

Example usage of the ænet-LAMMPS interface for molecular dynamics simulations with artificial neural network (ANN) potentials.

Contact: Michael Stephen Chen (misch@stanford.edu), Tobias Morawietz (tobias.morawietz.nn@gmail.com), Nong Artrith (nartrith@atomistic.net)

If you make use of the aenet-LAMMPS interface, please cite the following reference:

M.S. Chen, T. Morawietz, H. Mori, T.E. Markland, N. Artrith, AENET-LAMMPS and AENET-TINKER: Interfaces for Accurate and Efficient Molecular Dynamics Simulations with Machine Learning Potentials, in preparation (2021).

The database can be obtained from the Materials Cloud repository, DOI:

<https://doi.org/10.24435/materialscloud:dx-ct>

Tutorial: https://colab.research.google.com/drive/1Km8JVFM2DCeEIaE2n_WgMgLa7IU_IFh?usp=sharing or <https://github.com/atomisticnet/aenet-lammps/tutorial>

▼ 1. Downloading and extracting required codes

For this example, we will be using the [ænet](#) library version 2.0.4 and the [LAMMPS](#) release from 4 Feb 2020. Running the cell below downloads extracts both of these software packages into the working directory.

```
!wget https://github.com/atomisticnet/aenet/archive/refs/tags/v2.0.4.tar.gz
!wget https://download.lammps.org/tars/lammps-4Feb2020.tar.gz

!tar -xzvf lammps-4Feb2020.tar.gz
!tar -xzvf v2.0.4.tar.gz
```

Streaming output truncated to the last 5000 lines.

```
lammps-4Feb20/lib/gpu/lal_eam.cu
lammps-4Feb20/lib/gpu/lal_soft.cu
lammps-4Feb20/lib/gpu/lal_lj_expand.cpp
lammps-4Feb20/lib/gpu/lal_re_squared_ext.cpp
lammps-4Feb20/lib/gpu/lal_tersoff.cu
lammps-4Feb20/lib/gpu/lal_colloid.cpp
lammps-4Feb20/lib/gpu/lal_colloid.cu
lammps-4Feb20/lib/gpu/lal_tersoff_mod.cu
lammps-4Feb20/lib/gpu/lal_sw.cpp
lammps-4Feb20/lib/gpu/lal_dipole_lj_ext.cpp
lammps-4Feb20/lib/gpu/lal_buck.cpp
lammps-4Feb20/lib/gpu/README
lammps-4Feb20/lib/gpu/lal_lj_gromacs.cpp
lammps-4Feb20/lib/gpu/lal_born_coul_long_cs.cpp
```

```

lammps-4Feb20/lib/gpu/lal_coul_dsf.h
lammps-4Feb20/lib/gpu/lal_charmm_long.cpp
lammps-4Feb20/lib/gpu/lal_mie.cu
lammps-4Feb20/lib/gpu/lal_lj_class2_long.cpp
lammps-4Feb20/lib/gpu/lal_buck_coul_long.cu
lammps-4Feb20/lib/gpu/lal_neighbor_shared.cpp
lammps-4Feb20/lib/gpu/lal_lj_coul_long.cu
lammps-4Feb20/lib/gpu/Makefile.lammps.mac_ocl
lammps-4Feb20/lib/gpu/lal_re_squared_lj.cu
lammps-4Feb20/lib/gpu/lal_yukawa_ext.cpp
lammps-4Feb20/lib/gpu/lal_base_charge.h
lammps-4Feb20/lib/gpu/Makefile.xk7
lammps-4Feb20/lib/gpu/lal_lj_coul.cpp
lammps-4Feb20/lib/gpu/lal_gauss_ext.cpp
lammps-4Feb20/lib/gpu/lal_lj_cubic.h
lammps-4Feb20/lib/gpu/Makefile.lammps.mingw-cross
lammps-4Feb20/lib/gpu/lal_eam.cpp
lammps-4Feb20/lib/gpu/lal_coul_long_ext.cpp
lammps-4Feb20/lib/gpu/lal_lj_coul_ext.cpp
lammps-4Feb20/lib/gpu/lal_dipole_lj.cu
lammps-4Feb20/lib/gpu/lal_lj_coul_debye.cu
lammps-4Feb20/lib/gpu/lal_dpd_ext.cpp
lammps-4Feb20/lib/gpu/lal_uvm.cpp
lammps-4Feb20/lib/gpu/lal_device.cu
lammps-4Feb20/lib/gpu/lal_vashishta.cpp
lammps-4Feb20/lib/gpu/lal_lj_class2_long.h
lammps-4Feb20/lib/gpu/lal_neighbor_cpu.cu
lammps-4Feb20/lib/gpu/lal_buck_ext.cpp
lammps-4Feb20/lib/gpu/lal_dipole_lj.cpp
lammps-4Feb20/lib/gpu/lal_ellipsoid_extra.h
lammps-4Feb20/lib/gpu/lal_soft.h
lammps-4Feb20/lib/gpu/lal_lj.cu
lammps-4Feb20/lib/gpu/lal_base_dipole.h
lammps-4Feb20/lib/gpu/lal_table_ext.cpp
lammps-4Feb20/lib/gpu/lal_lj_coul_long_ext.cpp
lammps-4Feb20/lib/gpu/lal_zbl.cpp
lammps-4Feb20/lib/gpu/lal_tersoff_extra.h
lammps-4Feb20/lib/gpu/lal_coul.cu
lammps-4Feb20/lib/gpu/lal_tersoff.cpp
lammps-4Feb20/lib/gpu/lal_base_ellipsoid.cpp
lammps-4Feb20/lib/gpu/Makefile.mac_openc1
lammps-4Feb20/lib/gpu/lal_dipole_lj_sf.cpp
lammps-4Feb20/lib/gpu/Makefile.linux_multi
lammps-4Feb20/lib/gpu/lal_dpd.cpp

```

Now we download the ænet-LAMMPS code directly from the GitHub repository.

```
!git clone https://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@github.com/atomisticnet
```

```
Cloning into 'aenet-lammps'...
remote: Enumerating objects: 266, done.
remote: Counting objects: 100% (266/266), done.
remote: Compressing objects: 100% (133/133), done.
remote: Total 266 (delta 111), reused 195 (delta 71), pack-reused 0
Receiving objects: 100% (266/266), 10.14 MiB | 4.34 MiB/s, done.
Resolving deltas: 100% (111/111), done.
```

▼ 2. Compiling aenet

In the cell below, we build the aenet library that will be called by the aenet-LAMMPS interface. Note that in this example we use the OpenBLAS library, but other Makefiles linking alternative optimized linear algebra libraries are provided as part of aenet. For more details on compiling aenet, please see the install instructions found as part of the [aenet documentation](#). Also, parallelization will be left to LAMMPS so we should only compile a serial version of the aenet library.

```
%cd /content/aenet-2.0.4/lib/
!make
%cd ../src
!make clean
!make -f makefiles/Makefile.gfortran_openblas_serial lib
%cd /content/
```

```
/content/aenet-2.0.4/lib
tar xfvz Lbfgsb.3.0.tar.gz
./._Lbfgsb.3.0
Lbfgsb.3.0/
Lbfgsb.3.0/._algorithm.pdf
Lbfgsb.3.0/algorithm.pdf
Lbfgsb.3.0/blas.f
Lbfgsb.3.0/._code.pdf
Lbfgsb.3.0/code.pdf
Lbfgsb.3.0/driver1.f
Lbfgsb.3.0/driver1.f90
Lbfgsb.3.0/driver2.f
Lbfgsb.3.0/driver2.f90
Lbfgsb.3.0/driver3.f
Lbfgsb.3.0/driver3.f90
Lbfgsb.3.0/._iterate.dat
Lbfgsb.3.0/iterate.dat
Lbfgsb.3.0/lbfgsb.f
Lbfgsb.3.0/License.txt
Lbfgsb.3.0/linpack.f
Lbfgsb.3.0/Makefile
```

```

Lbfgsb.3.0/._Makefile
Lbfgsb.3.0/Makefile
Lbfgsb.3.0/._OUTPUTS
Lbfgsb.3.0/OUTPUTS/
Lbfgsb.3.0/README
Lbfgsb.3.0/timer.f
Lbfgsb.3.0/x.lbfgsb_77_1
Lbfgsb.3.0/x.lbfgsb_77_2
Lbfgsb.3.0/x.lbfgsb_77_3
Lbfgsb.3.0/x.lbfgsb_90_1
Lbfgsb.3.0/x.lbfgsb_90_2
Lbfgsb.3.0/x.lbfgsb_90_3
Lbfgsb.3.0/OUTPUTS/._output_77_1
Lbfgsb.3.0/OUTPUTS/output_77_1
Lbfgsb.3.0/OUTPUTS/._output_77_2
Lbfgsb.3.0/OUTPUTS/output_77_2
Lbfgsb.3.0/OUTPUTS/._output_77_3
Lbfgsb.3.0/OUTPUTS/output_77_3
Lbfgsb.3.0/OUTPUTS/._output_90_1
Lbfgsb.3.0/OUTPUTS/output_90_1
Lbfgsb.3.0/OUTPUTS/._output_90_2
Lbfgsb.3.0/OUTPUTS/output_90_2
Lbfgsb.3.0/OUTPUTS/._output_90_3
Lbfgsb.3.0/OUTPUTS/output_90_3
gfortran -c -O2 Lbfgsb.3.0/blas.f -o Lbfgsb.3.0/blas.o
gfortran -c -O2 Lbfgsb.3.0/lbfgsb.f -o Lbfgsb.3.0/lbfgsb.o
gfortran -c -O2 Lbfgsb.3.0/linpack.f -o Lbfgsb.3.0/linpack.o
gfortran -c -O2 Lbfgsb.3.0/timer.f -o Lbfgsb.3.0/timer.o
ar -crusv liblbfgsb.a Lbfgsb.3.0/blas.o Lbfgsb.3.0/lbfgsb.o Lbfgsb.3.0/li
ar: `u' modifier ignored since `D' is the default (see `U')
a - Lbfgsb.3.0/blas.o
a - Lbfgsb.3.0/lbfgsb.o
a - Lbfgsb.3.0/linpack.o
a - Lbfgsb.3.0/timer.o
gfortran -c -O2 -fPIC -o Lbfgsb.3.0/blas_pic.o Lbfgsb.3.0/blas.f
gfortran -c -O2 -fPIC -o Lbfgsb.3.0/lbfgsb_pic.o Lbfgsb.3.0/lbfgsb.f
gfortran -c -O2 -fPIC -o Lbfgsb.3.0/linpack_pic.o Lbfgsb.3.0/linpack.f
gfortran -c -O2 -fPIC -o Lbfgsb.3.0/timer_pic.o Lbfgsb.3.0/timer.f
gcc -shared Lbfgsb.3.0/blas_pic.o Lbfgsb.3.0/lbfgsb_pic.o Lbfgsb.3.0/linp

```

▼ 3. Compiling LAMMPS with ænet support

Note, for more detailed instructions on how to patch and compile LAMMPS with ænet support please see the [ænet-LAMMPS GitHub repository](#).

First, let us organize things so that the ænet header and library files are where we expect them to be when compiling things.

```
%cd /content/lammps-4Feb20/lib/
!mkdir -p aenet/lib
!mkdir -p aenet/include
%cd /content/lammps-4Feb20/lib/aenet/include
!ln -s /content/aenet-2.0.4/src/aenet.h
%cd /content/lammps-4Feb20/lib/aenet/lib
!ln -s /content/aenet-2.0.4/src/libaenet.* .
!ln -s /content/aenet-2.0.4/lib/liblbfgsb.* .

/content/lammps-4Feb20/lib
/content/lammps-4Feb20/lib/aenet/include
/content/lammps-4Feb20/lib/aenet/lib
```

Next, let us patch LAMMPS with the ænet-LAMMPS interface files. This entails copying over the provided USER-AENET folder into the LAMMPS src directory and replacing the LAMMPS Makefile. Since we compiled the ænet library using Makefile.gfortran_openblas_serial, we will use the corresponding Install.sh file for our custom USER-AENET package so as to make sure that OpenBLAS is linked during the compilation.

```
%cd /content/lammps-4Feb20/src/
! cp -r /content/aenet-lammps/USER-AENET .
! cp -f /content/aenet-lammps/Makefile-aenetlammps Makefile
! cp -f USER-AENET/Install.sh-gfortran_openblas_serial USER-AENET/Install.sh

/content/lammps-4Feb20/src
```

We need to flag the USER-AENET package to be included as part of our LAMMPS compilation and lastly we compile an MPI-parallelized LAMMPS executable.

```
%cd /content/lammps-4Feb20/src/
! make yes-user-aenet
! make mpi

/content/lammps-4Feb20/src
Gathering installed package information (may take a little while)
make[1]: Entering directory '/content/lammps-4Feb20/src'
Gathering git version information
make[1]: Leaving directory '/content/lammps-4Feb20/src'
Compiling LAMMPS for machine mpi
make[1]: Entering directory '/content/lammps-4Feb20/src/Obj_mpi'
cc -O -o fastdep.exe ../DEPEND/fastdep.c
make[1]: Leaving directory '/content/lammps-4Feb20/src/Obj_mpi'
make[1]: Entering directory '/content/lammps-4Feb20/src/Obj_mpi'
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -I../lib/aenet/inclu
mpicxx -g -O3 -DLAMMPS_GZIP -DLAMMPS_MEMALIGN=64 -I../lib/aenet/inclu
```


▼ 4. Running LAMMPS with ænet ANN potentials

An example LAMMPS molecular dynamics simulation of liquid water with an ænet ANN potential is provided as part of the ænet-LAMMPS package.

First we need to make sure that the ænet library file can be dynamically linked when we run LAMMPS.


```
%env LD_LIBRARY_PATH=/content/lammps-4Feb20/lib/aenet/lib:/usr/local/nvidia/lib:/usr
!echo $LD_LIBRARY_PATH
```

```
env: LD_LIBRARY_PATH=/content/lammps-4Feb20/lib/aenet/lib:/usr/local/nvidia/li
/content/lammps-4Feb20/lib/aenet/lib:/usr/local/nvidia/lib:/usr/local/nvidia/l
```

In the cell below we run the short example simulation. Some details concerning the simulation (see the LAMMPS input file md.lmp for more details):

- NVT simulation of liquid water at 300K
- Initial frame specified by 01_Start/firstframe.start file (64 water molecules in box with side lengths of 12.417 Angstroms)
- H.ann and O.ann are the ænet ANN potential files
- Simulation runs for 100 steps with 0.5 fs spacing between steps and writing out properties every 2.0fs
- Input file flags the use of the "[metal](#)" unit system since the ANN potential was trained using eV units for energies and Angstroms units for positions.
- Positions, velocities, forces, and energies are written out to files in the 02_Traj folder (traj.xyz, velocities.xyz, forces.xyz, and analysis_frames.dat respectively)

```
%cd /content/aenet-lammps/examples/water
!/content/lammps-4Feb20/src/lmp_mpi -in md.lmp
```

	28	330.23232	-30057.005	0	-30048.852	5347.1609
	32	319.03827	-30056.716	0	-30048.84	6956.5274
	36	316.10423	-30056.657	0	-30048.853	3009.7582
	40	299.62656	-30056.248	0	-30048.85	571.70686
	44	326.0215	-30056.911	0	-30048.862	545.76778
	48	312.05352	-30056.516	0	-30048.812	3383.9577
	52	318.83778	-30056.654	0	-30048.782	4847.6457
	56	300.95386	-30056.155	0	-30048.725	6217.3848
	60	302.54665	-30056.278	0	-30048.808	4371.6857
	64	304.476	-30056.331	0	-30048.814	2679.8174
	68	300.04551	-30056.189	0	-30048.781	3053.4613

```

72      314.64045      -30056.534      0      -30048.766      5653.102
76      293.68455      -30055.993      0      -30048.742      8959.0566
80      324.65481      -30056.783      0      -30048.768      5872.407
84      305.23793      -30056.259      0      -30048.723      3076.0805
88      324.61769      -30056.773      0      -30048.759      1100.5434
92      311.16735      -30056.459      0      -30048.777      4735.5056
96      308.70087      -30056.388      0      -30048.767      8820.4214
100     320.68558      -30056.668      0      -30048.751      7659.6949

```

Loop time of 805.919 on 1 procs for 100 steps with 192 atoms

Performance: 0.005 ns/day, 4477.326 hours/ns, 0.124 timesteps/s
95.7% CPU use with 1 MPI tasks x no OpenMP threads

MPI task timing breakdown:

Section	min time	avg time	max time	%varavg	%total
Pair	805.84	805.84	805.84	0.0	99.99
Neigh	0.041803	0.041803	0.041803	0.0	0.01
Comm	0.0035625	0.0035625	0.0035625	0.0	0.00
Output	0.023947	0.023947	0.023947	0.0	0.00
Modify	0.0053537	0.0053537	0.0053537	0.0	0.00
Other		0.0006583			0.00

```

Nlocal:      192 ave 192 max 192 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Nghost:      2302 ave 2302 max 2302 min
Histogram: 1 0 0 0 0 0 0 0 0 0
Neighs:       0 ave 0 max 0 min
Histogram: 1 0 0 0 0 0 0 0 0 0
FullNghs:    46754 ave 46754 max 46754 min
Histogram: 1 0 0 0 0 0 0 0 0 0

```

Total # of neighbors = 46754

Ave neighs/atom = 243.51

Neighbor list builds = 25

Dangerous builds = 0

System init for write_restart ...

Total wall time: 0:13:34

[73f8d0ac8026:05923] *** Process received signal ***

[73f8d0ac8026:05923] Signal: Segmentation fault (11)

[73f8d0ac8026:05923] Signal code: Address not mapped (1)

[73f8d0ac8026:05923] Failing at address: 0x7f907648920d

[73f8d0ac8026:05923] [0] /lib/x86_64-linux-gnu/libpthread.so.0(+0x12980)[0x

[73f8d0ac8026:05923] [1] /lib/x86_64-linux-gnu/libc.so.6(getenv+0xa5)[0x7f9

[73f8d0ac8026:05923] [2] /usr/lib/x86_64-linux-gnu/libtcmalloc.so.4(_ZN13TC

[73f8d0ac8026:05923] [3] /lib/x86_64-linux-gnu/libc.so.6(__cxa_finalize+0xf

[73f8d0ac8026:05923] [4] /usr/lib/x86_64-linux-gnu/libtcmalloc.so.4(+0x13cb

[73f8d0ac8026:05923] *** End of error message ***

