UNIVERSITY OF NOTRE DAME | ENGINEERING

Intro to MD: Setting Up a System in LAMMPS

Sep 3rd 2024 Group Meeting

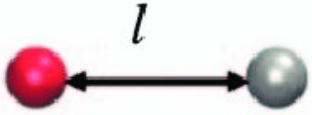
Outline

- What is Molecular Dynamics?
- What Do You Need To Set Up A Simulation?
- What Does That Look Like in LAMMPS?
- How To Build A System in LAMMPS

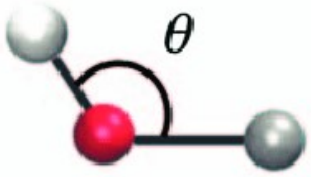
What is Molecular Dynamics?

It's Just Wiggles in Time

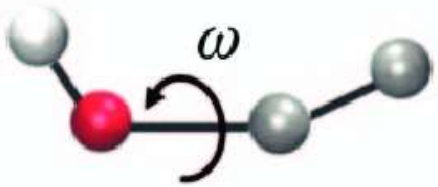
Bonded Interactions



Bond Stretching



Angle Bending



Torsion (Dihedral)

Non-Bonded Interactions

Electrostatics

Dispersion (VdW)

For an atom $'i'$:

$$E_i = E_{Bonded,i} + E_{Unbonded,i}$$

$$\boldsymbol{F_i} = m_i\,\boldsymbol{a_i} = -\frac{\partial E_i}{\partial \boldsymbol{x}}$$

$$\boldsymbol{v_i} = \frac{d\boldsymbol{a_i}}{dt};\ \ \boldsymbol{x_i} = \frac{d\boldsymbol{v_i}}{dt}$$

What Do You Need To Set Up A LAMMPS Simulation?

A Forcefield and Initial Coordinates – A `.data` File

```
LAMMPS Description

     377  atoms
     250  bonds
     125  angles
     0  dihedrals
     0  impropers

     4  atom types
     1  bond types
     1  angle types
     0  dihedral types
     0  improper types

  0.0 31.0342 xlo xhi
  0.0 31.0342 ylo yhi
  0.0 31.0342 zlo zhi

Masses

1 15.9994  # O
2 1.008  # H
3 22.9898  # Na
4 35.453  # Cl
```

```
Atoms  # full

1 1 1 -0.8476 0.0 0.0 0.0
2 1 2 0.4238 0.8164904 0.0 0.577359
3 1 2 0.4238 -0.8164904 0.0 0.577359
4 2 1 -0.8476 3.10342 0.01 0.01
5 2 2 0.4238 3.9199104 0.01 0.587359
6 2 2 0.4238 2.2869295999999997 0.01 0.587359
373 125 1 -0.8476 12.41368 12.453679999999999 12.493
374 125 2 0.4238 13.230170399999999 12.4536799999999
375 125 2 0.4238 11.5971896 12.453679999999999 13.07
376 126 3 1.0 4.7 4.7 4.7
377 127 4 -1.0 10.9 10.9 10.9

Bonds

1 1 1 2
2 1 1 3
3 1 4 5
4 1 4 6
249 1 373 374
250 1 373 375

Angles
```

How To Build A System in LAMMPS

MolTemplate + PackMol

MolTemplate:
- ✓ Assigns force field parameters to each atom
- × Creates limited initial configurations

PackMol:
- × Cannot assign FF parameters
- ✓ Creates a randomized initial configuration

MolTemplate + PackMol

- ✓ Use PackMol to creates the initial configuration (output – .xyz or .pdb)
- ✓ Use MolTemplate to assigns force field parameters to each atom and create the datafile (output .data file)

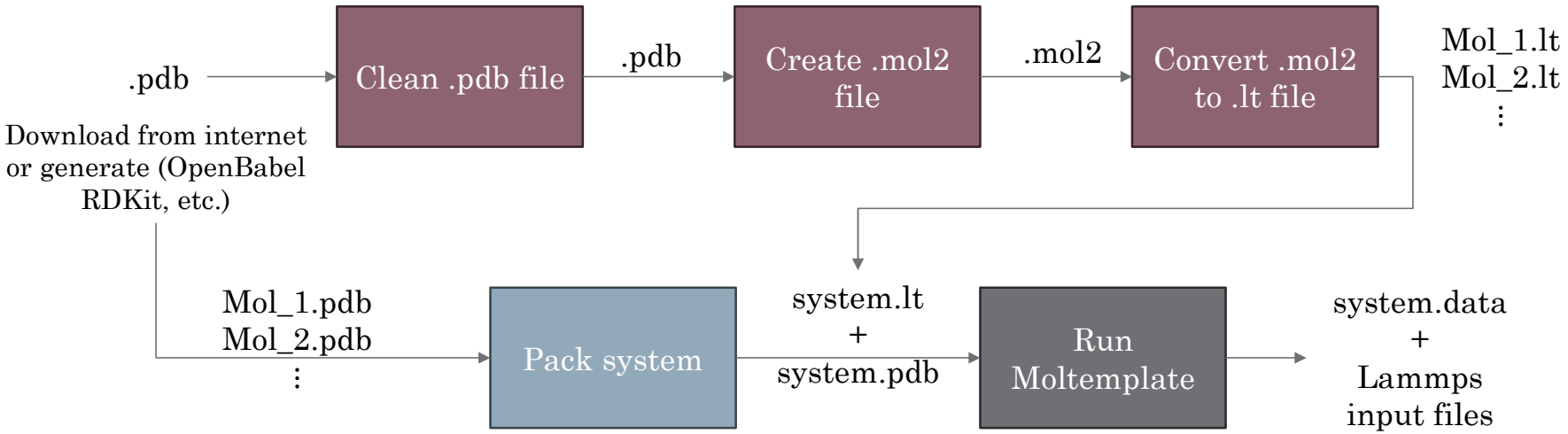
Create .mol2 files using Amber

Tutorial on Building A System

Emim-TF2 Using GAFF Parameters

MolTemplate + PackMol

- ✓ Use PackMol to creates the initial configuration (output – .xyz or .pdb)
- ✓ Use MolTemplate to assigns force field parameters to each atom and create the datafile (output .data file)



Legend: AmberTools | PackMol | MolTemplate