

LAMMPS 23Jun22

ウェブページ

<https://www.lammps.org>

バージョン

23Jun22 Update 2

ビルド環境

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

ビルドに必要なファイル

- lammps-stable.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

conda 環境

[lammps 29Sep21 CPU 版で作成したものを流用。](#)

lammps 本体

```
#!/bin/sh

VERSION=23Jun22
NAME=lammps-23Jun2022
INSTALL_PREFIX=/apl/lammps/2022-Jun23

BASEDIR=/home/users/${USER}/Software/LAMMPS/${VERSION}
LAMMPS_TARBALL=${BASEDIR}/lammps-stable.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 -s purge

# oneapi compiler (oneapi 2022.3.1 compiler classic 2022.2.1)
. ~/intel/oneapi/compiler/2022.2.1/env/vars.sh

. /apl/lammps/2022-Jun23/conda_init.sh

module -s load mkl/2022.2.1
module -s 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}
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 incompatible 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 \

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-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="-qmkl" \
-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

```

パッケージ

```

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 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

```

テスト

テストログのコピーを </apl/lammps/2022-Jun23/Testing/> に置いています。

```

The following tests FAILED:
 11 - AtomStyles (Failed)
 42 - ComputeGlobal (Failed)

```

94 - MolPairStyle:coul_diel (Failed)
100 - MolPairStyle:coul_shield (Failed)
102 - MolPairStyle:coul_slater_long (Failed)
137 - MolPairStyle:lj_class2_soft (Failed)
152 - MolPairStyle:lj_cut_soft (Failed)
158 - MolPairStyle:lj_expand_coul_long (Failed)
171 - MolPairStyle:lj_sdk_coul_long (Failed)
172 - MolPairStyle:lj_sdk_coul_table (Failed)
176 - MolPairStyle:lj_switch3_coulgauss_long (Failed)
200 - MolPairStyle:tip4p_long_soft (Failed)
203 - MolPairStyle:wf_cut (Failed)
211 - AtomicPairStyle:buck_coul_cut_qeq_point (Failed)
212 - AtomicPairStyle:buck_coul_cut_qeq_shielded (Failed)
229 - AtomicPairStyle:edip (Failed)
236 - AtomicPairStyle:meam (Failed)
237 - AtomicPairStyle:meam_spline (Failed)
238 - AtomicPairStyle:meam_sw_spline (Failed)
241 - AtomicPairStyle:reaxff-acks2 (Failed)
242 - AtomicPairStyle:reaxff-acks2_efield (Failed)
243 - AtomicPairStyle:reaxff (Failed)
244 - AtomicPairStyle:reaxff_lgvdw (Failed)
245 - AtomicPairStyle:reaxff_noqeq (Failed)
246 - AtomicPairStyle:reaxff_tabulate (Failed)
247 - AtomicPairStyle:reaxff_tabulate_flag (Failed)
264 - ManybodyPairStyle:comb (Failed)
272 - ManybodyPairStyle:ilp-graphene-hbn (Failed)
273 - ManybodyPairStyle:ilp-graphene-hbn_notaper (Failed)
277 - ManybodyPairStyle:icbop (Failed)
286 - ManybodyPairStyle:pace_product (Failed)
287 - ManybodyPairStyle:pace_recursive (Failed)
299 - ManybodyPairStyle:tersoff (Failed)
304 - ManybodyPairStyle:tersoff_shift (Failed)
314 - BondStyle:gaussian (Failed)
357 - KSpaceStyle:ewald_tri (Failed)
359 - KSpaceStyle:pppm_ad (Failed)
360 - KSpaceStyle:pppm_cg (Failed)
362 - KSpaceStyle:pppm_cg_tiled (Failed)
369 - KSpaceStyle:pppm_disp_tip4p (Failed)
377 - KSpaceStyle:pppm_tip4p (Failed)
382 - KSpaceStyle:scafacos_direct (Failed)
383 - KSpaceStyle:scafacos_ewald (Failed)
384 - KSpaceStyle:scafacos_fmm (Failed)
385 - KSpaceStyle:scafacos_fmm_tuned (Failed)
386 - KSpaceStyle:scafacos_p2nfft (Failed)
387 - FixTimestep:adapt_coul (Failed)
390 - FixTimestep:addforce_const (Failed)
392 - FixTimestep:addtorque_const (Failed)
411 - FixTimestep:nph (Failed)
412 - FixTimestep:nph_sphere (Failed)
414 - FixTimestep:npt_iso (Failed)
415 - FixTimestep:npt_sphere_aniso (Failed)
416 - FixTimestep:npt_sphere_iso (Failed)
440 - FixTimestep:rigid_npt_small (Failed)
454 - FixTimestep:smd_couple (Failed)
462 - FixTimestep:temp_csld (Failed)
483 - DihedralStyle:table_cut_linear (Failed)
485 - DihedralStyle:table_linear (Failed)
486 - DihedralStyle:table_spline (Failed)
496 - ImproperStyle:inversion_harmonic (Failed)

- ほとんどは軽微な数値エラーと、インテルコンパイラ利用時の lattice 関連。大筋では問題無いと判断。

メモ

- NETCDF を on にするとビルドに失敗するため、今回は回避。システム側のライブラリの問題の可能性が高い。

- システムの python 3.6 を使っていれば、conda 環境は不要であった可能性が高い。また、NETCDF も on にできたかもしれない。