LAMMPS 23Jun22 (Intel MPI)

Webpage

https://www.lammps.org

Version

23Jun22 Update 2

Build Environment

- Intel oneAPI Compiler Classic 2023.1.0
- Intel MKL 2023.1.0
- Intel MPI 2021.9.0

Files Required

- lammps-stable.tar.gz
- (some of files will be downloaded in the procedure below)

Build Procedure

```
#!/bin/sh

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

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

# load intel env (2023.1.0)
. ~/intel/oneapi/compiler/latest/env/vars.sh

module -s purge
module -s load intelmpi/2021.9.0
module -s load mkl/2023.1.0

export CC=mpiicc
export CXX=mpiicpc
export FC=mpiifort
export MPICC=mpiicc
export MPICXX=mpiicpc
export MPIFC=mpiifort

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 zxf ${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
# ML-IAP: failed to build
# KIM: CDDL is imcompatible with GPL
# LATTE: technical problem of cmake? (LAPACK and BLAS)
# MPIIO: not maintained?

cmake ../cmake \
  -DLAMMPS_MACHINE=rccs \
  -DENABLE_TESTING=on \
  -DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
  -DCMAKE_C_COMPILER=mpiicc \
  -DCMAKE_CXX_COMPILER=mpiicpc \
  -DCMAKE_Fortran_COMPILER=mpiifort \
  -DCMAKE_MPI_C_COMPILER=mpiicc \
  -DCMAKE_MPI_CXX_COMPILER=mpiicpc \
  -DCMAKE_MPI_Fortran_COMPILER=mpiifort \
  -DPython_EXECUTABLE=${PYTHONEXE} \
  -DPython_INCLUDE_DIR=${PYTHONINC} \
  -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=off \
-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=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="-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
```

Test Result

List of failed tests:

```
The following tests FAILED:
        11 - AtomStyles (Failed)
        35 - SimpleCommands (SEGFAULT)
        38 - Regions (Subprocess aborted)
        43 - ComputeGlobal (Failed)
        95 - MolPairStyle:coul_diel (Failed)
       101 - MolPairStyle:coul_shield (Failed)
       103 - MolPairStyle:coul_slater_long (Failed)
       138 - MolPairStyle:lj_class2_soft (Failed)
       153 - MolPairStyle:lj_cut_soft (Failed)
       159 - MolPairStyle:lj_expand_coul_long (Failed)
       172 - MolPairStyle:lj_sdk_coul_long (Failed)
       173 - MolPairStyle:lj_sdk_coul_table (Failed)
       177 - MolPairStyle:lj_switch3_coulgauss_long (Failed)
       201 - MolPairStyle:tip4p_long_soft (Failed)
       204 - MolPairStyle:wf_cut (Failed)
       212 - AtomicPairStyle:buck_coul_cut_qeq_point (Failed)
       213 - AtomicPairStyle:buck_coul_cut_qeq_shielded (Failed)
       230 - AtomicPairStyle:edip (Failed)
       237 - AtomicPairStyle:meam (Failed)
       238 - AtomicPairStyle:meam_spline (Failed)
       239 - AtomicPairStyle:meam_sw_spline (Failed)
       242 - AtomicPairStyle:reaxff-acks2 (Failed)
       243 - AtomicPairStyle:reaxff-acks2_efield (Failed)
       244 - AtomicPairStyle:reaxff (Failed)
       245 - AtomicPairStyle:reaxff_lgvdw (Failed)
       246 - AtomicPairStyle:reaxff_noqeq (Failed)
```

247 - AtomicPairStyle:reaxff_tabulate (Failed)
248 - AtomicPairStyle:reaxff_tabulate_flag (Failed)
265 - ManybodyPairStyle:comb (Failed)
273 - ManybodyPairStyle:ilp-graphene-hbn (Failed)
274 - ManybodyPairStyle:ilp-graphene-hbn_notaper (Failed)
278 - ManybodyPairStyle:lcbop (Failed)
287 - ManybodyPairStyle:pace_product (Failed)
288 - ManybodyPairStyle:pace_recursive (Failed)
300 - ManybodyPairStyle:tersoff (Failed)
305 - ManybodyPairStyle:tersoff_shift (Failed)
315 - BondStyle:gaussian (Failed)
358 - KSpaceStyle:ewald_tri (Failed)
360 - KSpaceStyle:pppm_ad (Failed)
361 - KSpaceStyle:pppm_cg (Failed)
363 - KSpaceStyle:pppm_cg_tiled (Failed)
370 - KSpaceStyle:pppm_disp_tip4p (Failed)
378 - KSpaceStyle:pppm_tip4p (Failed)
383 - KSpaceStyle:scafacos_direct (Failed)
384 - KSpaceStyle:scafacos_ewald (Failed)
385 - KSpaceStyle:scafacos_fmm (Failed)
386 - KSpaceStyle:scafacos_fmm_tuned (Failed)
387 - KSpaceStyle:scafacos_p2nfft (Failed)
388 - FixTimestep:adapt_coul (Failed)
391 - FixTimestep:addforce_const (Failed)
393 - FixTimestep:addtorque_const (Failed)
412 - FixTimestep:nph (Failed)
413 - FixTimestep:nph_sphere (Failed)
415 - FixTimestep:npt_iso (Failed)
416 - FixTimestep:npt_sphere_aniso (Failed)
417 - FixTimestep:npt_sphere_iso (Failed)
441 - FixTimestep:rigid_npt_small (Failed)
455 - FixTimestep:smd_couple (Failed)
463 - FixTimestep:temp_csld (Failed)
484 - DihedralStyle:table_cut_linear (Failed)
486 - DihedralStyle:table_linear (Failed)
487 - DihedralStyle:table_spline (Failed)
497 - ImproperStyle:inversion_harmonic (Failed)

Notes

- Python 3.6 is employed instead of python 3.9. NETCDF is enabled in this version, while ML-IAP is disabled to avoid compilation error.
- In case of OpenMPI build, there is significant performance degradation in LJ system. This version is free from that issue.
    - In the problematic case, "Comm" spends 10 or more times than "Pair" according to timing statistics.
    - "intel" package seems bit unstable, while Intel MPI is employed...