

## LAMMPS 23Jun22 with GPU support (Intel MPI)

### Webpage

<https://www.lammps.org>

### Version

23Jun22 Update 2

### 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.tar.gz
- (some of files will be downloaded in the script below)

### Build Procedure

```
#!/bin/sh

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

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

WORKDIR=/gwork/users/${USER}/lammps-23Sep2022-cuda
LAMMPS_WORKDIR=${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

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
# MK-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-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} \
-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

```

## テスト

以下のジョブで実行

```

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

NAME=lammmps-23Jun2022
WORKDIR=/gwork/users/${USER}/lammmps-23Sep2022-cuda
LAMMPS_WORKDIR=${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

```

## Test Results

### List of failed tests:

The following tests FAILED:

- 35 - SimpleCommands (SEGFAULT)
- 43 - ComputeGlobal (Failed)
- 68 - MolPairStyle:beck (SEGFAULT)
- 69 - MolPairStyle:born (SEGFAULT)
- 74 - MolPairStyle:born\_coul\_table\_cs (SEGFAULT)
- 76 - MolPairStyle:born\_coul\_wolf\_cs (SEGFAULT)
- 77 - MolPairStyle:buck (SEGFAULT)
- 78 - MolPairStyle:buck\_coul\_cut (SEGFAULT)
- 79 - MolPairStyle:buck\_coul\_long (SEGFAULT)
- 81 - MolPairStyle:buck\_coul\_table (SEGFAULT)
- 84 - MolPairStyle:buck\_long\_coul\_off (SEGFAULT)
- 86 - MolPairStyle:buck\_mdf (SEGFAULT)
- 88 - MolPairStyle:buck\_table\_coul\_off (SEGFAULT)
- 89 - MolPairStyle:buck\_table\_coul\_table (SEGFAULT)
- 95 - MolPairStyle:coul\_diel (SEGFAULT)
- 96 - MolPairStyle:coul\_dsf (SEGFAULT)
- 99 - MolPairStyle:coul\_long\_cs (SEGFAULT)
- 100 - MolPairStyle:coul\_long\_soft (SEGFAULT)
- 103 - MolPairStyle:coul\_slater\_long (Failed)
- 105 - MolPairStyle:coul\_streitz\_wolf (SEGFAULT)
- 106 - MolPairStyle:coul\_table (SEGFAULT)
- 119 - MolPairStyle:hybrid\_multiple (SEGFAULT)
- 122 - MolPairStyle:lj\_charmm\_coul\_charmm (SEGFAULT)
- 124 - MolPairStyle:lj\_charmm\_coul\_long (SEGFAULT)
- 125 - MolPairStyle:lj\_charmm\_coul\_long\_soft (SEGFAULT)
- 126 - MolPairStyle:lj\_charmm\_coul\_table (SEGFAULT)
- 127 - MolPairStyle:lj\_charmmfsw\_coul\_charmmfsw (SEGFAULT)
- 135 - MolPairStyle:lj\_class2\_coul\_long\_soft (SEGFAULT)
- 136 - MolPairStyle:lj\_class2\_coul\_table (SEGFAULT)
- 139 - MolPairStyle:lj\_cubic (SEGFAULT)
- 140 - MolPairStyle:lj\_cut (SEGFAULT)
- 142 - MolPairStyle:lj\_cut\_coul\_cut\_soft (SEGFAULT)
- 145 - MolPairStyle:lj\_cut\_coul\_long (SEGFAULT)
- 147 - MolPairStyle:lj\_cut\_coul\_long\_soft (SEGFAULT)
- 148 - MolPairStyle:lj\_cut\_coul\_table (SEGFAULT)
- 150 - MolPairStyle:lj\_cut\_coul\_wolf (SEGFAULT)
- 153 - MolPairStyle:lj\_cut\_soft (SEGFAULT)
- 154 - MolPairStyle:lj\_cut\_tip4p\_cut (SEGFAULT)
- 157 - MolPairStyle:lj\_cut\_tip4p\_table (SEGFAULT)
- 166 - MolPairStyle:lj\_long\_cut\_dipole\_long (SEGFAULT)
- 167 - MolPairStyle:lj\_long\_cut\_tip4p\_long (SEGFAULT)
- 168 - MolPairStyle:lj\_long\_dipole\_long (SEGFAULT)
- 170 - MolPairStyle:lj\_mdf (SEGFAULT)
- 173 - MolPairStyle:lj\_sdk\_coul\_table (SEGFAULT)
- 175 - MolPairStyle:lj\_smooth (SEGFAULT)
- 181 - MolPairStyle:lj\_table\_coul\_table (SEGFAULT)
- 182 - MolPairStyle:lj\_table\_tip4p\_long (SEGFAULT)
- 183 - MolPairStyle:lj\_table\_tip4p\_table (SEGFAULT)
- 184 - MolPairStyle:mie\_cut (SEGFAULT)
- 185 - MolPairStyle:mm3\_switch3\_coulgauss\_long (SEGFAULT)
- 187 - MolPairStyle:morse (SEGFAULT)
- 190 - MolPairStyle:nm\_cut (SEGFAULT)
- 191 - MolPairStyle:nm\_cut\_coul\_cut (SEGFAULT)
- 192 - MolPairStyle:nm\_cut\_coul\_long (SEGFAULT)
- 193 - MolPairStyle:nm\_cut\_coul\_table (SEGFAULT)
- 197 - MolPairStyle:soft (SEGFAULT)
- 204 - MolPairStyle:wf\_cut (SEGFAULT)
- 206 - MolPairStyle:zbl (SEGFAULT)
- 211 - AtomicPairStyle:born (SEGFAULT)

212 - AtomicPairStyle:buck\_coul\_cut\_geq\_point (Failed)  
213 - AtomicPairStyle:buck\_coul\_cut\_geq\_shielded (Failed)  
214 - AtomicPairStyle:colloid (SEGFAULT)  
216 - AtomicPairStyle:colloid\_multi\_tri (SEGFAULT)  
218 - AtomicPairStyle:colloid\_tiled\_tri (SEGFAULT)  
225 - AtomicPairStyle:eam\_fs (SEGFAULT)  
227 - AtomicPairStyle:eam\_he (SEGFAULT)  
228 - AtomicPairStyle:eam\_he\_real (SEGFAULT)  
230 - AtomicPairStyle:edip (SEGFAULT)  
231 - AtomicPairStyle:eim (SEGFAULT)  
232 - AtomicPairStyle:gauss (SEGFAULT)  
233 - AtomicPairStyle:hybrid-eam (SEGFAULT)  
234 - AtomicPairStyle:hybrid-eam\_fs (SEGFAULT)  
235 - AtomicPairStyle:kim\_lj (SEGFAULT)  
237 - AtomicPairStyle:meam (SEGFAULT)  
238 - AtomicPairStyle:meam\_spline (Failed)  
239 - AtomicPairStyle:meam\_sw\_spline (SEGFAULT)  
242 - AtomicPairStyle:reaxff-acks2 (SEGFAULT)  
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)  
254 - AtomicPairStyle:table\_linear (SEGFAULT)  
260 - ManybodyPairStyle:airebo\_00 (SEGFAULT)  
266 - ManybodyPairStyle:comb3 (SEGFAULT)  
268 - ManybodyPairStyle:drip\_real (SEGFAULT)  
273 - ManybodyPairStyle:ilp-graphene-hbn (Failed)  
274 - ManybodyPairStyle:ilp-graphene-hbn\_notaper (SEGFAULT)  
275 - ManybodyPairStyle:kolmogorov\_crespi\_full (SEGFAULT)  
279 - ManybodyPairStyle:lebedeva\_z (SEGFAULT)  
281 - ManybodyPairStyle:mliap\_nn (SEGFAULT)  
288 - ManybodyPairStyle:pace\_recursive (SEGFAULT)  
289 - ManybodyPairStyle:polymorphic\_sw (SEGFAULT)  
290 - ManybodyPairStyle:polymorphic\_tersoff (SEGFAULT)  
291 - ManybodyPairStyle:quip-sw (SEGFAULT)  
297 - ManybodyPairStyle:sw-mod-multi (SEGFAULT)  
298 - ManybodyPairStyle:sw-multi (SEGFAULT)  
301 - ManybodyPairStyle:ttersoff\_mod (SEGFAULT)  
306 - ManybodyPairStyle:ttersoff\_table (SEGFAULT)  
309 - ManybodyPairStyle:vashishta (SEGFAULT)  
310 - ManybodyPairStyle:vashishta\_table (SEGFAULT)  
349 - KSpaceStyle:ewald (SEGFAULT)  
350 - KSpaceStyle:ewald\_conp\_charge (SEGFAULT)  
352 - KSpaceStyle:ewald\_disp (SEGFAULT)  
356 - KSpaceStyle:ewald\_slab (SEGFAULT)  
357 - KSpaceStyle:ewald\_tilted (SEGFAULT)  
360 - KSpaceStyle:pppm\_ad (SEGFAULT)  
361 - KSpaceStyle:pppm\_cg (SEGFAULT)  
362 - KSpaceStyle:pppm\_cg\_ad (Failed)  
363 - KSpaceStyle:pppm\_cg\_tiled (Failed)  
365 - KSpaceStyle:pppm\_dipole (SEGFAULT)  
370 - KSpaceStyle:pppm\_disp\_tip4p (Failed)  
372 - KSpaceStyle:pppm\_nozforce (SEGFAULT)  
373 - KSpaceStyle:pppm\_slab (SEGFAULT)  
374 - KSpaceStyle:pppm\_stagger (SEGFAULT)  
375 - KSpaceStyle:pppm\_stagger\_tiled (SEGFAULT)  
378 - KSpaceStyle:pppm\_tip4p (SEGFAULT)  
379 - KSpaceStyle:pppm\_tip4p\_ad (SEGFAULT)  
381 - KSpaceStyle:pppm\_tip4p\_slab (SEGFAULT)  
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)  
393 - FixTimestep:addtorque\_const (Failed)  
459 - FixTimestep:spring\_rg (Failed)  
466 - FixTimestep:wall\_harmonic\_const (Failed)  
482 - DihedralStyle:quadratic (Failed)  
484 - DihedralStyle:table\_cut\_linear (Failed)  
486 - DihedralStyle:table\_linear (Failed)  
487 - DihedralStyle:table\_spline (Failed)

## Notes

- Please also check notes about CPU version.
- If Intel Compilers are employed in GPU version, non-negligible slowdown happens on LJ system (when -pk gpu is active). The same slowdown happens on GCC+OpenMPI version. This GCC+IntelMPI version is strangely free from that issue.