2022_09_21_LAMMPS_CMake_Adding ML-ATOMNN Package

Wednesday, September 21, 2022   11:56 AM

Adding the ML-ATOMNN Package

The procedure, here, is courtesy of Michal Kanski and Axel Kohlmey: https://matsci.org/t/adding-a-custom-package-to-lammps-cmake-configuration/44423.

> (Note that my use of "sudo" for compiling is highly recommended against. The LAMMPS source should be downloaded to a directory owned by a non-root user account, so that compiling can be done without "sudo".)

mkanski   1 ✏ 5d

It's fairly easy. You just need to add a new line (ML-ATOMNN) in $LAMMPSDIR/cmake/CMakeLists.txt around line 240 and copy your directory to $LAMMPSDIR/src
Additionally, because you need Eigen library, you need a custom cmake file (called ML-ATOMNN.cmake) at $LAMMPSDIR/cmake/Modules/Packages. Look at the file MACHDYN.cmake in the same directory to see how to handle requesting Eigen.

akohlmey Representative of LAMMPS
September 22

> s   sej423:
>
> See attached. Any additional advice?

You also need to add the ML-ATOMNN package name into this loop around line 500 in cmake/CMakeLists.txt

```
foreach(PKG_WITH_INCL KSPACE PYTHON ML-IAP VORONOI COLVARS ML-HDNNP MDI MOLFILE NETCDF
        PLUMED QMMM ML-QUIP SCAFACOS MACHDYN VTK KIM LATTE MSCG COMPRESS ML-PACE)
  if(PKG_${PKG_WITH_INCL})
    include(Packages/${PKG_WITH_INCL})
  endif()
endforeach()
```

This is required so that your added file in cmake/Modules/Packages/ is read and processed.

Copied the most up-to-date version of the ML-ATOMNN package to the G:\02_Temple folder.

```
scott@lammps-cmake:/mnt/g/02_Temple$ ls -la
total 256
drwxr-xr-x 2 root root      0 Aug 16 11:41 .
drwxr-xr-x 2 root root      0 Dec 31  1979 ..
drwxr-xr-x 2 root root      0 Jul  7 04:25 2022_05_10_LAMMPS_ICME_HPC_MississippiState
drwxr-xr-x 2 root root      0 Jul  7 04:25 2022_05_17_LAMMPS_Examples_AtC_no_atomsFE
drwxr-xr-x 2 root root      0 Jul  7 04:25 2022_05_23_LAMMPS_Examples_AtC_eam_energy
drwxr-xr-x 2 root root      0 Jul  7 04:25 2022_05_25_LAMMPS_Examples_AtC_cb_unistrain
drwxr-xr-x 2 root root      0 Jul  7 04:25 2022_06_02_LAMMPS_Examples_AtC_eam_energy_FEMOnly
drwxr-xr-x 2 root root      0 Jul  7 04:25 2022_06_07_LAMMPS_MissState_UniaxTens_Al99_PureAtom
drwxr-xr-x 2 root root      0 Jun 23 10:39 2022_06_17_LAMMPS_MissState_UniaxTens_Al99_PureAtom_Poissons
drwxr-xr-x 2 root root      0 Jul  7 04:25 2022_06_17_LAMMPS_MissState_UniaxTens_Al99_PureFE
drwxr-xr-x 2 root root      0 Jul  7 04:25 2022_06_18_LAMMPS_Examples_AtC_no_atomsFE_vel
drwxr-xr-x 2 root root      0 Jun 22 19:16 2022_06_20_LAMMPS_Examples_AtC_no_atomsFE_unit_Ar
drwxr-xr-x 2 root root      0 Jul 24 21:54 2022_06_24_01_LAMMPS_Temple_ANN_Ni_read_data
drwxr-xr-x 2 root root      0 Jul  8 15:50 2022_06_24_02_LAMMPS_Temple_ANN_Ni_lattice
drwxr-xr-x 2 root root      0 Jul  4 13:58 2022_07_03_VMD_Tutorial_UsingVMD
drwxr-xr-x 2 root root      0 Jul  6 11:28 2022_07_04_LAMMPS_NEU_Unit_FEA+Atom
drwxr-xr-x 2 root root      0 Jul 21 11:05 2022_07_07_LAMMPS_Examples_AtC_elastic_bar1d_Ar
drwxr-xr-x 2 root root      0 Jul 11 13:48 2022_07_08_LAMMPS_Examples_AtC_elastic_bar1d_Ni
drwxr-xr-x 2 root root      0 Jul 14 09:52 2022_07_09_LAMMPS_Examples_no_atomsFE_unit_Ni
drwxr-xr-x 2 root root      0 Jul 19 14:40 2022_07_14_LAMMPS_Examples_AtC_elastic_bar1d_Cu
drwxr-xr-x 2 root root      0 Jul 16 20:09 2022_07_14_LAMMPS_MissState_UniaxTens_Cu_PureAtom
drwxr-xr-x 2 root root      0 Jul 16 21:00 2022_07_16_LAMMPS_Examples_AtC_bar1d_Ar_SplitFE
drwxr-xr-x 2 root root      0 Jul 21 11:06 2022_07_19_01_LAMMPS_Examples_AtC_bar1d_ArToCu
drwxr-xr-x 2 root root      0 Jul 19 15:09 2022_07_19_02_LAMMPS_Examples_AtC_bar1d_Ar_ToRupt
drwxr-xr-x 2 root root      0 Jul 21 11:48 2022_07_21_LAMMPS_elastic_bar1d_unit_Ar
drwxr-xr-x 2 root root      0 Aug  5 09:43 2022_08_03_LibMultiScale_Example_atc_xiao_Al
drwxr-xr-x 2 root root      0 Aug  5 23:56 2022_08_05_LibMultiScale_Example_atc_xiao_Al_FCC
drwxr-xr-x 2 root root      0 Aug  6 07:49 2022_08_05_LibMultiScale_Example_atc_xiao_Ni_NNP
drwxr-xr-x 2 root root      0 Aug 18 10:25 2022_08_18_01_LibMultiScale_Example_single_scale_cont
drwxr-xr-x 2 root root      0 Aug 18 10:40 2022_08_18_02_LibMultiScale_Example_custom_atc_coupling
drwxr-xr-x 2 root root      0 Aug 18 12:51 2022_08_18_04_LAMMPS_UpdatedANNPkg_UniaxTens_NiNNP
drwxr-xr-x 2 root root      0 Aug 18 12:39 2022_08_18_05_LAMMPS_UpdatedANNPkg_Temple_ANN_Ni
drwxr-xr-x 2 root root      0 Aug 24 10:31 2022_08_24_LibMultiScale_Example_custom_bridge_coupling
drwxr-xr-x 2 root root      0 Aug 24 16:33 2022_08_24_LibMultiScale_Test_single_scale_MECA1D_test_1D_Energy
drwxr-xr-x 2 root root      0 Aug 25 10:00 2022_08_25_LibMultiScale_Test_single_scale_MECA1D_test_1D_KineticEnergy
drwxr-xr-x 2 root root      0 Aug 30 10:57 2022_08_30_LibMultiScale_Test_single_scale_AKANTU_pbc_isotropic
drwxr-xr-x 2 root root      0 Aug  5 09:43 2022_09_01_LibMultiScale_Example_atc_xiao_Al_uni
-r-xr-xr-x 1 root root  78662 Sep 15 12:17 ML-ATOMNN.zip
```

Copied the ZIP file over to "/opt/lammps/src".

```
scott@lammps-cmake:/mnt/g/02_Temple$ sudo cp ML-ATOMNN.zip /opt/lammps/src/
scott@lammps-cmake:/mnt/g/02_Temple$ cd /opt/lammps/src/
```

```
scott@lammps-cmake:/opt/lammps/src$ ls -la | grep -i ML-ATOMNN
-r-xr-xr-x  1 root root  78662 Sep 15 12:18 ML-ATOMNN.zip
```

Unzipped the ML-ATOMNN ZIP file into the directory.

```
scott@lammps-cmake:/opt/lammps/src$ sudo unzip ML-ATOMNN.zip
Archive:  ML-ATOMNN.zip
  inflating: ML-ATOMNN/ann_basis.cpp
  inflating: ML-ATOMNN/ann_basis.h
  inflating: ML-ATOMNN/ann_basis_angular.cpp
  inflating: ML-ATOMNN/ann_basis_angular.h
  inflating: ML-ATOMNN/ann_basis_radial.cpp
  inflating: ML-ATOMNN/ann_basis_radial.h
```
...

```
scott@lammps-cmake:/opt/lammps/src$ ls -la | grep -i ML-ATOMNN
drwxr-xr-x  3 root root   4096 Sep 15 12:21 ML-ATOMNN
-r-xr-xr-x  1 root root  78662 Sep 15 12:18 ML-ATOMNN.zip
```

Deleted the ZIP file.

```
scott@lammps-cmake:/opt/lammps/src$ sudo rm -iv ML-ATOMNN.zip
rm: remove regular file 'ML-ATOMNN.zip'? y
removed 'ML-ATOMNN.zip'
```

Navigated to the "/opt/lammps/cmake" folder and backed up the "CMakeLists.txt" file.

```
scott@lammps-cmake:/opt/lammps/cmake$ ls -la
total 152
drwxr-xr-x  8 root root  4096 Aug 15 13:07 .
drwxr-xr-x 16 root root  4096 Aug 15 13:10 ..
-rw-r--r--  1 root root 21635 Aug 15 13:07 CMakeLists.jpeg
-rw-r--r--  1 root root 26060 Aug 15 13:07 CMakeLists.png
-rw-r--r--  1 root root 38196 Aug 15 13:07 CMakeLists.txt
-rw-r--r--  1 root root  5654 Aug 15 13:07 CMakeLists.zlib
-rw-r--r--  1 root root  8276 Aug 15 13:07 CMakeSettings.json
-rw-r--r--  1 root root   151 Aug 15 13:07 .coveragerc.in
drwxr-xr-x  3 root root  4096 Aug 15 13:07 etc
drwxr-xr-x  2 root root  4096 Aug 15 13:07 gpu
drwxr-xr-x  2 root root  4096 Aug 15 13:07 iwyu
-rw-r--r--  1 root root   152 Aug 15 13:07 LAMMPSConfig.cmake.in
drwxr-xr-x  3 root root  4096 Aug 15 13:07 Modules
drwxr-xr-x  2 root root  4096 Aug 15 13:07 pkgconfig
drwxr-xr-x  2 root root  4096 Aug 15 13:07 presets
scott@lammps-cmake:/opt/lammps/cmake$ sudo cp -v CMakeLists.txt CMakeLists.txt.bak
'CMakeLists.txt' -> 'CMakeLists.txt.bak'
```

Edited the file. Added the "ML-ATOMNN" package to the standard packages list (around line 240).

```
scott@lammps-cmake:/opt/lammps/cmake$ sudo nano CMakeLists.txt
```

Added "ML-ATOMNN" to the list of standard packages in "$LAMMPSDIR/cmake/CMakeLists.txt"

```
  GNU nano 4.8
  EFF
  ELECTRODE
  EXTRA-COMPUTE
  EXTRA-DUMP
  EXTRA-FIX
  EXTRA-MOLECULE
  EXTRA-PAIR
  FEP
  GRANULAR
  H5MD
  INTERLAYER
  KIM
  KSPACE
  LATBOLTZ
  LATTE
  MACHDYN
  MANIFOLD
  MANYBODY
  MC
  MDI
  MEAM
  MESONT
  MGPT
  MISC
▎ ML-ATOMNN
  ML-HDNNP
  ML-IAP
  ML-PACE
  ML-QUIP
  ML-RANN
  ML-SNAP
  MOFFF
  MOLECULE
  MOLFILE
  MPIIO
  MSCG
  NETCDF
  ORIENT
  PERI
  PHONON
  PLUGIN
  PLUMED
  POEMS
                                                      [ line 242/988 (24%),
```

Created "ML-ATOMNN.cmake" in "$LAMMPSDIR/cmake/Modules/Packages" directory.

Looks like the "MACHDYN.cmake" file contains everything needed to find/build Eigen.

```
scott@lammps-cmake:/opt/lammps/cmake/Modules/Packages$ cat MACHDYN.cmake
find_package(Eigen3 NO_MODULE)
if(EIGEN3_FOUND)
  set(DOWNLOAD_EIGEN3_DEFAULT OFF)
else()
  set(DOWNLOAD_EIGEN3_DEFAULT ON)
endif()
option(DOWNLOAD_EIGEN3 "Download Eigen3 instead of using an already installed one)" ${DOWNLOAD_EIGEN3_DEFAULT})
if(DOWNLOAD_EIGEN3)
  message(STATUS "Eigen3 download requested - we will build our own")

  set(EIGEN3_URL "${LAMMPS_THIRDPARTY_URL}/eigen-3.4.0.tar.gz" CACHE STRING "URL for Eigen3 tarball")
  set(EIGEN3_MD5 "4c527a9171d71a72a9d4186e65bea559" CACHE STRING "MD5 checksum of Eigen3 tarball")
  mark_as_advanced(EIGEN3_URL)
  mark_as_advanced(EIGEN3_MD5)
  include(ExternalProject)
  ExternalProject_Add(Eigen3_build
    URL      ${EIGEN3_URL}
    URL_MD5 ${EIGEN3_MD5}
    CONFIGURE_COMMAND "" BUILD_COMMAND "" INSTALL_COMMAND ""
  )
  ExternalProject_get_property(Eigen3_build SOURCE_DIR)
  add_library(LAMMPS::EIGEN3 INTERFACE IMPORTED)
  set_target_properties(LAMMPS::EIGEN3 PROPERTIES INTERFACE_INCLUDE_DIRECTORIES "${SOURCE_DIR}")
  target_link_libraries(lammps PRIVATE LAMMPS::EIGEN3)
  add_dependencies(LAMMPS::EIGEN3 Eigen3_build)
else()
  find_package(Eigen3 NO_MODULE)
  mark_as_advanced(Eigen3_DIR)
  if(NOT EIGEN3_FOUND)
    message(FATAL_ERROR "Eigen3 not found, help CMake to find it by setting EIGEN3_INCLUDE_DIR, or set DOWNLOAD_EIGEN3=ON to download it")
  endif()
  target_link_libraries(lammps PRIVATE Eigen3::Eigen)
endif()

# PGI/Nvidia compiler internals collide with vector intrinsics support in Eigen3
if((CMAKE_CXX_COMPILER_ID STREQUAL "PGI") OR (CMAKE_CXX_COMPILER_ID STREQUAL "NVHPC"))
  target_compile_definitions(lammps PRIVATE -DEIGEN_DONT_VECTORIZE)
endif()

target_compile_definitions(lammps PRIVATE -DEIGEN_NO_CUDA)
```

Simply copied to new file named "ML-ATOMNN.cmake".

```
scott@lammps-cmake:/opt/lammps/cmake/Modules/Packages$ sudo cp -v MACHDYN.cmake ML-ATOMNN.cmake
'MACHDYN.cmake' -> 'ML-ATOMNN.cmake'
```

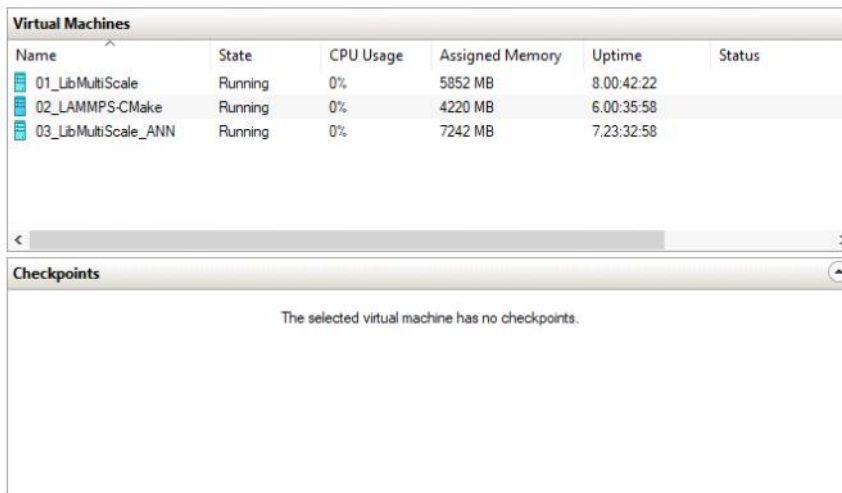Added the word "ML-ATOMNN" to "lammps/cmake/CMakeLists.txt".

```
foreach(PKG_WITH_INCL KSPACE PYTHON ML-IAP VORONOI COLVARS ML-HDNNP MDI MOLFILE NETCDF
        PLUMED QMMM ML-QUIP SCAFACOS MACHDYN VTK KIM LATTE MSCG COMPRESS ML-PACE ML-ATOMNN)
  if(PKG_${PKG_WITH_INCL})
    include(Packages/${PKG_WITH_INCL})
  endif()
endforeach()
```

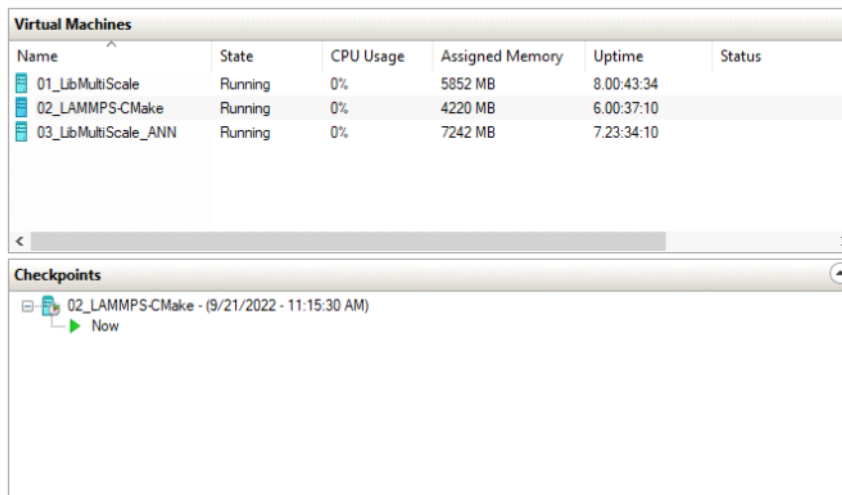Added ML-ATOMNN package to CMake build.

```
scott@lammps-cmake:/opt/lammps/build$ sudo cmake -D PKG_ML-ATOMNN=yes ../cmake
-- Running check for auto-generated files from make-based build system
-- Could NOT find BLAS (missing: BLAS_LIBRARIES)
-- LAPACK requires BLAS
-- A library with LAPACK API not found. Please specify library location.
-- Could NOT find BLAS (missing: BLAS_LIBRARIES)
-- Could NOT find FFMPEG (missing: FFMPEG_EXECUTABLE)
-- Checking for module 'fftw3'
--   No package 'fftw3' found
-- Generating style headers...
-- Generating package headers...
-- Generating lmpinstalledpkgs.h...
-- Could NOT find ClangFormat (missing: ClangFormat_EXECUTABLE) (Required is at least version "8.0")
-- The following tools and libraries have been found and configured:
 * Git
 * OpenMP
 * Threads
 * PkgConfig

-- <<< Build configuration >>>
   LAMMPS Version:   20220623
   Operating System: Linux Ubuntu 20.04
   Build type:       RelWithDebInfo
   Install path:     /root/.local
   Generator:        Unix Makefiles using /usr/bin/make
-- Enabled packages: ATC;KSPACE;MANYBODY;ML-ATOMNN;MOLECULE;RIGID
```

Removed all checkpoints on the VM.

Virtual Machines

Name	State	CPU Usage	Assigned Memory	Uptime	Status
01_LibMultiScale	Running	0%	5852 MB	8.00:42:22	
02_LAMMPS-CMake	Running	0%	4220 MB	6.00:35:58	
03_LibMultiScale_ANN	Running	0%	7242 MB	7.23:32:58	

Checkpoints

The selected virtual machine has no checkpoints.

Created a new one.

Virtual Machines

Name	State	CPU Usage	Assigned Memory	Uptime	Status
01_LibMultiScale	Running	0%	5852 MB	8.00:43:34	
02_LAMMPS-CMake	Running	0%	4220 MB	6.00:37:10	
03_LibMultiScale_ANN	Running	0%	7242 MB	7.23:34:10	

Checkpoints

- 02_LAMMPS-CMake - (9/21/2022 - 11:15:30 AM)
  - ▶ Now

Recompiled LAMMPS. Worked.

```
scott@lammps-cmake:/opt/lammps/build$ sudo make
-- Running check for auto-generated files from make-based build system
-- Could NOT find BLAS (missing: BLAS_LIBRARIES)
-- LAPACK requires BLAS
-- A library with LAPACK API not found. Please specify library location.
-- Could NOT find BLAS (missing: BLAS_LIBRARIES)
-- Could NOT find FFMPEG (missing: FFMPEG_EXECUTABLE)
-- Checking for module 'fftw3'
--   No package 'fftw3' found
-- Could NOT find Eigen3 (missing: Eigen3_DIR)
-- Eigen3 download requested - we will build our own
-- Generating style headers...
-- Generating package headers...
-- Generating lmpinstalledpkgs.h...
-- Could NOT find ClangFormat (missing: ClangFormat_EXECUTABLE) (Required is at least version "8.0")
-- The following tools and libraries have been found and configured:
 * Git
 * OpenMP
 * Threads
 * PkgConfig
```
…

In the subsequent steps, Eigen3 was downloaded and installed.

```
Scanning dependencies of target Eigen3_build
[ 11%] Creating directories for 'Eigen3_build'
[ 11%] Performing download step (download, verify and extract)
for 'Eigen3_build'
-- Downloading...
   dst='/opt/lammps/build/Eigen3_build-
prefix/src/eigen-3.4.0.tar.gz'
   timeout='none'
-- Using
src='https://download.lammps.org/thirdparty/eigen-3.4.0.tar.gz
'
-- [download 1% complete]
-- [download 2% complete]
-- [download 3% complete]
-- [download 4% complete]
-- [download 5% complete]
```

```
-- [download 6% complete]
-- [download 7% complete]
-- [download 8% complete]
-- [download 9% complete]
-- [download 10% complete]
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-- [download 90% complete]
-- [download 91% complete]
-- [download 92% complete]
-- [download 93% complete]
-- [download 94% complete]
-- [download 95% complete]
-- [download 96% complete]
```

```
-- [download 97% complete]
-- [download 98% complete]
-- [download 99% complete]
-- [download 100% complete]
-- verifying file...
        file='/opt/lammps/build/Eigen3_build-
prefix/src/eigen-3.4.0.tar.gz'
-- Downloading... done
-- extracting...
      src='/opt/lammps/build/Eigen3_build-
prefix/src/eigen-3.4.0.tar.gz'
      dst='/opt/lammps/build/Eigen3_build-prefix/src/Eigen3
_build'
-- extracting... [tar xfz]
-- extracting... [analysis]
-- extracting... [rename]
-- extracting... [clean up]
-- extracting... done
[ 11%] No patch step for 'Eigen3_build'
[ 11%] No update step for 'Eigen3_build'
[ 11%] No configure step for 'Eigen3_build'
[ 11%] No build step for 'Eigen3_build'
[ 11%] No install step for 'Eigen3_build'
[ 11%] Completed 'Eigen3_build'
[ 11%] Built target Eigen3_build

...
```

Finished compiling without any errors.

```
[ 78%] Building CXX object
CMakeFiles/lammps.dir/opt/lammps/src/RIGID/fix_rigid_nph_small
.cpp.o
[ 78%] Building CXX object
CMakeFiles/lammps.dir/opt/lammps/src/RIGID/fix_rigid_npt.cpp.o
[ 79%] Building CXX object
CMakeFiles/lammps.dir/opt/lammps/src/RIGID/fix_rigid_npt_small
.cpp.o
[ 79%] Building CXX object
CMakeFiles/lammps.dir/opt/lammps/src/RIGID/fix_rigid_nve.cpp.o
[ 79%] Building CXX object
CMakeFiles/lammps.dir/opt/lammps/src/RIGID/fix_rigid_nve_small
.cpp.o
[ 79%] Building CXX object
CMakeFiles/lammps.dir/opt/lammps/src/RIGID/fix_rigid_nvt.cpp.o
[ 79%] Building CXX object
CMakeFiles/lammps.dir/opt/lammps/src/RIGID/fix_rigid_nvt_small
.cpp.o
[ 79%] Building CXX object
CMakeFiles/lammps.dir/opt/lammps/src/RIGID/fix_rigid_small.cpp
.o
[ 79%] Building CXX object
CMakeFiles/lammps.dir/opt/lammps/src/RIGID/fix_shake.cpp.o
[ 79%] Linking CXX static library liblammps.a
[ 79%] Built target lammps
[ 79%] Linking CXX executable lmp
[ 79%] Built target lmp
[100%] Built target linalg
```

Tested on an Ni NNP potential example job. Worked.

```
scott@lammps-cmake:/mnt/g/02_Temple/2022_08_18_05_LAMMPS_UpdatedANNPkg_Temple_ANN_Ni$ sudo /opt/lammps/build/lmp -in lmp_md_npt_T300.in
LAMMPS (23 Jun 2022 - Update 1)
OMP_NUM_THREADS environment is not set. Defaulting to 1 thread. (src/comm.cpp:98)
  using 1 OpenMP thread(s) per MPI task
Reading data file ...
  orthogonal box = (0 0 0) to (3.45 3.45 3.45)
  1 by 1 by 1 MPI processor grid
  reading atoms ...
  4 atoms
  read_data CPU = 0.020 seconds
Replicating atoms ...
  orthogonal box = (0 0 0) to (10.35 10.35 10.35)
  1 by 1 by 1 MPI processor grid
  108 atoms
  replicate CPU = 0.001 seconds
terminate called after throwing an instance of 'std::runtime_error'
  what():  Token::next(): no tokens left
Aborted
scott@lammps-cmake:/mnt/g/02_Temple/2022_08_18_05_LAMMPS_UpdatedANNPkg_Temple_ANN_Ni$ sudo /opt/lammps/build/lmp -in lmp_md_npt_T300.in
LAMMPS (23 Jun 2022 - Update 1)
OMP_NUM_THREADS environment is not set. Defaulting to 1 thread. (src/comm.cpp:98)
  using 1 OpenMP thread(s) per MPI task
Reading data file ...
  orthogonal box = (0 0 0) to (3.45 3.45 3.45)
  1 by 1 by 1 MPI processor grid
  reading atoms ...
  4 atoms
  read_data CPU = 0.008 seconds
Replicating atoms ...
  orthogonal box = (0 0 0) to (10.35 10.35 10.35)
  1 by 1 by 1 MPI processor grid
  108 atoms
  replicate CPU = 0.001 seconds
*************** SPECIES MAP ***************
type nnp name
1 0 Ni
*************** SPECIES MAP ***************
NNH Ni
==============================================================
********************* NN - HAMILTONIAN *********************
ATOM    = name Ni mass 58.693 energy -4187.67
NSPECIES = 1
N_INPUT  = 30
N_INPUTR = 16
N_INPUTA = 14
```