed)
295 - AtomicPairStyle:reaxff_tabulate (Failed)
296 - AtomicPairStyle:reaxff_tabulate_flag (Failed)
315 - ManybodyPairStyle:drip (Failed)
316 - ManybodyPairStyle:drip_real (Failed)
317 - ManybodyPairStyle:edip_multi (Failed)
321 - ManybodyPairStyle:ilp-graphene-hbn (Failed)
322 - ManybodyPairStyle:ilp-graphene-hbn_notaper (Failed)
325 - ManybodyPairStyle:kolmogorov_crespi_z (Failed)
326 - ManybodyPairStyle:lcbop (Failed)
336 - ManybodyPairStyle:pace_product (Failed)
337 - ManybodyPairStyle:pace_recursive (Failed)
342 - ManybodyPairStyle:rann (Failed)
345 - ManybodyPairStyle:snap (Failed)
353 - ManybodyPairStyle:tersoff (Failed)
362 - ManybodyPairStyle:uf3 (Failed)
369 - BondStyle:gaussian (SEGFAULT)
372 - BondStyle:harmonic_restrain (Failed)
373 - BondStyle:harmonic_shift (Failed)
412 - KSpaceStyle:ewald_conp_charge (Failed)
422 - KSpaceStyle:pppm_ad (Failed)
423 - KSpaceStyle:pppm_cg (Failed)
424 - KSpaceStyle:pppm_cg_ad (Failed)
425 - KSpaceStyle:pppm_cg_tiled (Failed)
434 - KSpaceStyle:pppm_disp_tip4p (Failed)
442 - KSpaceStyle:pppm_tip4p (Failed)
457 - FixTimestep:addtorque_const (Failed)
464 - FixTimestep:deform_tri (Failed)
470 - FixTimestep:efield_variable (Failed)
471 - FixTimestep:heat (Failed)
482 - FixTimestep:nph_sphere (Failed)
484 - FixTimestep:npt_iso (Failed)
486 - FixTimestep:npt_sphere_iso (Failed)
495 - FixTimestep:nvt-psllod (Failed)
496 - FixTimestep:nvt-sllod (Failed)
514 - FixTimestep:rigid_npt_small (Failed)
528 - FixTimestep:smd_couple (Failed)
541 - FixTimestep:wall_lj1043_const (Failed)
544 - FixTimestep:wall_morse_const (Failed)
545 - FixTimestep:wall_region_harmonic_const (Failed)
552 - DihedralStyle:cosine_squared_restricted (Failed)
561 - DihedralStyle:quadratic (Failed)
563 - DihedralStyle:table_cut_linear (Failed)
564 - DihedralStyle:table_cut_spline (Failed)

Notes

- [Please check article of GCC13 version.](#)
- Tests show more errors than the GCC version.