

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 \

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-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.