LAMMPS 29Sep21

ウェブページ

https://www.lammps.org

バージョン

29Sep21

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_29Sep2021.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

システムの python 3.9 ではビルドにエラーが出たため、簡単な環境を /apl/lammps/2021-Sep29/ 以下に整備。
詳細な導入手順を紛失... yaml, scipy, numpy, pandas, mpi4py, mkl, cython などが導入済。

lammps 本体

```
#!/bin/sh

VERSION=29Sep21
NAME=lammps-stable_29Sep2021
INSTALL_PREFIX=/apl/lammps/2021-Sep29

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

# load intel compiler (onapi 2022.3.1, compiler 2022.2.1)
. ~/intel/oneapi/compiler/2022.2.1/env/vars.sh

. /apl/lammps/2021-Sep29/conda_init.sh

module load mkl/2022.2.1
module 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} lammps_erase
  rm -rf lammps_erase &
fi

tar zxf ${LAMMPS_TARBALL}

cd ${NAME}
# for intel pacakge
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 imcompatible 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_AWPMD=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 \
  -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 MESSAGE 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

以下のテストでエラー。エラーログは /apl/lammps/2021-Sep29/Testing 以下にコピーしてあります。

```
The following tests FAILED:
```

10 - AtomStyles (Failed)
88 - MolPairStyle:coul_diel (Failed)
94 - MolPairStyle:coul_shield (Failed)
117 - MolPairStyle:lj_charmm_coul_long_soft (Failed)
130 - MolPairStyle:lj_class2_soft (Failed)
139 - MolPairStyle:lj_cut_coul_long_soft (Failed)
145 - MolPairStyle:lj_cut_soft (Failed)
151 - MolPairStyle:lj_expand_coul_long (Failed)
164 - MolPairStyle:lj_sdk_coul_long (Failed)
165 - MolPairStyle:lj_sdk_coul_table (Failed)
169 - MolPairStyle:lj_switch3_coulgauss_long (Failed)
192 - MolPairStyle:tip4p_long_soft (Failed)
195 - MolPairStyle:wf_cut (Failed)
203 - AtomicPairStyle:buck_coul_cut_qeq_point (Failed)
204 - AtomicPairStyle:buck_coul_cut_qeq_shielded (Failed)
221 - AtomicPairStyle:edip (Failed)
224 - AtomicPairStyle:hybrid-eam (Failed)
228 - AtomicPairStyle:meam (Failed)
229 - AtomicPairStyle:meam_spline (Failed)
230 - AtomicPairStyle:meam_sw_spline (Failed)
233 - AtomicPairStyle:reaxff (Failed)
234 - AtomicPairStyle:reaxff_lgvdw (Failed)
235 - AtomicPairStyle:reaxff_noqeq (Failed)
236 - AtomicPairStyle:reaxff_tabulate (Failed)
246 - ManybodyPairStyle:bop (Failed)
247 - ManybodyPairStyle:bop_save (Failed)
248 - ManybodyPairStyle:comb (Failed)
250 - ManybodyPairStyle:drip (Failed)
251 - ManybodyPairStyle:drip_real (Failed)
256 - ManybodyPairStyle:ilp-graphene-hbn (Failed)
257 - ManybodyPairStyle:ilp-graphene-hbn_notaper (Failed)
258 - ManybodyPairStyle:kolmogorov_crespi_full (Failed)
261 - ManybodyPairStyle:lcbop (Failed)
262 - ManybodyPairStyle:lebedeva_z (Failed)
263 - ManybodyPairStyle:meam (Failed)
269 - ManybodyPairStyle:nb3b_harmonic (Failed)
270 - ManybodyPairStyle:pace_product (Failed)
271 - ManybodyPairStyle:pace_recursive (Failed)
272 - ManybodyPairStyle:polymorphic_sw (Failed)
273 - ManybodyPairStyle:polymorphic_tersoff (Failed)
281 - ManybodyPairStyle:tersoff (Failed)
286 - ManybodyPairStyle:tersoff_shift (Failed)
287 - ManybodyPairStyle:tersoff_table (Failed)
295 - BondStyle:gaussian (Failed)
312 - AngleStyle:cosine_delta (Failed)
314 - AngleStyle:cosine_shift (Failed)
336 - KSpaceStyle:ewald_tri (Failed)
338 - KSpaceStyle:pppm_ad (Failed)
339 - KSpaceStyle:pppm_cg (Failed)
341 - KSpaceStyle:pppm_cg_tiled (Failed)
347 - KSpaceStyle:pppm_disp_tip4p (Failed)
354 - KSpaceStyle:pppm_tip4p (Failed)
359 - KSpaceStyle:scafacos_direct (Failed)
360 - KSpaceStyle:scafacos_ewald (Failed)
361 - KSpaceStyle:scafacos_fmm (Failed)
362 - KSpaceStyle:scafacos_fmm_tuned (Failed)
363 - KSpaceStyle:scafacos_p2nfft (Failed)
364 - FixTimestep:adapt_coul (Failed)
367 - FixTimestep:addforce_const (Failed)
368 - FixTimestep:addforce_variable (Failed)
369 - FixTimestep:addtorque_const (Failed)
372 - FixTimestep:aveforce_variable (Failed)
374 - FixTimestep:drag (Failed)
378 - FixTimestep:heat (Failed)
381 - FixTimestep:momentum (Failed)

```
383 - FixTimestep:nph (Failed)
384 - FixTimestep:nph_sphere (Failed)
386 - FixTimestep:npt_iso (Failed)
387 - FixTimestep:npt_sphere_aniso (Failed)
388 - FixTimestep:npt_sphere_iso (Failed)
389 - FixTimestep:npt_sphere_tri (Failed)
397 - FixTimestep:nvt (Failed)
399 - FixTimestep:oneway (Failed)
412 - FixTimestep:rigid_npt_small (Failed)
424 - FixTimestep:shake_angle (Failed)
426 - FixTimestep:smd_couple (Failed)
429 - FixTimestep:spring_couple (Failed)
430 - FixTimestep:spring_rg (Failed)
432 - FixTimestep:spring_tether (Failed)
433 - FixTimestep:temp_berendsen (Failed)
434 - FixTimestep:temp_csld (Failed)
435 - FixTimestep:temp_csvr (Failed)
436 - FixTimestep:temp_rescale (Failed)
455 - DihedralStyle:table_cut_linear (Failed)
457 - DihedralStyle:table_linear (Failed)
458 - DihedralStyle:table_spline (Failed)
466 - ImproperStyle:harmonic (Failed)
468 - 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。