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

  ls 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

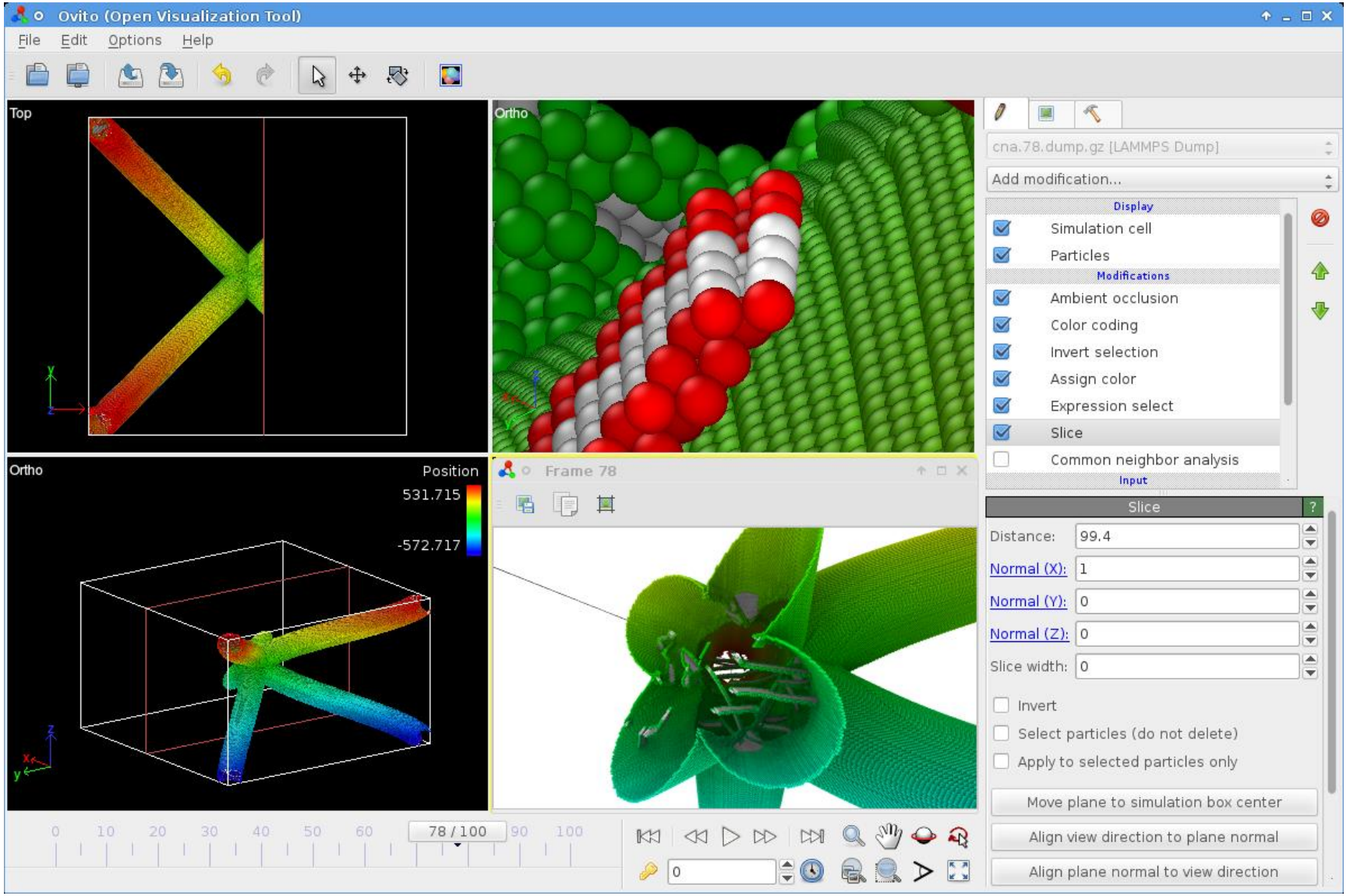
Task: go to “/usr/bin” or “C:\Windows\System32”, list the files in the current folder and the parent folder

Using OVITO to visualize MD trajectory

https://ovito.org

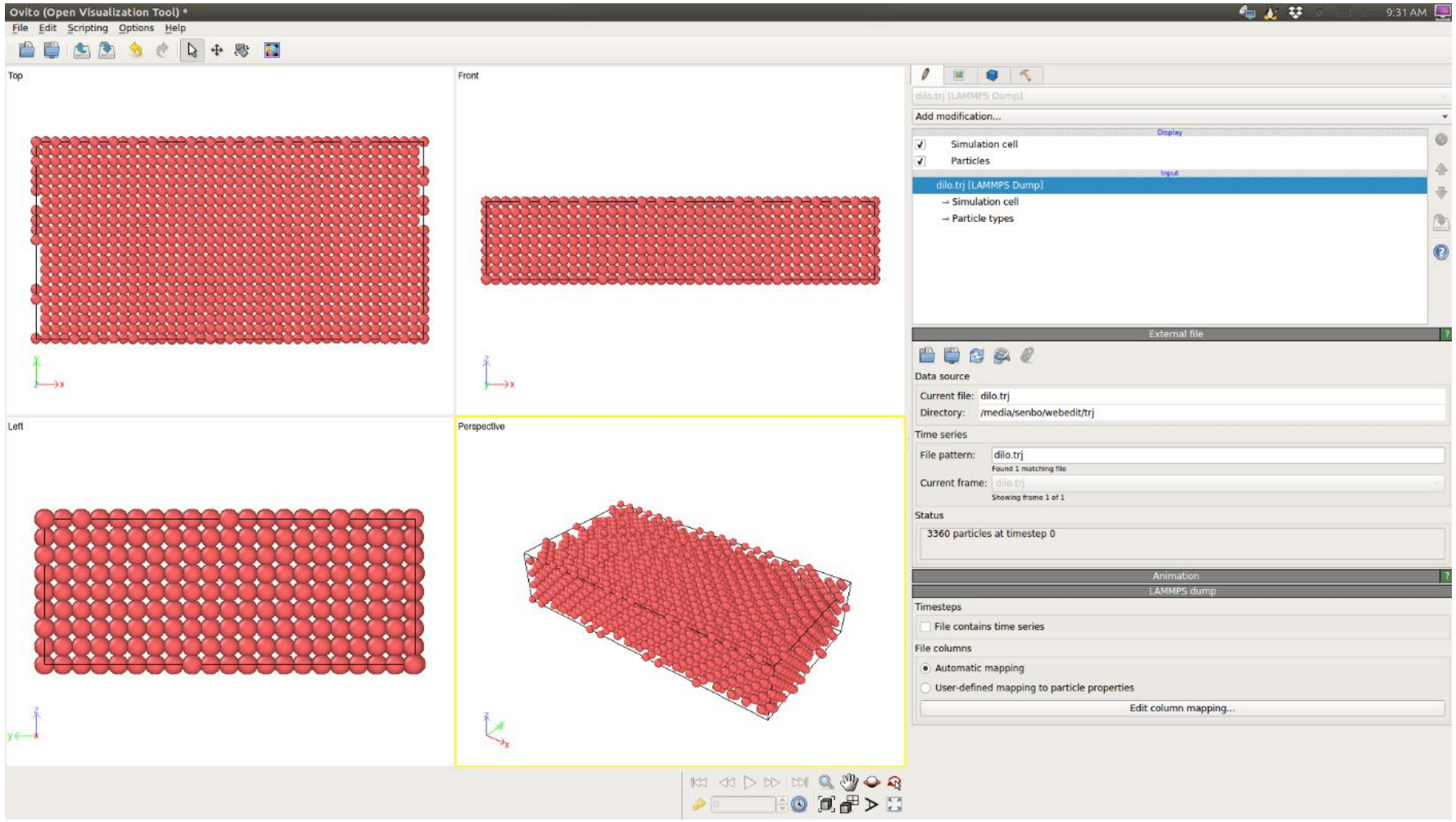
OVITO
Open Visualization Tool

Install and open ovito



Using OVITO to visualize MD trajectory

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



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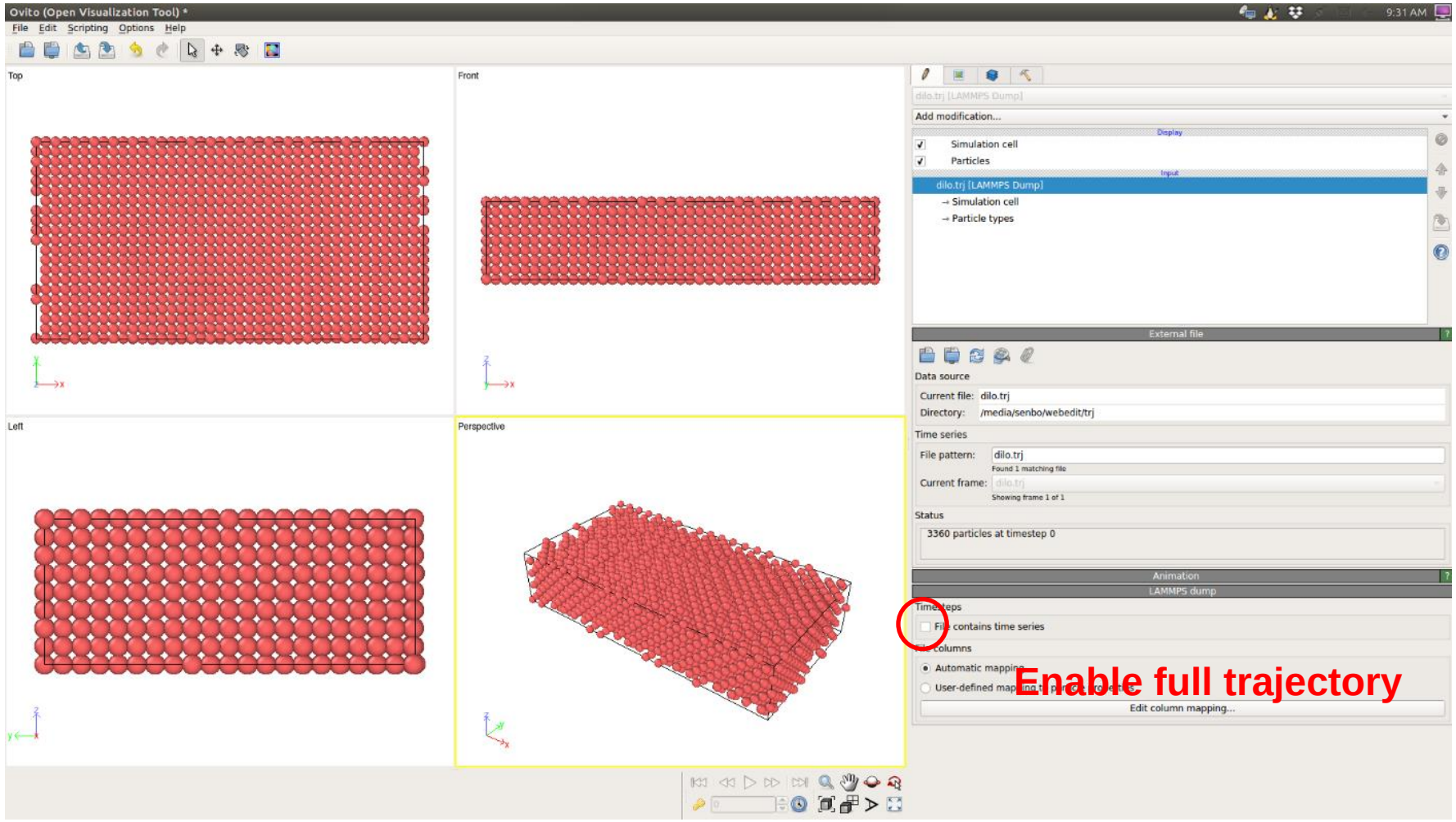

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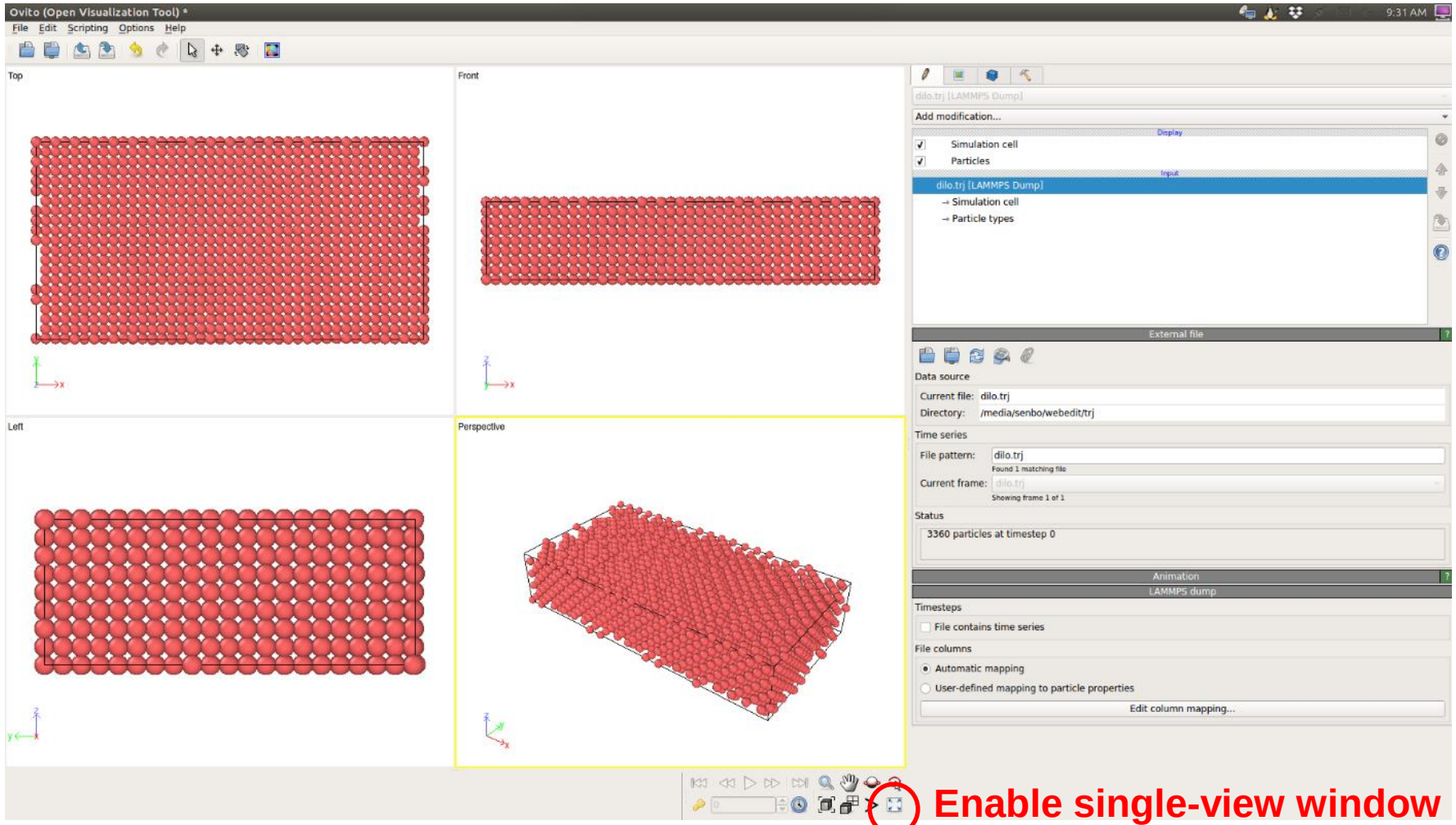

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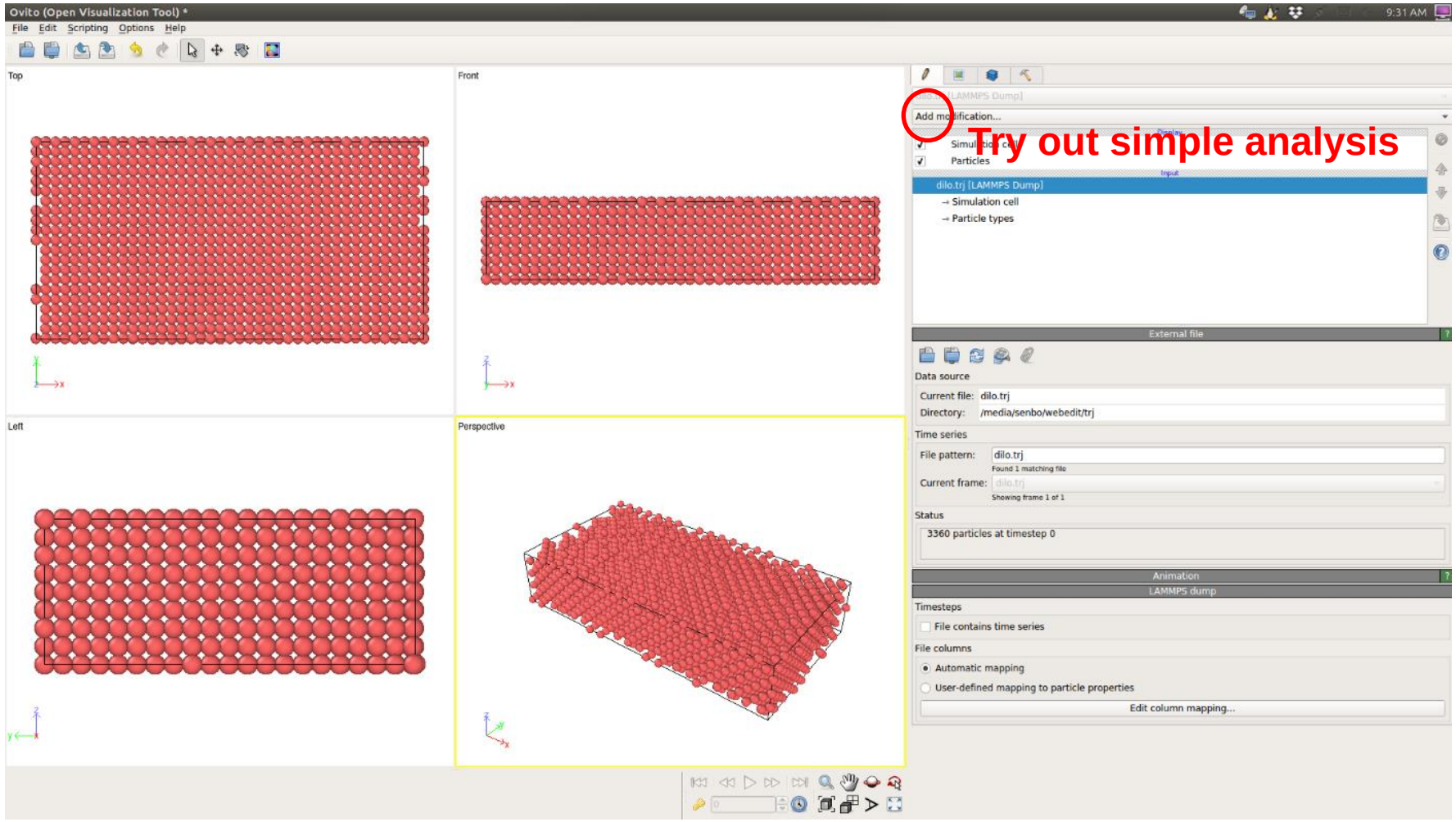

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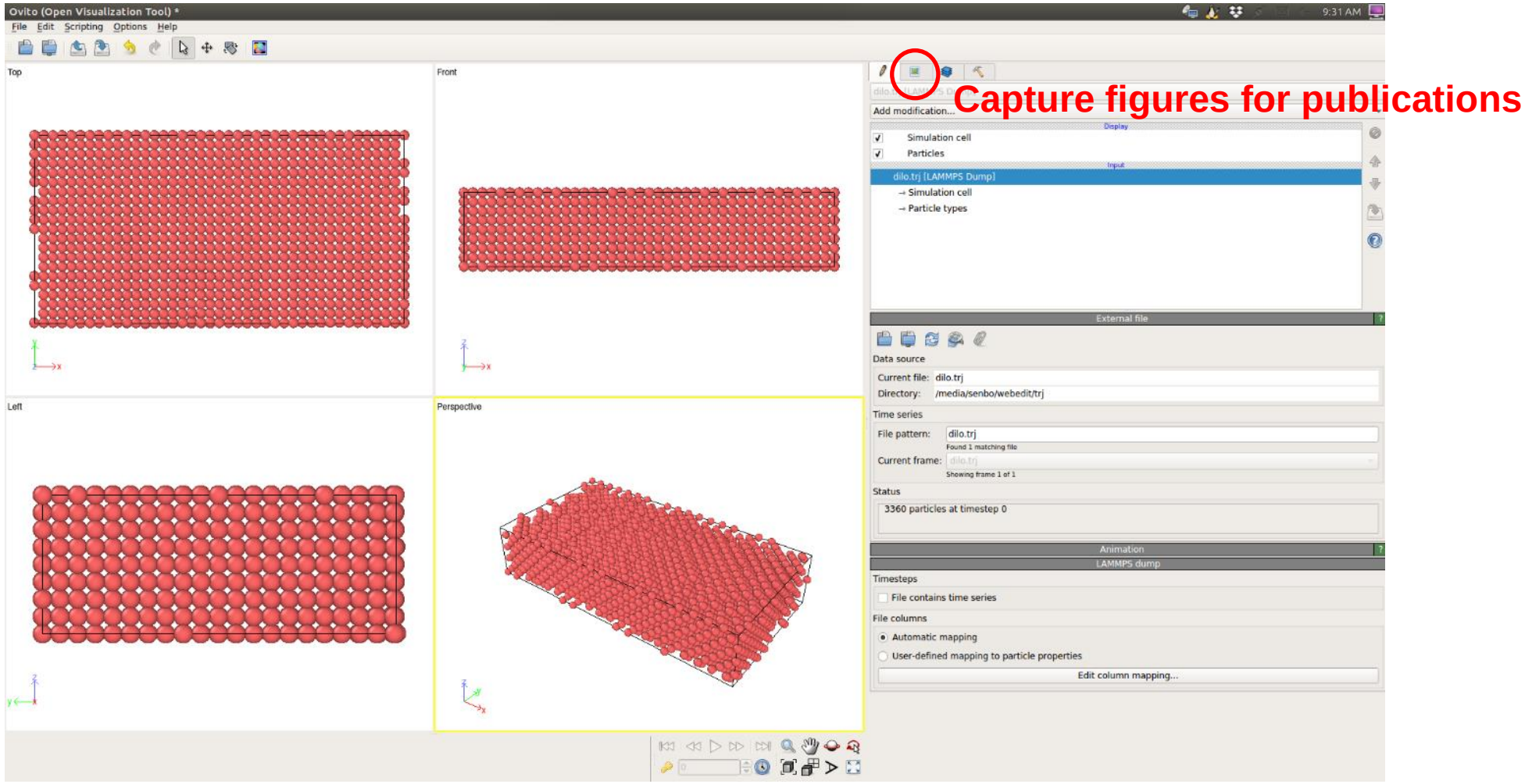


Download lammps

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

Task:

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

lmp (or lmp_serial in linux)

Short introduction to lammps

How to run it: *lmp –in inputFile*

or *lmp_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 “>”

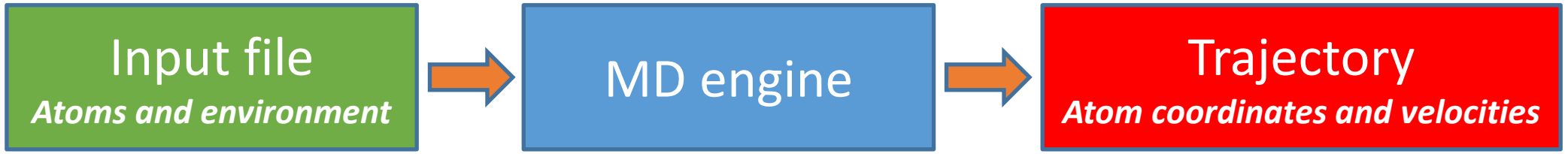
Short introduction to lammps

- 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

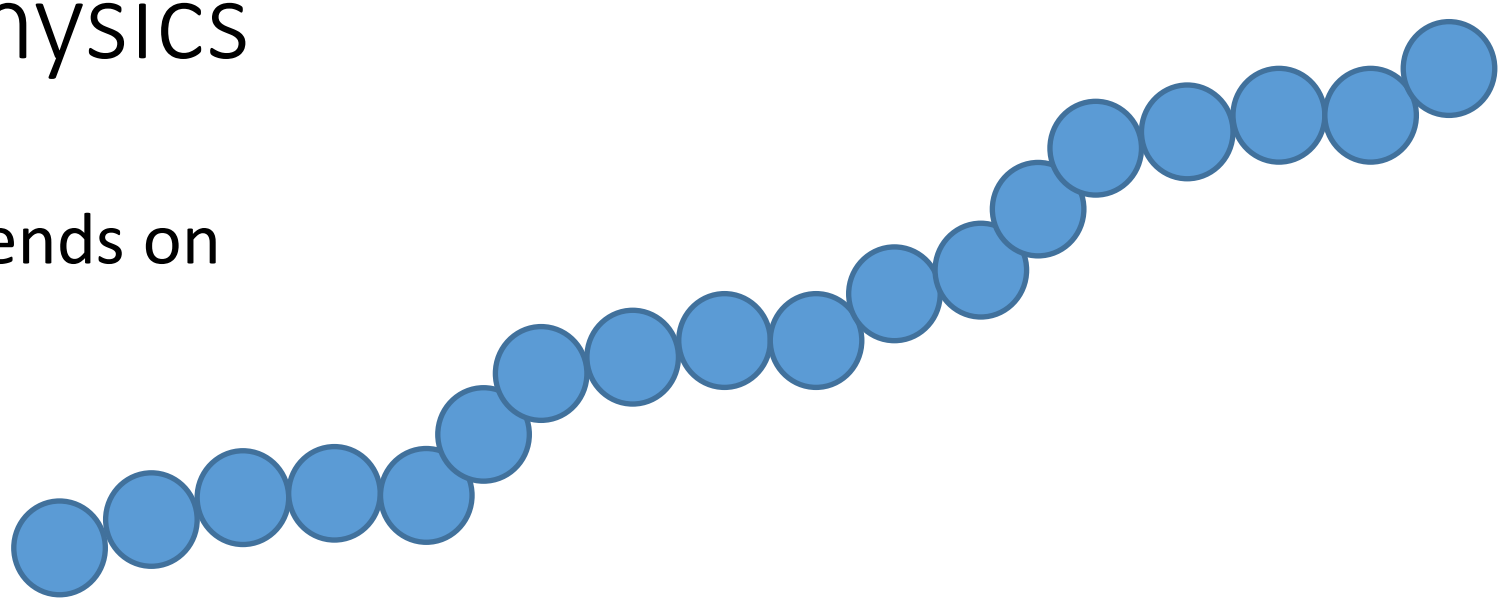
How Lammps dose MD:



Building a fully flexible polymer chain

Brief polymer physics

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



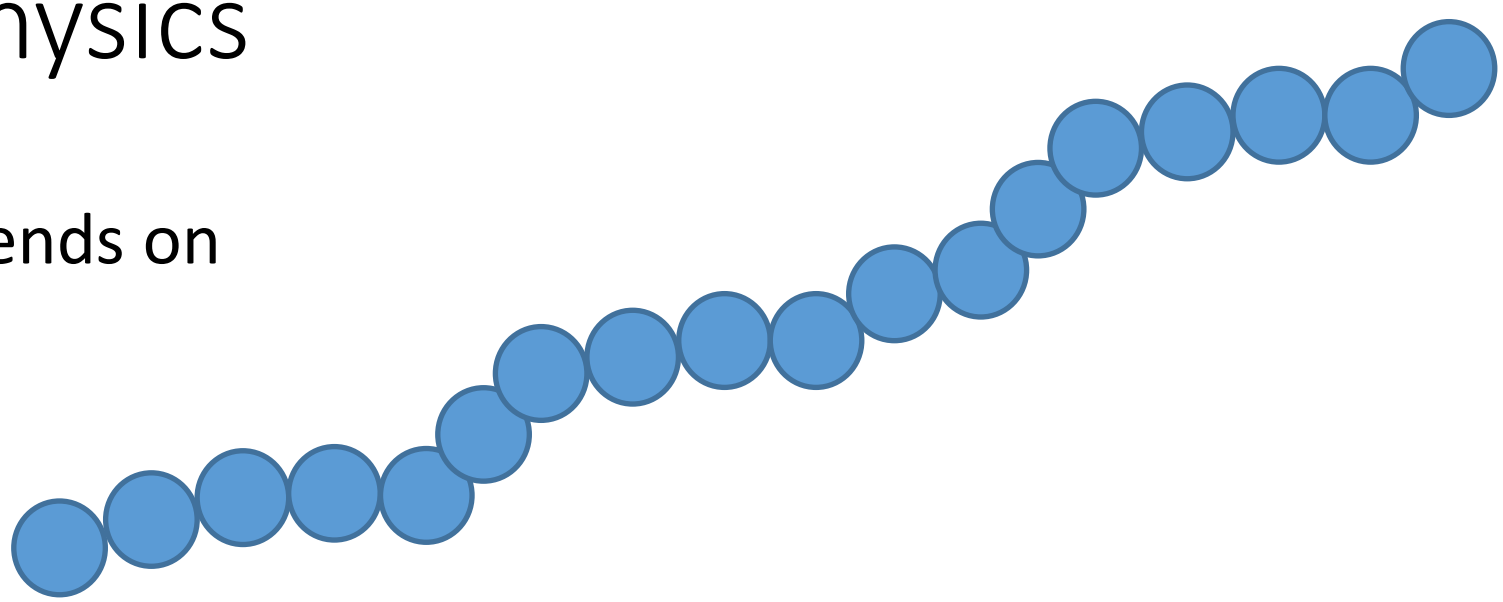
The simplest model for polymer chains: fully flexible model

Polymer monomers by beads

Neighbor monomers bonded by free joints (covalent bonds)

Building a fully flexible polymer chain

Brief polymer physics



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The simplest model for polymer chains: fully flexible model

Polymer monomers by beads

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Assignment 1: model and simulate fully flexible chain melts

Potentials

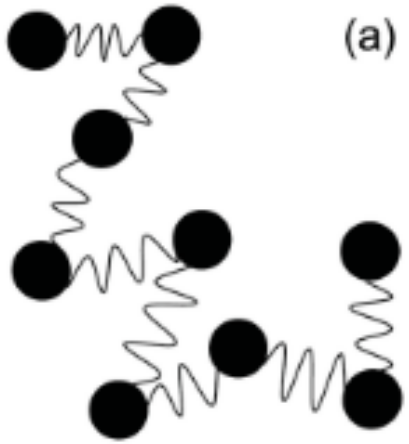
Finite extensible nonlinear elastic (FENE) bond

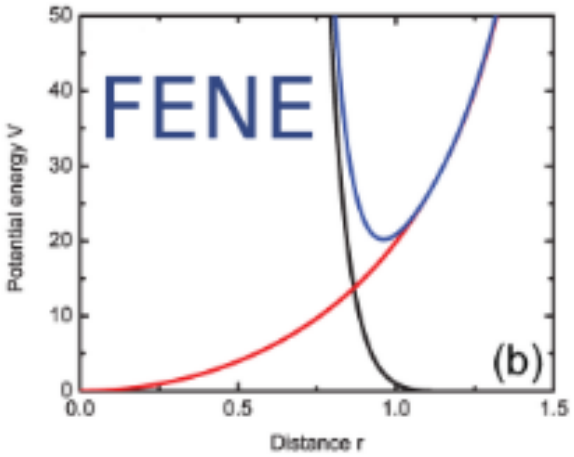
Weeks-Chandler-Andersen (WCA) potential

$$E = -0.5KR_o^2 \, ln\left[1 - \left(\frac{r}{R_o}\right)^2\right] + 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \epsilon$$

Attractive

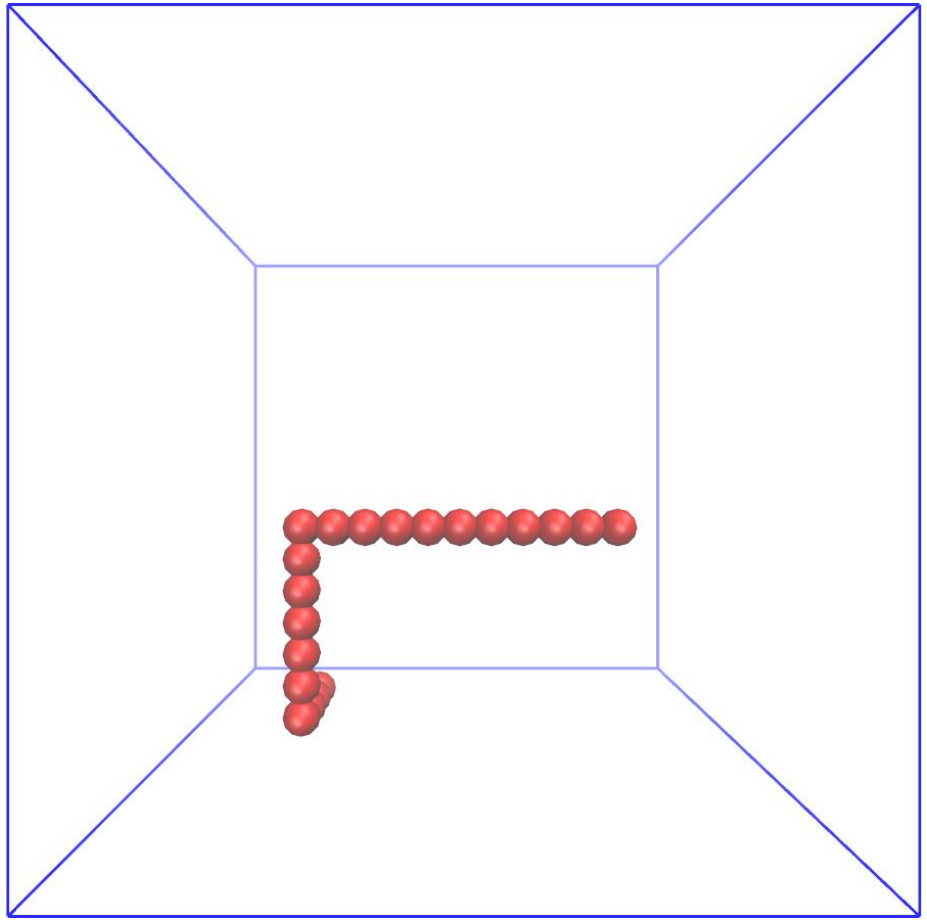
Repulsive





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

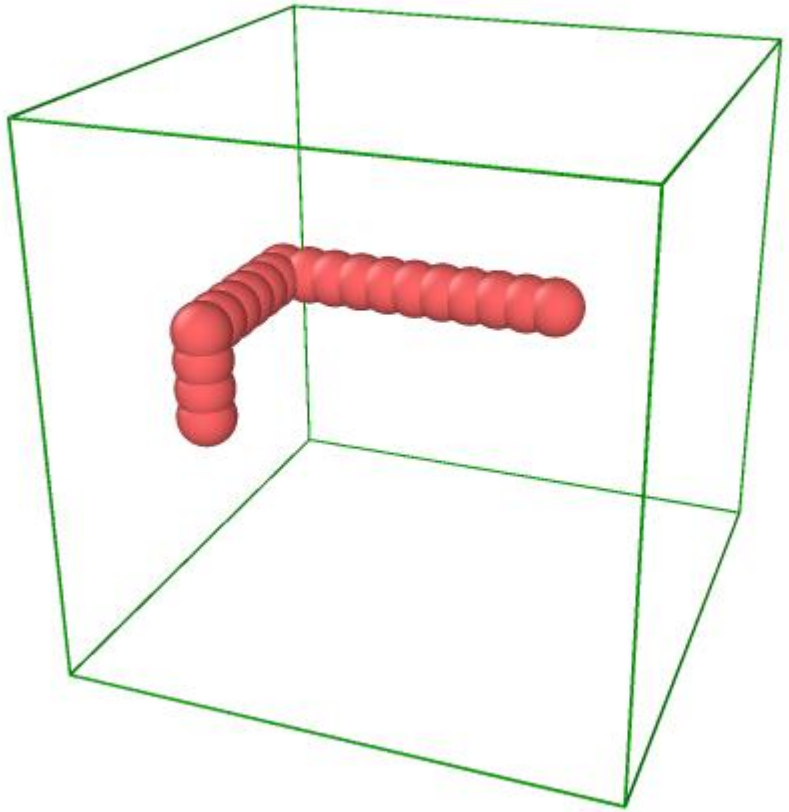
What is needed:

1. 3D coordinates of all beads

2. Neighbor beads pairs

How is the simulation looks like:

vmd movie

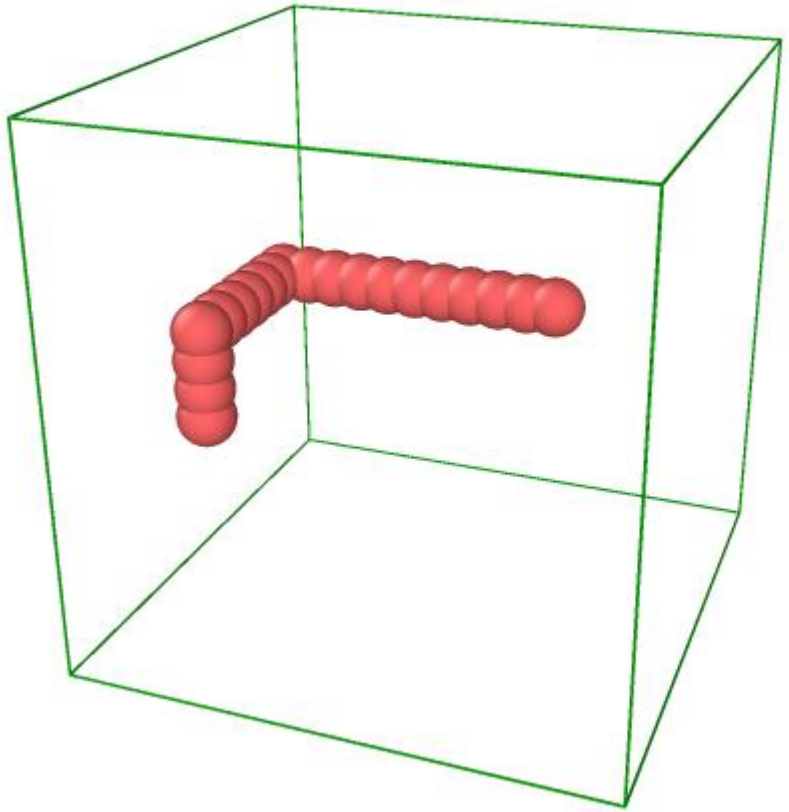


Building one single polymer chain

Two files for Lammps:

data file: structure information

input file: simulation control



Setting up simple run in Lammps

input file:

Number of atoms

number of bonds

Number of atom & bond types

Masses of atoms

Atoms

bonds

Example

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           lj
atom_style      bond

read_data       datafile

pair_style      lj/cut   1.122461
pair_modify     shift   yes
pair_coeff      1  1  1.0   1.0   1.122461

bond_style      fene
bond_coeff      * 30.0 1.5 1.0 1.0

#dump           1 all atom 100 traj.lammpstrj

timestep        0.01
velocity        all  create  1.0  12345

fix             1 all nvt temp 1.0 1.0 100
run             50000
```