

LAMMPS 29Sep21 Update 3 (intel MPI)

Webpage

<https://www.lammps.org>

Version

29Sep21 Update 3

Build Environment

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

Files Required

- lammps-stable_29Sep2021_update3.tar.gz
- (some of files will be downloaded during the build)

Build Procedure

```
#!/bin/sh

VERSION=29Sep21
NAME=lammps-stable_29Sep2021_update3
INSTALL_PREFIX=/apl/lammps/2021-Sep29-impi

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

# 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
PYTHONLIB=/usr/lib64/libpython3.6m.so

cd ${WORKDIR}
if [ -d ${NAME} ]; then
```

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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=${INSTALL_PREFIX} \
-DCMAKE_C_COMPILER=mpiicc \
-DCMAKE_CXX_COMPILER=mpiicpc \
-DCMAKE_Fortran_COMPILER=mpiifort \
-DCMAKE_MPI_C_COMPILER=mpiicc \
-DCMAKE_MPI_CXX_COMPILER=mpiicpc \
-DCMAKE_MPI_Fortran_COMPILER=mpiifort \
-DPython_EXECUTABLE=${PYTHONEXE} \
-DPython_INCLUDE_DIR=${PYTHONINC} \
-DPython_LIBRARY=${PYTHONLIB} \
-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_ASHERE=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=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 \

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-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 Results

The following tests FAILED:

```

10 - AtomStyles (Failed)
32 - SimpleCommands (SEGFAULT)
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)

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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:lcobp (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)

Notes

- This is an updated version. There are some differences from [the previous build](#) at the source code level.
- Please check notes of [2022-Jun23 version](#). Problems of this and 2022-Jun23 version are almost identical.