

## LAMMPS 29Sep21 Update 3 with GPU support (intel MPI)

### Webpage

<https://www.lammps.org>

### Version

29Sep21 Update 3

### Build Environment

- GCC 11.2.1 (gcc-toolset-11)
- Intel MKL 2023.1.0
- Intel MPI 2021.9.0
- CUDA 11.6

### Files Required

- lammps-stable\_29Sep2021\_update3.tar.gz
- (some of files will be downloaded during the build procedure below)

### Build Procedure

```
#!/bin/sh

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

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

WORKDIR=/gwork/users/${USER}/lammps-29Sep2021-cuda
LAMMPS_WORKDIR=${WORKDIR}/${NAME}

GPU_ARCH=sm_80
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
module -s load gcc-toolset/11
module -s load intelmpi/2021.9.0
module -s load mkl/2023.1.0
module -s load cuda/11.6

export CC=mpicc
export CXX=mpicxx
export FC=mpif90
export MPICC=mpicc
export MPICXX=mpicxx
export MPIFC=mpif90

PYTHONEXE=/usr/bin/python3.6m
PYTHONINC=/usr/include/python3.6m
PYTHONLIB=/usr/lib64/libpython3.6m.so

cd ${WORKDIR}
```

```

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

tar zxf ${LAMMPS_TARBALL}

cd ${NAME}
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-cuda \
-DENABLE_TESTING=on \
-DCMAKE_INSTALL_PREFIX=${INSTALL_PREFIX} \
-DCMAKE_C_COMPILER=mpicc \
-DCMAKE_CXX_COMPILER=mpicxx \
-DCMAKE_Fortran_COMPILER=mpif90 \
-DCMAKE_MPI_C_COMPILER=mpicc \
-DCMAKE_MPI_CXX_COMPILER=mpicxx \
-DCMAKE_MPI_Fortran_COMPILER=mpif90 \
-DPython_EXECUTABLE=${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_ASPHERE=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=on \  
-DGPU\_API=cuda \  
-DGPU\_ARCH=\${GPU\_ARCH} \  
-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="-Wl,--no-as-needed -lmkl_intel_lp64 -lmkl_gnu_thread -lmkl_core -lgomp -lpthread -lm -ldl" \
-DCMAKE_BUILD_TYPE=Release

make VERBOSE=1 -j ${PARALLEL}
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 liblammmps_rccs-cuda.so ]; then
  ln -s liblammmps_rccs-cuda.so liblammmps.so
fi
if [ -f liblammmps_rccs-cuda.so.0 ]; then
  ln -s liblammmps_rccs-cuda.so.0 liblammmps.so.0
fi

```

## Tests

```

#!/bin/sh
#PBS -l select=1:ncpus=16:mpiprocs=8:ompthreads=2:ngpus=2
#PBS -l walltime=24:00:00

NAME=lammmps-stable_29Sep2021_update3
WORKDIR=/gwork/users/${USER}/lammmps-29Sep2021-cuda
LAMMPS_WORKDIR=${WORKDIR}/${NAME}

#-----
umask 0022
export LANG=C
ulimit -s unlimited

module -s purge
module -s load gcc-toolset/11
module -s load intelmpi/2021.9.0
module -s load mkl/2023.1.0
module -s load cuda/11.6

export CC=mpicc
export CXX=mpicxx
export FC=mpif90
export MPICC=mpicc
export MPICXX=mpicxx
export MPIFC=mpif90

cd ${LAMMPS_WORKDIR}
cd build

```

make test # there may be errors...

## Test Results

The following tests FAILED:

32 - SimpleCommands (SEGFAULT)  
66 - MolPairStyle:born\_coul\_long\_cs (SEGFAULT)  
70 - MolPairStyle:buck (SEGFAULT)  
71 - MolPairStyle:buck\_coul\_cut (SEGFAULT)  
72 - MolPairStyle:buck\_coul\_long (SEGFAULT)  
73 - MolPairStyle:buck\_coul\_long\_cs (SEGFAULT)  
77 - MolPairStyle:buck\_long\_coul\_off (SEGFAULT)  
78 - MolPairStyle:buck\_long\_cut\_coul\_long (SEGFAULT)  
79 - MolPairStyle:buck\_mdf (SEGFAULT)  
81 - MolPairStyle:buck\_table\_coul\_off (SEGFAULT)  
84 - MolPairStyle:coul\_cut (SEGFAULT)  
88 - MolPairStyle:coul\_diel (SEGFAULT)  
89 - MolPairStyle:coul\_dsf (SEGFAULT)  
90 - MolPairStyle:coul\_exclude (SEGFAULT)  
97 - MolPairStyle:coul\_streitz\_long (SEGFAULT)  
100 - MolPairStyle:coul\_table\_cs (SEGFAULT)  
107 - MolPairStyle:gauss\_cut (SEGFAULT)  
111 - MolPairStyle:hybrid\_multiple (SEGFAULT)  
112 - MolPairStyle:lennard\_mdf (SEGFAULT)  
114 - MolPairStyle:lj\_charmm\_coul\_charmm (SEGFAULT)  
116 - MolPairStyle:lj\_charmm\_coul\_long (SEGFAULT)  
118 - MolPairStyle:lj\_charmm\_coul\_table (SEGFAULT)  
120 - MolPairStyle:lj\_charmmfsw\_coul\_long (SEGFAULT)  
121 - MolPairStyle:lj\_charmmfsw\_coul\_table (SEGFAULT)  
132 - MolPairStyle:lj\_cut (SEGFAULT)  
137 - MolPairStyle:lj\_cut\_coul\_long (SEGFAULT)  
140 - MolPairStyle:lj\_cut\_coul\_table (SEGFAULT)  
147 - MolPairStyle:lj\_cut\_tip4p\_long (SEGFAULT)  
150 - MolPairStyle:lj\_expand (SEGFAULT)  
152 - MolPairStyle:lj\_expand\_coul\_table (SEGFAULT)  
155 - MolPairStyle:lj\_long\_coul\_long (SEGFAULT)  
163 - MolPairStyle:lj\_sdk (SEGFAULT)  
173 - MolPairStyle:lj\_table\_coul\_table (SEGFAULT)  
175 - MolPairStyle:lj\_table\_tip4p\_table (SEGFAULT)  
178 - MolPairStyle:mm3\_switch3\_coulgauss\_table (SEGFAULT)  
182 - MolPairStyle:nm\_cut (SEGFAULT)  
186 - MolPairStyle:python\_hybrid (SEGFAULT)  
188 - MolPairStyle:soft (SEGFAULT)  
191 - MolPairStyle:tip4p\_long (SEGFAULT)  
193 - MolPairStyle:tip4p\_table (SEGFAULT)  
199 - AtomicPairStyle:adp (SEGFAULT)  
203 - AtomicPairStyle:buck\_coul\_cut\_qeq\_point (Failed)  
204 - AtomicPairStyle:buck\_coul\_cut\_qeq\_shielded (Failed)  
206 - AtomicPairStyle:colloid\_multi (SEGFAULT)  
207 - AtomicPairStyle:colloid\_multi\_tri (SEGFAULT)  
213 - AtomicPairStyle:eam\_cd (SEGFAULT)  
214 - AtomicPairStyle:eam\_cd\_old (SEGFAULT)  
221 - AtomicPairStyle:edip (Failed)  
222 - AtomicPairStyle:eim (SEGFAULT)  
224 - AtomicPairStyle:hybrid-eam (SEGFAULT)  
225 - AtomicPairStyle:hybrid-eam\_fs (SEGFAULT)  
229 - AtomicPairStyle:meam\_spline (SEGFAULT)  
230 - AtomicPairStyle:meam\_sw\_spline (SEGFAULT)  
231 - AtomicPairStyle:momb (SEGFAULT)  
233 - AtomicPairStyle:reaxff (SEGFAULT)  
234 - AtomicPairStyle:reaxff\_lgvdw (Failed)  
235 - AtomicPairStyle:reaxff\_noqeq (Failed)  
236 - AtomicPairStyle:reaxff\_tabulate (Failed)  
238 - AtomicPairStyle:table\_linear (SEGFAULT)

240 - AtomicPairStyle:table\_spline (SEGFAULT)  
241 - AtomicPairStyle:yukawa\_colloid (SEGFAULT)  
242 - ManybodyPairStyle:airebo (SEGFAULT)  
243 - ManybodyPairStyle:airebo\_00 (SEGFAULT)  
244 - ManybodyPairStyle:airebo\_m (SEGFAULT)  
245 - ManybodyPairStyle:airebo\_m00 (SEGFAULT)  
246 - ManybodyPairStyle:bop (SEGFAULT)  
247 - ManybodyPairStyle:bop\_save (Failed)  
250 - ManybodyPairStyle:drip (Failed)  
251 - ManybodyPairStyle:drip\_real (Failed)  
256 - ManybodyPairStyle:ilp-graphene-hbn (SEGFAULT)  
257 - ManybodyPairStyle:ilp-graphene-hbn\_notaper (SEGFAULT)  
258 - ManybodyPairStyle:kolmogorov\_crespi\_full (Failed)  
259 - ManybodyPairStyle:kolmogorov\_crespi\_full\_notaper (SEGFAULT)  
262 - ManybodyPairStyle:lebedeva\_z (Failed)  
263 - ManybodyPairStyle:meam (SEGFAULT)  
275 - ManybodyPairStyle:rann (SEGFAULT)  
277 - ManybodyPairStyle:snap (SEGFAULT)  
290 - ManybodyPairStyle:vashishta (SEGFAULT)  
291 - ManybodyPairStyle:vashishta\_table (SEGFAULT)  
331 - KSpaceStyle:ewald\_disp (SEGFAULT)  
333 - KSpaceStyle:ewald\_nozforce (SEGFAULT)  
336 - KSpaceStyle:ewald\_tri (SEGFAULT)  
337 - KSpaceStyle:pppm (SEGFAULT)  
338 - KSpaceStyle:pppm\_ad (SEGFAULT)  
339 - KSpaceStyle:pppm\_cg (SEGFAULT)  
340 - KSpaceStyle:pppm\_cg\_ad (SEGFAULT)  
341 - KSpaceStyle:pppm\_cg\_tiled (SEGFAULT)  
342 - KSpaceStyle:pppm\_dipole (SEGFAULT)  
347 - KSpaceStyle:pppm\_disp\_tip4p (Failed)  
349 - KSpaceStyle:pppm\_slab (SEGFAULT)  
354 - KSpaceStyle:pppm\_tip4p (Failed)  
357 - KSpaceStyle:pppm\_tip4p\_slab (SEGFAULT)  
358 - KSpaceStyle:pppm\_tri (SEGFAULT)  
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)  
381 - FixTimestep:momentum (Failed)  
453 - DihedralStyle:quadratic (Failed)  
455 - DihedralStyle:table\_cut\_linear (Failed)  
457 - DihedralStyle:table\_linear (Failed)  
458 - DihedralStyle:table\_spline (Failed)

## Notes

- Please check pages of [CPU](#) and [2022-Jun23 Intel MPI+GPU](#) versions.