Installation of MLIP and ARTn

This is a PDF document that explains step by step how to install MLIP-2 and ARTn it contains screenshots for detailed explanation.

Note: The commands to execute are after the sign \$

MLIP-2 Installation

The instructions can be found in the next link <u>Home · Wiki · Alexander Shapeev / MLIP-2 Tutorials · GitLab</u>

- 1. Make a directory with the name mlip-2 using: mkdir mlip 2
- 2. Go to the directory and clone the mlip-2 gitlab repository:

\$ cd mlip 2

\$ git clone https://gitlab.com/ashapeev/mlip-2.git

```
[oupc@cedar2 mlip_2]$ git clone <a href="https://gitlab.com/ashapeev/mlip-2.git">https://gitlab.com/ashapeev/mlip-2.git</a>
Cloning into 'mlip-2'...
remote: Enumerating objects: 2352, done.
remote: Counting objects: 100% (96/96), done.
remote: Compressing objects: 100% (51/51), done.
remote: Total 2352 (delta 58), reused 75 (delta 45), pack-reused 2256 (from 1)
Receiving objects: 100% (2352/2352), 47.39 MiB | 8.84 MiB/s, done.
Resolving deltas: 100% (1185/1185), done.
Updating files: 100% (400/400), done.
```

3. Then in the same directory clone the interface mlip-2 repository:

\$ git clone https://gitlab.com/ashapeev/interface-lammps-mlip-2.git

```
[oupc@cedar2 mlip_2]$ git clone https://gitlab.com/ashapeev/interface-lammps-mlip-2.git
Cloning into 'interface-lammps-mlip-2'...
remote: Enumerating objects: 101, done.
remote: Counting objects: 100% (77/77), done.
remote: Compressing objects: 100% (70/70), done.
remote: Total 101 (delta 38), reused 13 (delta 7), pack-reused 24 (from 1)
Receiving objects: 100% (101/101), 30.98 KiB | 47.00 KiB/s, done.
Resolving deltas: 100% (43/43), done.
```

4. As the last step clone the lammps repository in the same directory:

\$ git clone -b stable https://github.com/lammps/lammps.git mylammps

```
[oupc@cedar2 mlip_2]$ git clone -b stable https://github.com/lammps/lammps.git mylammps Cloning into 'mylammps'...
remote: Enumerating objects: 432526, done.
remote: Counting objects: 100% (2211/2211), done.
remote: Compressing objects: 100% (501/501), done.
remote: Total 432526 (delta 2068), reused 1710 (delta 1710), pack-reused 430315 (from 3)
Receiving objects: 100% (432526/432526), 794.80 MiB | 21.73 MiB/s, done.
Resolving deltas: 100% (355738/355738), done.
Updating files: 100% (13885/13885), done.
```

- 5. Then go to mylammps directory, and then go to the src directory:
 - \$ cd mylammps/src/
- 6. Install the next packages using the next commands:
 - \$ make yes-EXTRA-COMPUTE
 - \$ make yes-kspace
 - \$ make yes-manybody
 - \$ make yes-plugin
 - \$ make yes-replica

7. Go to the interface directory and change the next line of the file install.sh:

\$ cd ../../interface-lammps-mlip-2/

\$ vi install.sh

```
##!/bin/sh

LAMMPS_PATH=$1

TARGET=$2
curdir=$(pwd)

if [ ! -f "lib mlip_interface.a" ]; then echo Error: copy lib_mlip_interface.a to this directory.; echo
LIP root folder"; exit 1; fi
if [ ! -d "$LAMMPS_PATH/src" ]; then echo Error: run ./install.sh \<path-to-lammps\> \<lammps-target\>;
./preinstall.sh $1

cd $LAMMPS_PATH/src
make mpi-stubs
make $TARGET -lgfortran #intel_cpu_intelmpi
cd $curdir
cp $LAMMPS_PATH/src/lmp_$TARGET .
```

Change it for (to edit the document press i)

make mode=shared \$TARGET -lgfortran #intel_cpu_intelmpi

```
#!/bin/sh

LAMMPS_PATH=$1

TARGET=$2

curdir=$(pwd)

if [ ! -f "lib_mlip_interface.a" ]; then echo Error: copy lib_mlip

LIP root folder"; exit 1; fi

if [ ! -d "$LAMMPS_PATH/src" ]; then echo Error: run ./install.sh

./preinstall.sh $1

cd $LAMMPS_PATH/src

make mpi-stubs

make mode=shared $TARGET -lgfortran #intel_cpu_intelmpi

cd $curdir

p $LAMMPS_PATH/src/lmp_$TARGET .

~
```

Exit and save the changes pressing esc and then :wq

- 8. For the next step go to the mlip-2 directory and executed the next commads:
 - \$ cd ../mlip-2
 - \$./configure
 - \$ make mlp

9. When the command above finishes execute:

\$ make libinterface

- 10. Copy lib mlip interface.a in the interface-lammps-mlip-2 directory:
 - \$ cp lib/lib mlip interface.a ../interface-lammps-mlip-2/
- 11. Go to interface-lammps-mlip-2 directory and execute install.sh:
 - \$ cd ../ interface-lammps-mlip-2/
 - \$./install.sh ../mylammps mpi

```
[oupc@cedar2 interface-lammps-mlip-2]$ ./unstall.sh ../mylammps mpi
//home/oupc/mlip_2/interface-lammps-mlip-2
Uninstalling package user-mlip
Installing package information (may take a little white)
Installing package information (may take
```

This is the last step, so now you are able to use MLIP-2.

ARTn installation

For better details you can go to this page <u>Installation</u> — plugin-ARTn v0.1 documentation

1. For the first step you need to clone the ARTn repository: \$ git clone https://gitlab.com/mammasmias/artn-plugin.git

```
[oupc@cedar5 ~]$ git clone <a href="https://gitlab.com/mammasmias/artn-plugin.git">https://gitlab.com/mammasmias/artn-plugin.git</a>
Cloning into 'artn-plugin'...
remote: Enumerating objects: 17549, done.
remote: Counting objects: 100% (1931/1931), done.
remote: Compressing objects: 100% (1211/1211), done.
remote: Total 17549 (delta 1255), reused 1025 (delta 708), pack-reused 15618 (from 1) Receiving objects: 100% (17549/17549), 112.22 MiB | 25.21 MiB/s, done. Resolving deltas: 100% (9569/9569), done. Updating files: 100% (629/629), done.
[oupc@cedar5 ~]$ ls
artn-plugin mlip_2
                                              scratch
 [oupc@cedar5 ~]$
```

- 2. Then enter the folder artn-plugin make a folder named build and enter to that folder: \$ cd artn-plugin && mkdir build && cd build
- 3. Execute the next commands:

\$ cmake .. -DWITH LAMMPS=yes -DLAMMPS ROOT=/path/to/lammps

```
Comake .. -DWITH LAMMPS=yes -DLAMMPS ROOT=/path/to/lammps

oupc@cedar5 build]$ cmake .. -DWITH_LAMMPS=yes -DLAMMPS_ROOT=/home/oupc/mlip_2/mylammps/

- The CXX compiler identification is GNU 12.3.1

- The C compiler identification is GNU 12.3.1

- The Fortran compiler identification is GNU 12.3.1

- Detecting CXX compiler ABI info

- Detecting CXX compiler ABI info

- Detecting CXX compiler ABI info - done

- Check for working CXX compiler identification is GNU 12.3.1

- Detecting CXX compile features

- Detecting CXX compile features - done

- Detecting CXX compile features - done

- Detecting C compiler ABI info

- Detecting C compiler ABI info - done

- Check for working C compiler: /cvmfs/soft.computecanada.ca/gentoo/2023/x86-64-v3/usr/x86_64-pc-linux-gnu/gcc-bin/12/gcc - skipped

- Detecting C compiler ABI info

- Detecting C compiler ABI info

- Detecting C compiler features

- Detecting Fortran compiler ABI info

- Detecting Fortran segment - not found

- Performing Test CMAKE HAVE_LIBC_PTHREAD - Success

- Found Threads: TRUE

- Looking for Fortran sgemm

- Found Threads: TRUE
```

```
[oupc@cedar5 build]$ cmake --build . --target artn -j16
[ 1%] Building Fortran object CMakeFiles/artn.dir/src/precision.f90.o
[ 3%] Building Fortran object CMakeFiles/artn.dir/src/artn_info.f90.o
[ 4%] Building Fortran object CMakeFiles/artn.dir/src/artn_debuse 600
     7%] Building CXX object CMakeFiles/artn.dir/Files_LAMMPS/artnplugin.cpp.o
   7%] Building CXX object CMakeFiles/artn.dir/Files_LAMMPS/fix_artn.cpp.o
10%] Building Fortran object CMakeFiles/artn.dir/src/m_tools.f90.o
   10%] Building Fortran object CMakeFiles/artn.dir/src/m_option.f90.o
25%] Building Fortran object CMakeFiles/artn.dir/src/units.f90.o
25%] Building Fortran object CMakeFiles/artn.dir/src/string_tools.f90.o
   25%] Building Fortran object CMakeFiles/artn.dir/src/sum force.f90.o
   25%] Building Fortran object CMakeFiles/artn.dir/src/pbc.f90.o
25%] Building Fortran object CMakeFiles/artn.dir/src/diag.f90.o
   25%] Building Fortran object CMakeFiles/artn.dir/src/center.f90.o
```

- 4. Go to the previous folder and execute the next command: \$ cd ..
 - \$./configure --with-lammps LAMMPS PATH=/home/oupc/mlip 2/mylammps/

```
[oupc@cedar5 build]$ cd .
[oupc@cedar5 artn-plugin]$ ./configure --with-lammps LAMMPS_PATH=/home/oupc/mlip_2/mylammps/checking build system type... x86_64-pc-linux-gnu
checking host system type... x86_64-pc-linux-gnu
>> host x86_64-pc-linux-gnu
>> host_cpu x86_64
>> host vendor pc
>> host_os linux-gnu
>> build x86_64-pc-linux-gnu
>> build_cpu x86_64
>> build vendor pc
>> build os linux-gnu
  Searching system architecture
checking ARCH... x86_64
>> arch x86 64
try_f90 gfortran f90 ifx ifort nvfortran pgf90 nagfor
try_mpif90 mpif90 mpifort mpiifx mpiifort
try_cc mpicxx gcc
try_cxx mpicxx gcc
```

5. For the last step compile Implib

```
[oupc@cedar5 artn-plugin]$ make lmplib
( cd src && make && cd - )
make[1]: Entering directory '/home/oupc/artn-plugin/src'
Getting version info from git
Getting version info from git
gfortran -JObj -IObj -FPIC -c -g -00 -funroll-loops dgeev.f -o Obj/dgeev.o
gfortran -JObj -IObj -c -g -02 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interface -Wimplicit
=f2008 -ffree-line-length-512 -fPIC -g -02 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interf
pedantic -std=f2008 -ffree-line-length-512 -fPIC -cpp -funroll-loops artn_info.f90 -o Obj/artn_info.o
gfortran -JObj -IObj -c -g -02 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interf
pedantic -std=f2008 -ffree-line-length-512 -fPIC -cpp -funroll-loops prectsion.f90 -o Obj/precision.o
gfortran -JObj -IObj -c -g -02 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interf
pedantic -std=f2008 -ffree-line-length-512 -fPIC -cpp -funroll-loops prectsion.f90 -o Obj/precision.o
gfortran -JObj -IObj -c -g -02 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interf
pedantic -std=f2008 -ffree-line-length-512 -fPIC -cpp -funroll-loops m_tools.f90 -o Obj/m_tools.o
afortran -JObj -IObj -c -g -02 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interf
pedantic -std=f2008 -ffree-line-length-512 -fPIC -cpp -funroll-loops m_tools.f90 -o Obj/m_tools.o
pedantic -std=f2008 -ffree-line-length-512 -fPIC -cpp -funroll-loops m_tools.f90 -o Obj/m_tools.o
gfortran -JObj -IObj -c -g -O2 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interface -Wimplicit
=f2008 -ffree-line-length-512 -fPIC -cpp -funroll-loops units.f90 -o Obj/units.o
gfortran -JObj -IObj -c -g -O2 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interface -Wimplicit
=f2008 -ffree-line-length-512 -fPIC -cpp -funroll-loops units.f90 -o Obj/units.o
gfortran -JObj -IObj -c -g -O2 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interface -Wimplicit
=f2008 -ffree-line-length-512 -fPIC -cpp -funroll-loops m_artn_data.f90 -o Obj/m_artn_data.o
gfortran -JObj -IObj -c -g -O2 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interface -Wimplicit
=f2008 -ffree-line-length-512 -fPIC -g -O2 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interface -Wimplicit-interface -free-line-length-512 -fPIC -cpp -funroll-loops m_error.f90 -o Obj/m_error.o
gfortran -JObj -IObj -c -g -O2 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wimplicit-interface -Wimplicit
=f2008 -ffree-line-length-512 -fPIC -g -O2 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interface -free-line-length-512 -fPIC -g -op -funroll-loops m_error.f90 -o Obj/m_error.o
gfortran -JObj -IObj -c -g -O2 -fcheck=bounds -Wunused -Wall -Wconversion-extra -Wextra -Wimplicit-interface -free-line-length-512 -fPIC -g -op -funroll-loops string_tools.f90 -o Obj/string_tools.o
     string_tools.f90:32:44:
                                                                                        character(len=:), allocatable :: ctmp(:)
    Warning: '.ctmp' is used uninitialized [-Wuninitialized] string_tools.f90:109:26:
                                                                           end subroutine read line
```

You finish the installation now you are able to use ARTn