LAMMPS 29Sep21

ウェブページ

https://www.lammps.org

バージョン

29Sep21

ビルド環境

- Intel Parallel Studio XE 2018 update 4
- gcc 7.3.1 (devtoolset-7)
- cmake 3.16.3

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

```
#!/bin/sh

VERSION=29Sep21
NAME=lammps-stable_29Sep2021
INSTALL_PREFIX=/local/apl/lx/lammps${VERSION}

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

WORKDIR=/work/users/${USER}
LAMMPS_WORKDIR=${WORKDIR}/${NAME}

VMD_MOLFILE_INC=/local/apl/lx/vmd193/lib/plugins/include

PARALLEL=12

#------------------------------------------------------------------
umask 0022
export LANG=C

module purge
module load scl/devtoolset-7
module load intel_parallelstudio/2018update4
module load cmake/3.16.3

export CC=mpiicc
export CXX=mpiicpc
export FC=mpiifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export MPIFC=mpiifort
export PYTHON_EXECUTABLE=/usr/bin/python3

cd ${WORKDIR}
if [ -d ${NAME} ]; then
  mv ${NAME} lammps_erase
  rm -rf lammps_erase &
fi

tar zxf ${LAMMPS_TARBALL}
```

```
cd ${NAME}
mkdir build && cd build

# Disabled PKGs:
# 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

cmake ../cmake \
  -DLAMMPS_MACHINE=rccs \
  -DENABLE_TESTING=on \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_C_COMPILER=mpiicc \
  -DCMAKE_CXX_COMPILER=mpiicpc \
  -DCMAKE_Fortran_COMPILER=mpiifort \
  -DCMAKE_MPI_C_COMPILER=mpiicc \
  -DCMAKE_MPI_CXX_COMPILER=mpiicpc \
  -DCMAKE_MPI_Fortran_COMPILER=mpiifort \
  -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" \
  -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_FFMPEG=yes \
  -DFFMPEG_EXECUTABLE=/local/apl/lx/ffmpeg-4.4/bin/ffmpeg \
  -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_SKX=yes \
-DKokkos_ENABLE_OPENMP=yes \
-DPKG_KSPACE=on \
-DPKG_LATBOLTZ=on \
-DPKG_LATTE=on \
-DDOWNLOAD_LATTE=yes \
-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=on \
-DPKG_MSCG=off \
-DPKG_NETCDF=on \
-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="-mkl" \
  -DCMAKE_BUILD_TYPE=Release

#make -j ${PARALLEL}
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

- 有効なパッケージ

```
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 LATTE MACHDYN MANIFOLD MANYBODY MC MEAM MESONT MESSAGE MGPT MISC
ML-IAP ML-PACE ML-RANN ML-SNAP MOFFF MOLECULE MOLFILE MPIIO NETCDF 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
```

- 無効なパッケージ
  - ADIOS, MDI, VTK: skipped
  - MSCG: システムの gsl のバージョンでは対応できないため
  - MESSAGE: (ZeroMQ のサポートのみ無効)
  - QUIP: 自動ビルド失敗
  - ML-HDNNP: 自動ビルド失敗
  - KIM: ライセンスの問題; CDDL は GPL と混ぜられないため
    - ビルド自体は可能。ただし、ライブラリ(libkim-api)を手動でインストール先にコピーする必要がありそう

テスト

以下のテストでエラー。エラーログは /local/apl/lx/lammps29Sep21/Testing 以下にもコピーしてあります。

```
The following tests FAILED:
        10 - AtomStyles (Failed)
```

83 - MolPairStyle:coul_diel (Failed)
89 - MolPairStyle:coul_shield (Failed)
112 - MolPairStyle:lj_charmm_coul_long_soft (Failed)
125 - MolPairStyle:lj_class2_soft (Failed)
134 - MolPairStyle:lj_cut_coul_long_soft (Failed)
140 - MolPairStyle:lj_cut_soft (Failed)
146 - MolPairStyle:lj_expand_coul_long (Failed)
159 - MolPairStyle:lj_sdk_coul_long (Failed)
160 - MolPairStyle:lj_sdk_coul_table (Failed)
164 - MolPairStyle:lj_switch3_coulgauss_long (Failed)
187 - MolPairStyle:tip4p_long_soft (Failed)
190 - MolPairStyle:wf_cut (Failed)
198 - AtomicPairStyle:buck_coul_cut_qeq_point (Failed)
199 - AtomicPairStyle:buck_coul_cut_qeq_shielded (Failed)
216 - AtomicPairStyle:edip (Failed)
219 - AtomicPairStyle:hybrid-eam (Failed)
223 - AtomicPairStyle:meam (Failed)
224 - AtomicPairStyle:meam_spline (Failed)
225 - AtomicPairStyle:meam_sw_spline (Failed)
228 - AtomicPairStyle:reaxff (Failed)
229 - AtomicPairStyle:reaxff_lgvdw (Failed)
230 - AtomicPairStyle:reaxff_noqeq (Failed)
231 - AtomicPairStyle:reaxff_tabulate (Failed)
241 - ManybodyPairStyle:bop (Failed)
242 - ManybodyPairStyle:bop_save (Failed)
243 - ManybodyPairStyle:comb (Failed)
245 - ManybodyPairStyle:drip (Failed)
246 - ManybodyPairStyle:drip_real (Failed)
251 - ManybodyPairStyle:ilp-graphene-hbn (Failed)
252 - ManybodyPairStyle:ilp-graphene-hbn_notaper (Failed)
253 - ManybodyPairStyle:kolmogorov_crespi_full (Failed)
256 - ManybodyPairStyle:lcbop (Failed)
257 - ManybodyPairStyle:lebedeva_z (Failed)
258 - ManybodyPairStyle:meam (Failed)
263 - ManybodyPairStyle:mliap_so3 (Failed)
264 - ManybodyPairStyle:nb3b_harmonic (Failed)
265 - ManybodyPairStyle:pace_product (Failed)
266 - ManybodyPairStyle:pace_recursive (Failed)
267 - ManybodyPairStyle:polymorphic_sw (Failed)
268 - ManybodyPairStyle:polymorphic_tersoff (Failed)
281 - ManybodyPairStyle:tersoff_shift (Failed)
282 - ManybodyPairStyle:tersoff_table (Failed)
290 - BondStyle:gaussian (Failed)
307 - AngleStyle:cosine_delta (Failed)
309 - AngleStyle:cosine_shift (Failed)
333 - KSpaceStyle:pppm_ad (Failed)
334 - KSpaceStyle:pppm_cg (Failed)
336 - KSpaceStyle:pppm_cg_tiled (Failed)
349 - KSpaceStyle:pppm_tip4p (Failed)
354 - KSpaceStyle:scafacos_direct (Failed)
355 - KSpaceStyle:scafacos_ewald (Failed)
356 - KSpaceStyle:scafacos_fmm (SEGFAULT)
357 - KSpaceStyle:scafacos_fmm_tuned (Failed)
358 - KSpaceStyle:scafacos_p2nfft (Failed)
359 - FixTimestep:adapt_coul (Failed)
362 - FixTimestep:addforce_const (Failed)
363 - FixTimestep:addforce_variable (Failed)
364 - FixTimestep:addtorque_const (Failed)
367 - FixTimestep:aveforce_variable (Failed)
369 - FixTimestep:drag (Failed)
373 - FixTimestep:heat (Failed)
376 - FixTimestep:momentum (Failed)
378 - FixTimestep:nph (Failed)
379 - FixTimestep:nph_sphere (Failed)
381 - FixTimestep:npt_iso (Failed)

```
382 - FixTimestep:npt_sphere_aniso (Failed)
383 - FixTimestep:npt_sphere_iso (Failed)
384 - FixTimestep:npt_sphere_tri (Failed)
392 - FixTimestep:nvt (Failed)
394 - FixTimestep:oneway (Failed)
407 - FixTimestep:rigid_npt_small (Failed)
419 - FixTimestep:shake_angle (Failed)
421 - FixTimestep:smd_couple (Failed)
424 - FixTimestep:spring_couple (Failed)
425 - FixTimestep:spring_rg (Failed)
427 - FixTimestep:spring_tether (Failed)
428 - FixTimestep:temp_berendsen (Failed)
429 - FixTimestep:temp_csld (Failed)
430 - FixTimestep:temp_csvr (Failed)
431 - FixTimestep:temp_rescale (Failed)
450 - DihedralStyle:table_cut_linear (Failed)
452 - DihedralStyle:table_linear (Failed)
453 - DihedralStyle:table_spline (Failed)
461 - ImproperStyle:harmonic (Failed)
463 - ImproperStyle:inversion_harmonic (Failed)
```

軽微な数値エラー以外のエラーについて

- "lattice" コマンドの挙動の違い(gcc vs intel)に依存する数値エラーと思われるもの。(29Oct20 の時と同様)
  - 198 - AtomicPairStyle:buck_coul_cut_qeq_point (Failed)
  - 199 - AtomicPairStyle:buck_coul_cut_qeq_shielded (Failed)
  - 216 - AtomicPairStyle:edip (Failed)
  - 225 - AtomicPairStyle:meam_sw_spline (Failed)
  - 228 - AtomicPairStyle:reaxff (Failed)
  - 229 - AtomicPairStyle:reaxff_lgvdw (Failed)
  - 230 - AtomicPairStyle:reaxff_noqeq (Failed)
  - 231 - AtomicPairStyle:reaxff_tabulate (Failed)
  - 354 - KSpaceStyle:scafacos_direct (Failed)
  - 355 - KSpaceStyle:scafacos_ewald (Failed)
  - 357 - KSpaceStyle:scafacos_fmm_tuned (Failed)
  - 358 - KSpaceStyle:scafacos_p2nfft (Failed)
- その他
  - 10 - AtomStyles (Failed): quarternion の値だけに大きなエラー。29Oct20 の時と同様
  - 356 - KSpaceStyle:scafacos_fmm (SEGFAULT): 不明(未検証)。
  - 256 - ManybodyPairStyle:lcbop (Failed): 不明(未検証)。29Oct20 の時と同様
  - 290 - BondStyle:gaussian (Failed): 不明(未検証)。

メモ

- intel20 ではエラーが少しだけ増え、速度も上がらないようなので前回と同じく intel18 でビルド
  - 他のバージョンは未検証
- KIM はライセンス(CDDL)の関係で導入不可。(今後のバージョンでは導入可能になるかもしれない。)
- QUIP, ML-HDNNP はビルドに失敗したため外した。詳細な検証は行っていない。