The MOL2LAMMPS – conversion routines.
Documentation and user guide.

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Note: These routines are still work in progress. Please do contact me if there are any issues.

Synopsis:
MOL2LAMMPS is a set of open-source conversion scripts than enable a user to generate working LAMMPS input files for various MD or other studies. The toolkit is designed with the intention for studies of molecular crystals however can still be used for non-crystalline systems.

Aim:
LAMMPS is a very versatile MD software however, creating LAMMPS input files on-the-fly is often difficult. There are a few commercial software GUI that have been designed to do this (e.g. SCIENOMICS, MATERIALS DESIGN, see **figure 1**) which work quite well, however even though the majority of the initial workflow can be treated in such a fashion. (i.e. loading a structure into GUI and hitting a few buttons) in most realistic research endeavors utilizing MD, detailed manipulation of inputs is always required. MOL2LAMMPS presents a zero-cost alternative to the LAMMPS input file generation available in expensive commercial software engines.

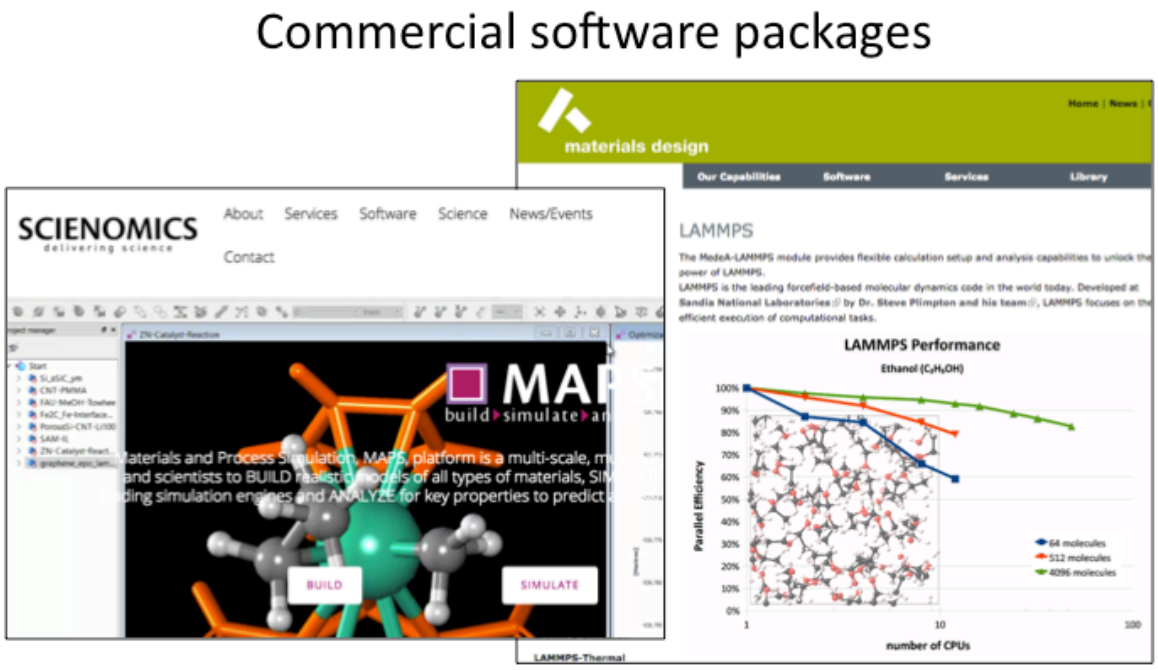

Figure 1. Such commercial software enable importing basic coordinates for molecular file formats and generating LAMMPS input files. They are software with many features. A crucial feature in all of these software is to act as a 3rd party client and build input files for the program LAMMPS.

Features:

Force field tables currently facilitated.

- Dreiding FF(named after Andre Dreiding, inventor of the Drieding Stereomodel kit)
- Generalized amber force field.

How it works:

MOL2LAMMPS exploits the MSI2LMP[1] program which is available as part of the LAMMPS distribution. Users begin with a model in .mol2 format which is easily achievable via the use of a free version of mercury[2] or openbabel[3]. The .mol2 is then converted into the .car and .mdf files which are read in by the program MSI2LMP, wherein the user must specify the choice of force field (.frc table) the outputs are then further edited with a 'polishing' script.

Dependencies:

The mol2lamps routines currently require setup of MSI2LMP, both PYTHON and PERL interpreters as well as the openbabel libraries with python bindings[4]. All dependencies are reasonably popular open source community codes. The program Antechamber [5] is required for making FF assignments with GAFF. The installers can be downloaded from the following website.

Running of MOL2LAMMPS:

Using MOL2LAMMPS scripts requires the following four steps (see **figure 2**):

1. Preparation of .mol2 file.
2. Run mol2car.py.
3. Run fixmsi2lammps.pl.
4. Test that the LAMMPS inputs are working.

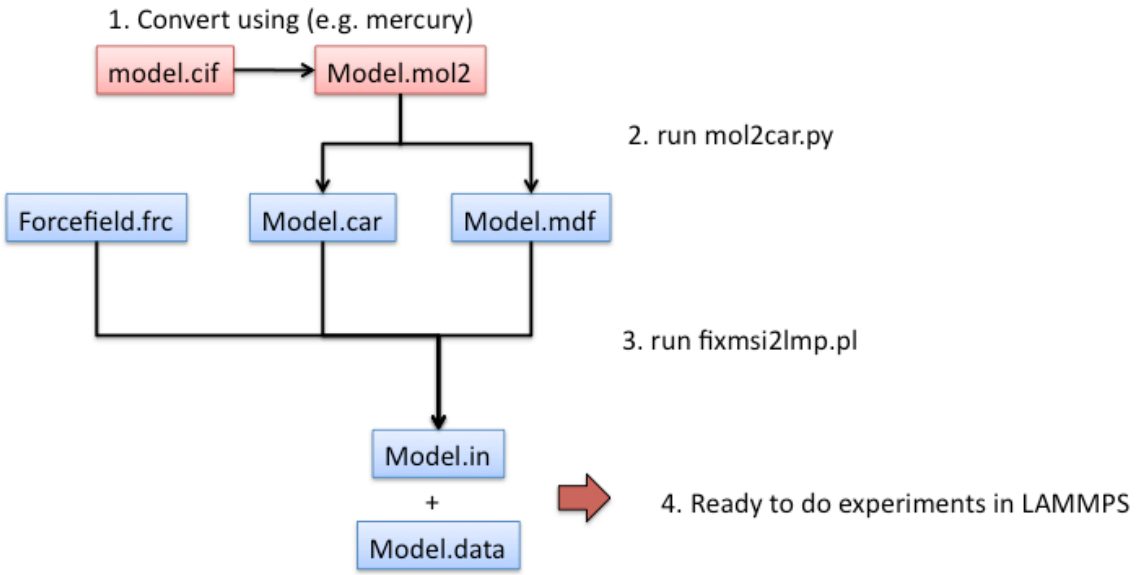

Figure 2. Flow chart for use of MOL2LAMMPS tools.

Conversion Scripts and features:

In this section we detail the individual programs, running and features

The mol2car.py script:
Mol2car is the .mol2 to .car conversion interface. It is run from the command line as follows.
$python mol2car.py [rootname] [options]

[rootname]: user specified rootname for all associated files (extension not inclusive)

[options]:
1. Select Force Field (drd of gaff)
2. Switch to run antechamber as part of the workflow (1 or 0)

The fixmsi2lmp.pl script:
There are several variations of this Perl script that can be modified depending on how the user see fit. Currently there are fixed versions available for the Dreiding or GAFF force fields. It is run from the command line as follows.

$fix_msi2lmp_out.pl [rootname] [options]

[rootname]: user specified rootname for all associated files (extension not inclusive)

[options]:

1. Periodicity (s or p)
2. Replicate option (number > 0)
3. improper flag (none or 'blank')

fix_msi_for_hbond.py:
In the event that you are using the Dreiding FF and you would like to setup the separate H-bond terms the you will also need to use the additional python script. IT should make the appropriate edits to your input files after you have setup all your LAMMPS inputs for Drieding FF. You can run as follows:

$ python fix_msi_for_hbond.py [rootname]

[rootname]: user specified rootname for all associated files (extension not inclusive)

Example usage:

(these examples are provided with the current distribution)

- Ethane single molecule from smiles string.

$ echo CC > ethane.smi
$ babel ethane.smi ethane.mol2 --gen3D
$ mol2car.py ethane drd 0
$ fix_msi2lmp_out.pl ethane s 1 none
$ lmp_mac_2015 -in ethane.in
$ vmd ethane_prod.lammpstrj

- Box of methanol using Dreiding parameters.
# use mol2car to simualte ethane with Dreiding FF via the following commands
$ echo CO > methanol.smi
$ babel methanol.smi methanol.mol2 --gen3D
$ mol2car.py methanol drd 0
$ fix_msi2lmp_out.pl methanol p 3 none
$ fix_msi_for_hbond.py methanol
now edit the methanol_hbond.data file and change the box extents such that

0.213200000 3.290100000 xlo xhi
-1.375600000 3.406800000 ylo yhi
-1.095700000 3.464400000 zlo zhi

$lmp_mac_2015 -in methanol_hbond.in
$vmd methanol_prod.lammpstrj

- Setup deformation of aspirin form II – Curious readers may be interested to note that the following scripts were actually developed out of attempts to model thermal diffuse scattering from Aspirin crystals [6]. In this example we start with the form II crystal and apply a postulated shear deformation in which slippage of layers will occur. The .mol2 file has already been prepared already (ACSALA17_qeq.mol2).

```
$mol2car.py ACSALA17_qeq gaff 1
$fix_msi2lmp_gaff.pl ACSALA17_qeq p 1
$lmp_mac_2015 -in ACSALA17_deform.in
```

How to cite:

If you do end up using or modifying these scripts for your own scientific works pls. make a reference to article [6].

References:

[1] https://github.com/lammps/lammps/tree/master/tools/msi2lmp

[2] https://www.ccdc.cam.ac.uk/solutions/csd-system/components/mercury/

[3] http://openbabel.org/wiki/Main_Page

[4] http://openbabel.org/docs/current/UseTheLibrary/PythonInstall.html

[5] http://ambermd.org/#AmberTools

[6] Chan, E. (2015). "On the use of molecular dynamics simulation to calculate X-ray thermal diffuse scattering from molecular crystals." Journal of Applied Crystallography **48**(5): 1420-1428.

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