Introduction to LAMMPS

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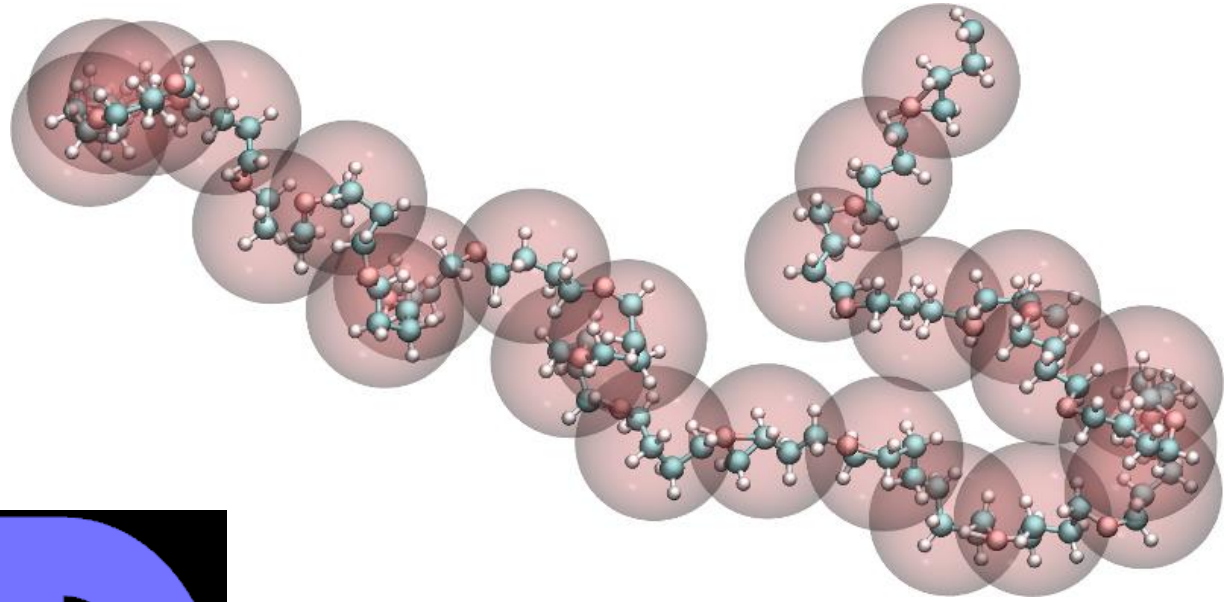
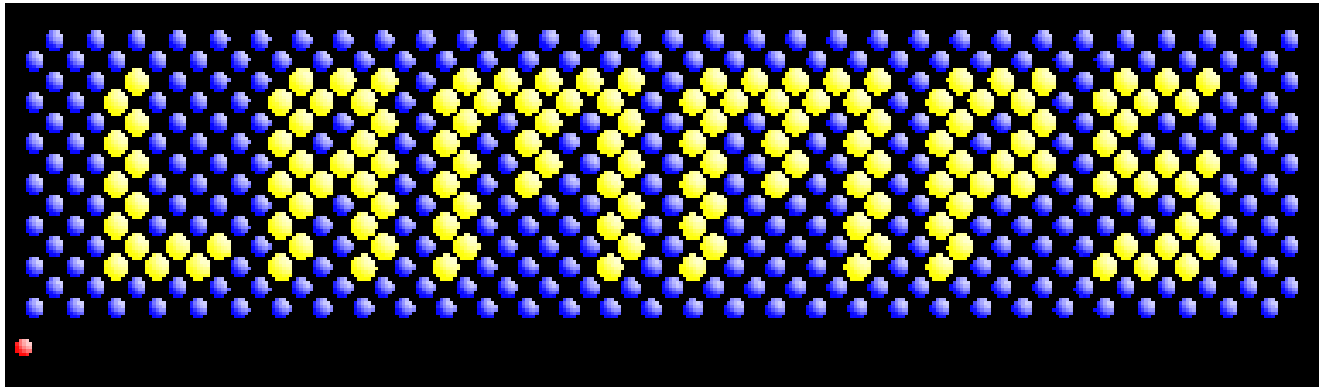
In previous sessions

- We talked discussed about
  - MD simulation
  - The reference code
  - VMD



LAMMPS

- LAMMPS = Large-scale Atomic/Molecular Massively Parallel Simulator
- LAMMPS is a classical molecular dynamics simulation code designed to run efficiently on parallel computers
- Developed by Sandia National Laboratories



References

- LAMMPS manual, source, and tutorials can be found at http://lammps.sandia.gov/
- LAMMPS documentation can be found at http://lammps.sandia.gov/doc/Manual.html

- LAMMPS can be downloaded from http://lammps.sandia.gov/download.html or http://lammps.sandia.gov/tars/

  (for selecting source version or using wget in linux)

Compiling LAMMPS

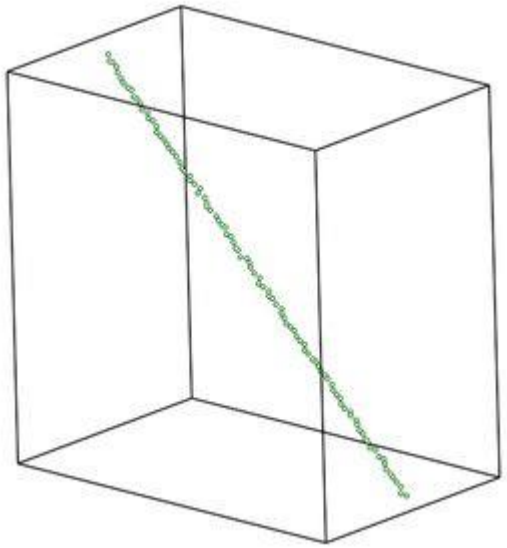
- Download LAMMPS
  - wget http://lammps.sandia.gov/tars/lammps-stable.tar.gz
- Unzipping
  - tar -zxf lammps-stable.tar.gz
- Making/Compiling
  - cd lammps-16Feb16/src/
  - make serial
- Including/Excluding functions/packages
  - make ps (to view currently included packages)
  - make yes-PKGNAME (include PKGNAME)
  - make no-PKGNAME (exclude PKGNAME) *Recompile after changing pkg

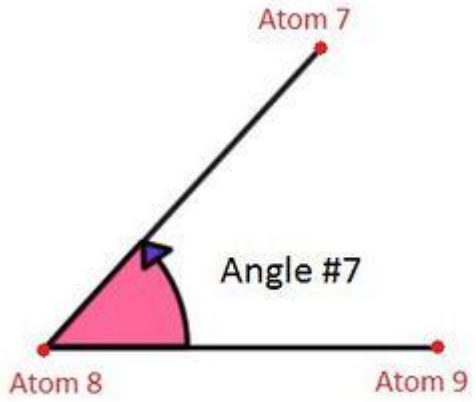
Using LAMMPS

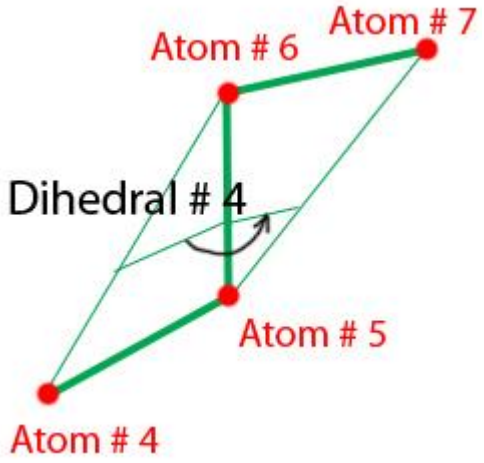
- LAMMPS executes the instructions in an input script
- The structure of an input script typically has 4 parts
  1. Initialization
  2. Atom definition
  3. Settings
  4. Run a simulation
- Detailed documentation of commands can be found at http://lammps.sandia.gov/doc/Section_commands.html#cmd-2

Sample problem

- Chain polymer with bond, angle, dihedral and pair interaction







Sample Input Script

```
# Initialization
units           real
boundary        f f f
atom_style      molecular
read_data       data.poly

# Potential information
neighbor        5.0 bin
bond_style      harmonic
bond_coeff      1 50 2.2
angle_style     harmonic
angle_coeff     1 30 160
dihedral_style  harmonic
dihedral_coeff  1 40.0 1 2
pair_style      lj/cut 10.5
pair_coeff      1 1 0.112 4.01 10.5


#########################################################
# Equilibration (Langevin dynamics at 300 K)

velocity        all create 300.0 1231
fix             1 all nve
fix             2 all langevin 300.0 300.0 100.0 904297
thermo_style    custom step temp pe etotal epair ebond eangle edihed
thermo          5000
timestep        1

dump            1 all xyz 50 conformation.xyz

run             100000
```

Data File Format

- In the sample input script, we used the command *read_data* to read atom/bond/angle/dihedral data from an external file
- Data file format
  - header
  - body

- Detailed documentation at http://lammps.sandia.gov/doc/read_data.html

```
# Model for PE

     10     atoms
      9     bonds
      8     angles
      7     dihedrals

         1     atom types
         1     bond types
         1     angle types
         1     dihedral types

    -100.0   100.0 xlo xhi
    -100.0   100.0 ylo yhi
    -100.0   100.0 zlo zhi

Masses

         1          14.02

Atoms

         1         1         1   0 0 0
         2         1         1   0 0 2
         3         1         1   0 0 4
         4         1         1   0 0 6
         5         1         1   0 0 8
         6         1         1   0 0 10
         7         1         1   0 0 12
         8         1         1   0 0 14
         9         1         1   0 0 16
        10         1         1   0 0 18
```

```
Bonds

         1         1         1         2
         2         1         2         3
         3         1         3         4
         4         1         4         5
         5         1         5         6
         6         1         6         7
         7         1         7         8
         8         1         8         9
         9         1         9        10

Angles

         1         1         1         2         3
         2         1         2         3         4
         3         1         3         4         5
         4         1         4         5         6
         5         1         5         6         7
         6         1         6         7         8
         7         1         7         8         9
         8         1         8         9        10

Dihedrals

         1         1         1         2         3         4
         2         1         2         3         4         5
         3         1         3         4         5         6
         4         1         4         5         6         7
         5         1         5         6         7         8
         6         1         6         7         8         9
         7         1         7         8         9        10
```

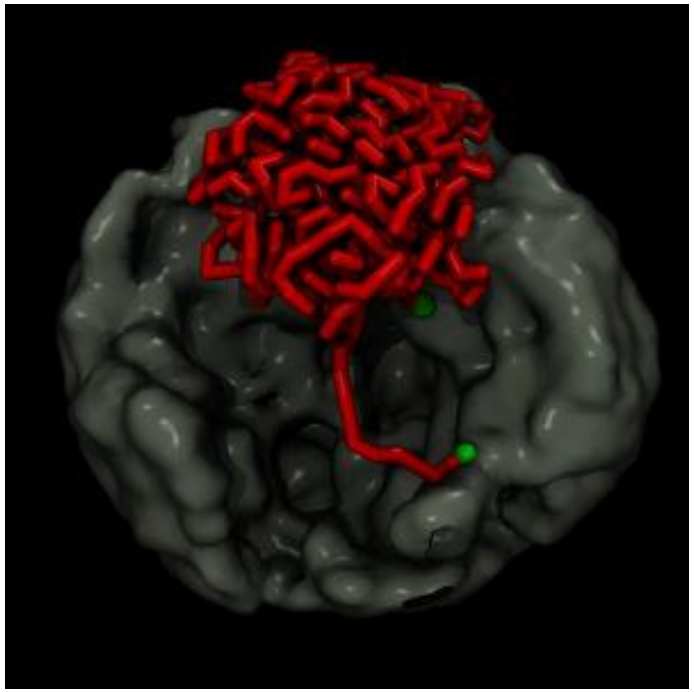
Executing LAMMPS

- LAMMPS executable
  - LAMMPS_FOLDER/src/lmp_serial
- Executing lammps
  - ./lmp_serial –i run.in (run.in is the input script for LAMMPS)

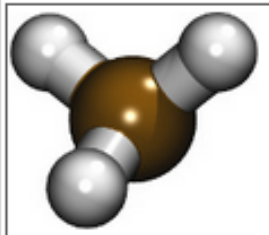
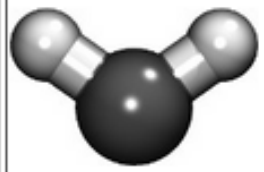
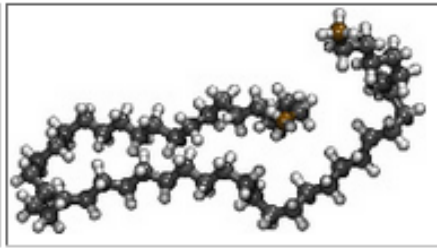
MolTemplate

- A convenient molecule builder that comes with LAMMPS
- Documentation can be found at http://www.moltemplate.org/

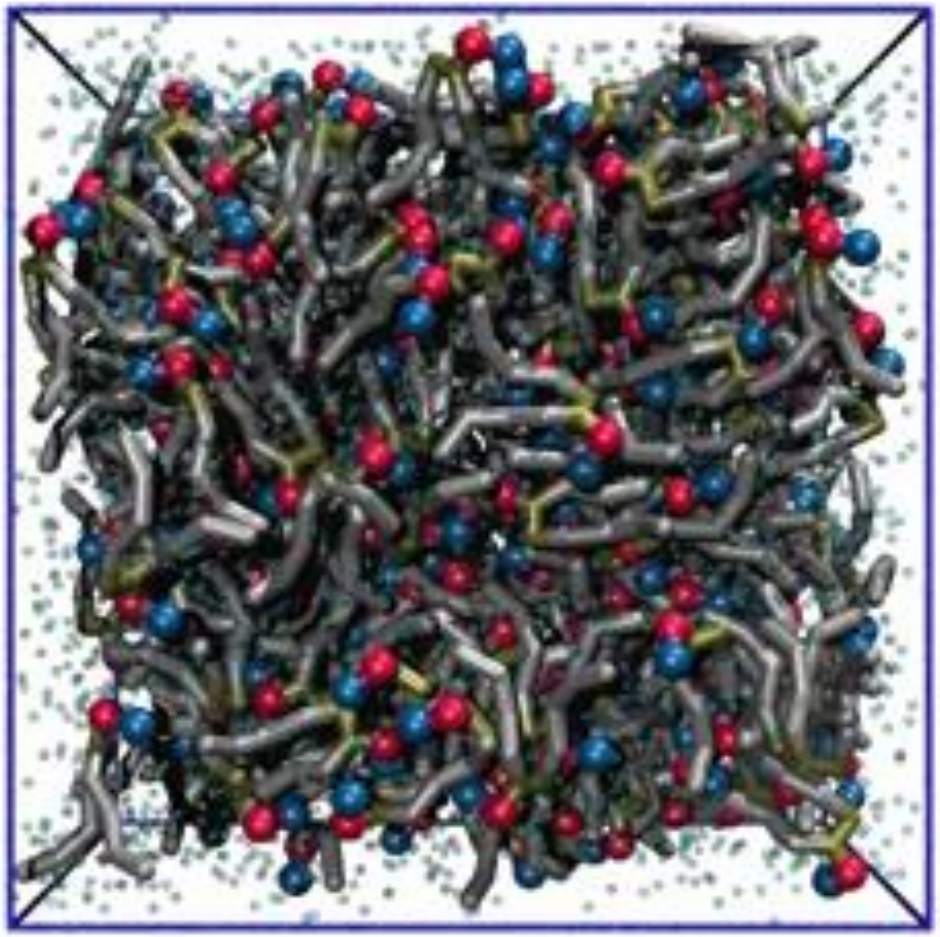
- Translate *.lt files input LAMMPS scripts and data files



Building large molecules from small ones

Building a simple polymer (using the OPLSAA force field) (click below for input files)						
Requirements:	*This example requires that LAMMPS is built with the optional **USER-MISC** package. You must also download and edit the oplsaa.prm file, and use it to create the oplsaa_subset.prm and oplsaa.lt files. (See **README.TXT**)*					
	+		→	 ...	→ 1ns	
ch3group.lt		**ch2group.lt**		**alkane50.lt** **system.lt** (Note: more **complex shapes** are possible)		**README.TXT** **run.in.min** **run.in.nvt**
Build Using:	`oplsaa_moltemplate.py oplsaa_subset.prm` `moltemplate.sh system.lt`					

Example



http://www.moltemplate.org/videos/martini_DPPC_bilayer/martini_DPPC_bilayer_formation_crf15_LR.mp4

Any Question?

Programming Exercise #3

- Programming Exercises can be found on the website of this course
- https://softphys.wordpress.com/

- Programming Exercise #3
- https://softphys.wordpress.com/2016/04/08/programming-exercise-3/