

## LAMMPS 29Aug2024 - Intel

### ウェブページ

<https://www.lammps.org>

### バージョン

29Aug2024

### ビルド環境

- 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

### ビルドに必要なファイル

- lammps-stable\_29Aug2024.tar.gz
- (一部ファイルは以下スクリプト中で取得)

### ビルド手順

```
#!/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} \
```

```
-DGSL_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

```

## 有効なパッケージ

```

AMOEBА 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 REPLICА RHEO RIGID SHOCK SMTBQ SPH
SPIN SRD TALLY UEF VORONOI YAFF

```

## テスト

テストログのコピーが [/apl/lammps/2024-Aug29-intel/Testing](#) 以下にあります。

```

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)

## メモ

- [GCC13 版の記事をご確認ください。](#)
- GCC 版に比べてテストで多くのエラーが発生しています。