MD Tutorial 1&2

Commands, installation and running lammps

Filesystem in windows and linux

• Windows

C:\Users\Senbo\Documents\

• Linux

/home/senbo/Documents

Path: absolute vs. relative

Current folder (.) and parent folder (..)

Important commands

• List files in the current folder

Is and *dir*

• Change folder location

cd

Make a new folder

mkdir folderName

Delete a file

rm filename and del filename

Remove a folder

rmdir folderName

Task: go to "/usr/bin" or "C:\Windows\System32", list the files in the current folder and the parent folder

https://ovito.org



Install and open ovito



Find 1 MD trajectory here : <u>http://folk.ntnu.no/senbox/trj/</u>

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Find 1 MD trajectory here : <u>http://folk.ntnu.no/senbox/trj/</u> Download it to your computer and load into ovito.

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Download lammps

http://lammps.sandia.gov/download.html

Task:

- 1. Unzip lammps to some folder and try installing it.
- 2. Try running lammps using the command:

Imp (or Imp_serial in linux)

Short introduction to lammps

How to run it: *Imp –in inputFile* or *Imp_serial < inputFile*

Task: go to *Example/melt* folder, and do a test run. The input file in this folder is: *in.melt*

- Pay attention to the output in your screen, try to understand (guess) what it tries to tell you.
- Try to store this screen output to a text-based file by ">"

Short introduction to lammps

- It is not the only package for Molecular Dynamics (MD) simulations
- It is fast, flexible (not very user friendly)
- Has limited analysis tool

• ...

- Provides interfaces to other software
- Has big user community (google-able for problems)

Typical inputs for a MD simulation

- Atoms: coordinates, properties, connection
- Simulation environments: box, pressure, temperature

How Lammps dose MD:



Building a fully flexible polymer chain

Brief polymer physics

- Polymer dynamics depends on
 - Chain length
 - Chain bending stiffness
 - Entanglement

• ...

The simplest model for polymer chains: fully flexible model Polymer monomers by beads Neighbor monomers bonded by free joints (covalent bonds)

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The simplest model for polymer chains: fully flexible model Polymer monomers by beads Neighbor monomers bonded by free joints (covalent bonds)

Assignment 1: model and simulate fully flexible chain melts

Potentials



Attractive



What to do?

- 1. Model fully flexible chains
- 2. Define bonding connections
- 3. Run simulations and perform analysis



Building one single polymer chain

Coarse-graining:

One bead = one monomer

What is needed:

1. 3D coordinates of all beads

2. Neighbor beads pairs

How is the simulation looks like:

vmd movie



Building one single polymer chain

Two files for Lammps:

data file: structure information

input file: simulation control



Setting up simple run in Lammps input file: Example Number of atoms number of bonds *Number of atom & bond types* Masses of atoms Atoms bonds

Polymer Chain data file 20 atoms 19 bonds 1 atom types 1 bond types 0 20 xlo xhi 0 20 ylo yhi 0 20 zlo zhi Masses 1 1.00 Atoms 1 1 1 5.0 2.0 10.0 Bonds 1 1 1 2

Running simulations

input file:

Choose units system for the system

Read atomistic structure

Setup non-bonded and boned interactions

Choose time step and generate initial velocity

Choose simulation ensemble

Set simulation length and run

	# Polymer Chain input file	
	units atom_style	lj bond
	read_data	datafile
	pair_style pair_modify pair_coeff	lj/cut 1.122461 shift yes 1 1 1.0 1.0 1.122461
	bond_style bond_coeff	fene * 30.0 1.5 1.0 1.0
5	#dump	1 all atom 100 traj.lammpstrj
	timestep velocity	0.01 all create 1.0 12345
	fix run	1 all nvt temp 1.0 1.0 100 50000