Importing External LAMMPS Forcefield into MedeA

Introduction

MedeA supports many types of forcefields suitable for modeling and simulating different types of materials. For most of the supported forcefield types MedeA includes as many forcefield parameter sets as possible. For example, the metallic forcefield under the EAM framework includes almost all of the available forcefield parameters from the NIST Interatomic Potentials Repository Project website (https://www.ctcms.nist.gov/potentials/). However, there are times when you would like to use a particular forcefield parameter set that has not been included within MedeA. This may be a new set of forcefield parameters that has just been published or a set of parameters that has been re-optimized or refined by you and/or your colleagues.

This tutorial demonstrates the steps required to directly import externally existing forcefield parameter sets into MedeA without the necessity of converting them to native MedeA forcefield (frc) files. We will use the COMB3 forcefield for ZrO_2 as an example. This tutorial contains the following sections:

- Creating a template frc file for COMB3 forcefield.
- Constructing a customized flowchart for importing external COMB3 parameters.
- Validation against stand-alone LAMMPS
- Appendix: Forcefields supported in MedeA-LAMMPS

1. Create a template frc file for COMB3 forcefield

Frc file: ingredients/forcefields/comb3_template.frc

First, start the MedeA program, click **Forcefields** >> **Read…** then from the "*Open Forcefield File*" window navigate to the "*MD/2.0/data/Forcefields.kit/inorganic*" directory, click on comb3.frc and click **Open**. It does seem like nothing has happened, but if you click **Forcefields** >> **Choose**, you should see **comb3** as the selected forcefield. Click **Forcefields** >> **Export…** and save the comb3.frc to a custom directory on your local hard drive, for example, "*MD/2.0/data/Forcefields/custom*" as comb3_template.frc.

Start your favorite text editor (such as Wordpad on Windows or Vim on Linux) and open the saved comb3_template.frc file. This is what the top part of the comb3_template.frc should look like:

```
!MD forcefield 1
#version        comb3.frc       1.0     29-October-2014

#elements Ti H C N O Cu Zn Zr

#description

COMB3 (Charge-Optimized Many-Body 3) forcefield developed by T. Liang, T.-R. Shan, Y.-T. Cheng

Contains parameters for Ti, H, C, N, O, Cu, Zn, and Zr (though it should be noted that only sp

#define comb3 default

!Ver Ref                Function             Label
!--- ---    ------------------------------   ------
 1.0  1     atom_types                       comb3
 1.0  1     tersoff_cutoff                   comb3
 1.0  1     atomic_self_energy               comb3
 1.0  1     pair_self_energy                 comb3
 1.0  1     Streitz_Mintmire_charge_density  comb3
 1.0  1     cutoffs                          comb3
 1.0  1     polarizability                   comb3
 1.0  1     short_range_energy               comb3
 1.0  1     short_range_energy_pairs         comb3
 1.0  1     bond_order_atoms                 comb3
 1.0  1     bond_order_pairs                 comb3
 1.0  1     bond_order_pairs_2               comb3
 1.0  1     tersoff_nonbond                  comb3
 1.0  1     flags                            comb3
 1.0  1     Ucorr                            comb3
 1.0  1     templates                        comb3
 1.0  1     bond_increments                  comb3

#atom_types     comb3

!Ver  Ref  Type    Mass      Element  Comment
!---- ---  ----  ----------  -------  ----------------------------------------
  1.0   1    Ti    47.867        Ti    Titanium
  1.0   1    H      1.007970     H     Hydrogen
  1.0   1    C     12.011150     C     Carbon
  1.0   1    N     14.006700     N     Nitrogen
  1.0   1    O     15.999400     O     Oxygen
  1.0   1    Cu    63.546000     Cu    Copper
  1.0   1    Zn    65.380000     Zn    Zinc
  1.0   1    Zr    91.224000     Zr    Zirconium

#tersoff_cutoff     comb3

>           1                                                                  rij <= Rmin(ij)
> Fc(rij) = 1/2*{1 + cos(pi*(rij-Rmin(ij))/(Rmax(ij)-Rmin(ij)))}   Rmin(ij) < rij <= Rmax(ij)
>           0                                                                  rij > Rmax(ij)

!Ver  Ref     I  J           Rmin            Rmax
!---- ---    -- --   -------------- --------------
  1.0   1     C  C   1.7            2
  1.0   1     Cu C   2.5            2.8
  1.0   1     Cu Cu  3.2            3.5
  1.0   1     H  C   1.6            1.9
  1.0   1     H  Cu  2              2.3
```

The first 10 lines and the first section titled "#define comb3 default" provide some basic information of the COMB3 forcefield and its sections - this is the part that we do not need to change. We will edit the following sections, start from the second section titled "atom_types comb3". If you have a new COMB3 forcefield for Li_2S, then you would need to add Li and S to the list of supported atom types. If you just have refined set of parameters for ZrO_2, then there is no need to edit this section.

Starting from the third section titled "tersoff_cutoff comb3" to the 16th section titled "Ucorr" are where the COMB3 frc file define parameters for atoms, pairs of atoms, angles in an angle, and angles in a dihedral. You will need to edit all these parts, but please don't feel intimated! Because your edits are going to be very simple. For example, for the "tersoff_cutoff comb3" section, you will delete all but the first line of parameters and change the first line to look like the following:

```
#tersoff_cutoff     comb3

>           1                                                          rij <= Rmin(ij)
> Fc(rij) = 1/2*{1 + cos(pi*(rij-Rmin(ij))/(Rmax(ij)-Rmin(ij)))}   Rmin(ij) < rij <= Rmax(ij)
>           0                                                          rij > Rmax(ij)

!Ver  Ref     I  J           Rmin            Rmax
!---- ---    -- --   -------------- --------------
  1.0   1     *  *            1.7             2

#atomic_self_energy     comb3
```

where the asterisk "*" sign indicates all atom types – there is just one line of change! This change essentially defines all tersoff_cutoff parameters for all atom pairs to be the same. *Rmin* and *Rmax* parameters can be any numbers – making them the same as the first set is a good idea. You would need to repeat the procedure for all remaining sections by keeping only the first line and replacing all I, J, and K with "*" - till your COMB3 frc file looks like the attached one. For the second from the last section titled "templates comb3", be sure to add the additional elements you have defined in the second section "atom_types comb3". Straightforward modifications, right?

After all of the above changes, please make sure the "comb3_template.frc" file is saved in the "*MD/2.0/data/Forcefields/custom*" directory on your local hard drive. If you are running the calculations on a remote JobServer and TaskServer, make sure the same custom directory "*MD/2.0/data/Forcefields/custom*" is also created on the JobServer computer and the "comb3_template.frc" file is also saved there.

Once a template frc file has been created for COMB3, it can be used with all other COMB3 forcefield parameter files. The only thing to make sure is that the "atom_type" section includes all atom types in the parameter file. Similarly, a template frc file can be created for the EAM forcefield for importing external EAM parameter files.

2. Constructing a customized flowchart

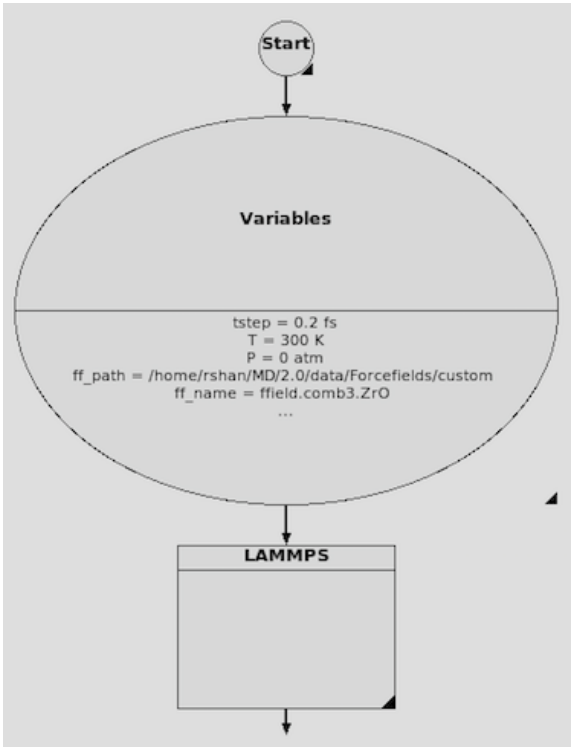
Flowchart: ingredients/flowchart/importing external LAMMPS forcefields.flow

Structure: ingredients/structure/mZrO2.sci

First, have a ZrO_2 structure active in MedeA. You can load the attached monoclinic ZrO_2 "*mZrO2.sci*" via **File** >> **Open structure from disk** and navigate to the directory where you saved the structure file. Alternatively, you can load any ZrO_2 structure from the InfoMaticA module.

Next you need to assign the ZrO_2 structure a forcefield. Instead of using the default **comb3.frc** from the "*MD/2.0/data/Forcefields.kit/inorganic*" directory, please load the **comb3_template.frc** that you just created from the "*MD/2.0/data/Forcefields/custom*" directory.

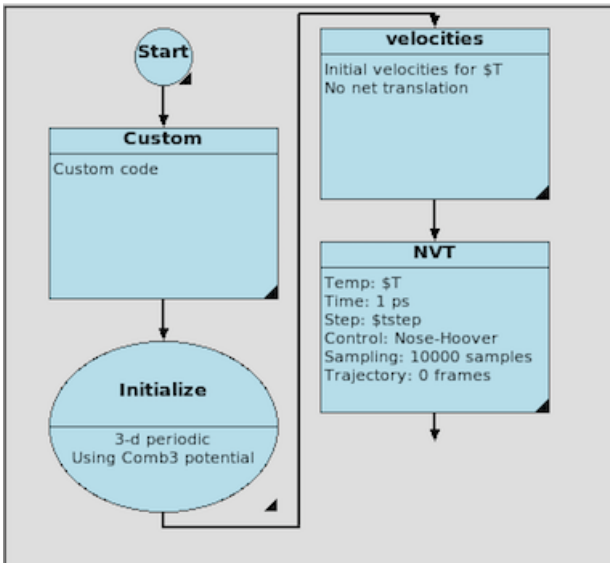
The next step is to construct a flowchart with a custom stage to use the above COMB3 template frc file comb3_template.frc. Click **Job Control** >> **New Job…** to start the flowchart interface. The flowchart contains a minimal of two stages, a **Variables** and a **LAMMPS** stage, that should like the following:



The **Variables** stage contains variables for controlling the simulation, such as timestep size (*tstep*), temperature (*T*), and pressure (*P*), but the most important variables are the last two: *ff_path* and *ff_name*. Variable "*ff_path"* identifies the directory where the custom comb3_template.frc file is saved on the local drive and on the JobServer (/home/rshan/ *MD/2.0/data/Forcefields/custom*), and variable "*ff_name*" identifies the name of the COMB3 forcefield parameter file (in this case "ffield.comb3.ZrO" which is available in the directory ingredients/forcefields) from an external source. It is very important that this file "ffield.comb3.ZrO" is also saved to the "*MD/2.0/data/Forcefields/custom"* directory.

There should be two files in the "MD/2.0/data/Forcefields/custom" directory: *comb3_template.frc* and *ffield.comb3.ZrO*.

The **LAMMPS** stage in this example contains 4 sub-stages: **Custom**, **Initialize**, **Velocities**, and **NVT** stages.



The **Custom** stage is just a one-line code which copies the aforementioned external COMB3 forcefield parameter file "ffield.comb3.ZrO" to overwrite the default MedeA forcefield file "parameters.dat".:

```
shell cp $ff_path/$ff_name parameters.dat
```

The remaining stages can keep the default settings, except for changing the Time to 1 ps for the NVT run for illustrative purpose. Please load the attached flowchart "*importing external LAMMPS*

forcefields.flow" whenever you are in doubt. To load the flowchart, click **Job Control** >> **New Job…**, then on the top right corner click "Open User…" and navigate to the directory where you saved the flowchart. Close flowcharts, give the job a name, and click **Run** to run the job.

The purpose of the comb3_template.frc file is to assign atom types for the active structure window. The atom types are assigned and the default forcefield parameters are written to the "parameters.dat". In the Custom stage you copied the external COMB3 parameter file to the parameter.dat file so that LAMMPS reads the external COMB3 parameters from the parameter.dat file.

3. Validation against stand-alone LAMMPS

Click Job **Control** >> **View and Control Jobs** to view the job. The bottom part of the Job.out prints the thermodynamic variables from the simulation:

```
Stage 2.4: NVT integration for 1 ps with a timestep of 0.2 fs
       T is 300 K

      Property         Value   +/- Uncertainty    Units      After Steps   % Run
------------------  ----------     ----------- ------------ ------------ -------
                t:     1000.0                 fs
                T:        385 +/- 34          K                      3500    70.0%
                P:     -73200 +/- 3000        atm                    1000    20.0%
                V:    9001.31 +/- 0           Ang^3                     0     0.0%
              rho:    5.81935 +/- 0           g/mL                      0     0.0%
  Etotal did not converge in 5000 steps
           Etotal:    -551430 +/- 370         kJ/mol                 4000    80.0%

             Epot:    -554640 +/- 340         kJ/mol                 3500    70.0%
             Ekin:       3690 +/- 320         kJ/mol                 3500    70.0%
             Evdw:    -298050 +/- 550         kJ/mol                 3000    60.0%
            Ecoul:    -256600 +/- 1900        kJ/mol                    0     0.0%
              Sxx:      45200 +/- 2100        atm                    1000    20.0%
              Syy:      60500 +/- 9600        atm                     500    10.0%
              Szz:     114300 +/- 1600        atm                    2500    50.0%
              Syz:        160 +/- 870         atm                       0     0.0%
              Sxz:     -83700 +/- 7900        atm                       0     0.0%
              Sxy:       1900 +/- 2200        atm                       0     0.0%


LAMMPS stage completed on Mon 10 April 2017 at 14:38:22 MDT after 556 s (0:09:16)
```

It shows all thermodynamic variables are reasonable. Next you can compare the results of the NVTs from MedeA to that from stand-alone LAMMPS.

	Step	Pressure	Volume	Temperature	Potential Energy
MedeA-LAMMPS	0	896346.43	9001.313	300.0	-1848.5147
LAMMPS (31March2017)	0	896346.43	9001.313	300.0	-1848.5147

Without surprises, all thermodynamic variables from MedeA-LAMMPS at the 0th step are exactly the same as the stand-alone LAMMPS (31March3017 version).

Comparing thermodynamic variables from the 0th step is a good indication if the LAMMPS executables from different sources are resulting in the same calculated properties.

Even after 5000 steps (1 ps) the thermodynamic variables are exactly the same:

	Step	Pressure	Volume	Temperature	Potential Energy
MedeA-LAMMPS	5000	-77641.029	9001.313	341.04163	-5755.8012
LAMMPS (31March2017)	5000	-77641.029	9001.313	341.04163	-5755.8012

Conclusions

In this tutorial we showed you the steps required to import external LAMMPS forcefield parameter sets into MedeA to be used with MedeA-supported forcefields. First, we showed you the creation of a template frc file for the forcefield, then the steps for constructing a custom flowchart to read the external parameter file. Lastly, we validated the results from MedeA-LAMMPS using the imported forcefield parameter file against stand-alone LAMMPS. Using this approach, any external forcefield parameter files can be imported into MedeA to be used with forcefields that are suppoted by MedeA-LAMMPS.

Appendix: Forcefields supported in MedeA-LAMMPS

Here is a list of forcefields currently supported in MedeA-LAMMPS

- Organic forcefields:
  - PCFF/PCFF+
  - Compass/Compass+
  - OPLS-AA/OPLS-AA+
  - AUA/AUA+
  - Trappe+
- Inorganic forcefields:
  - COMB3
  - Buckingham
  - Morse
  - BKS
  - Clay-FF
  - CVFF
- Metallic forcefields
  - EAM (all LAMMPS eam, eam/fs, and eam/alloy variants)
- Semiconductor forcefields
  - Tersoff
  - Stillinger-Weber