LAMMPS 23Jun22

Webpage

https://www.lammps.org

Version

23Jun22 Update 2

Build Environment

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

Files Required

- lammps-stable.tar.gz
- (some of files will be downloaded during the installation)

Build Procedure

conda environment

Conda (miniforge) environment prepared for lammps 29Sep21 CPU version is used.

lammps

```
#!/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} 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
# 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
```

Enabled Packages

```
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
```

Tests

Copy of test log is available at /apl/lammps/2022-Jun23/Testing/.

```
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:lcbop (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)

- Most errors are minor numerical ones or "lattice" command problem when intel compiler is employed. There may not be serious problems.

Notes

- If NETCDF is set to on, the build failed. We thus disabled NETCDF this time. This may be due to the problem of system library.
- The compilation errors could be avoided if python 3.6 of the system was employed... We will try it in the next time.