

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

```

AMOEBAS 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 REPLICARHEO 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。