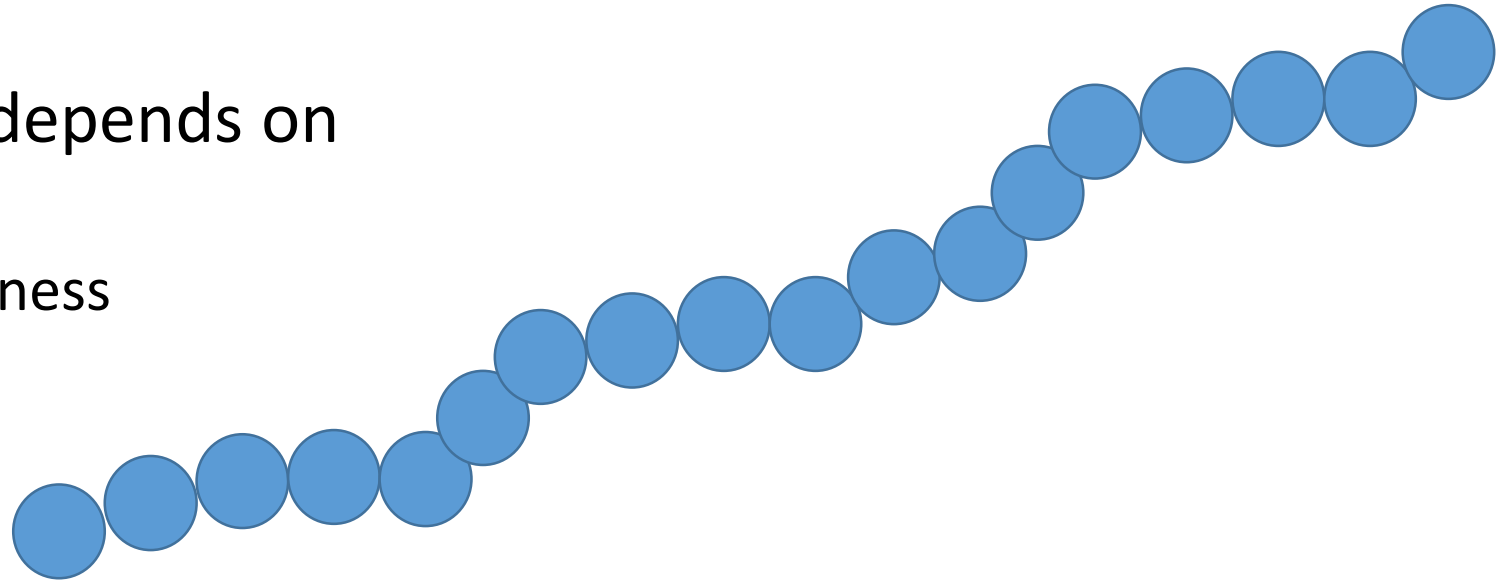
Lammps Tutorial 3&4

output control in lammps
data and restart files, analysis,
building more complex polymer system

Polymer chain dynamics

- 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)

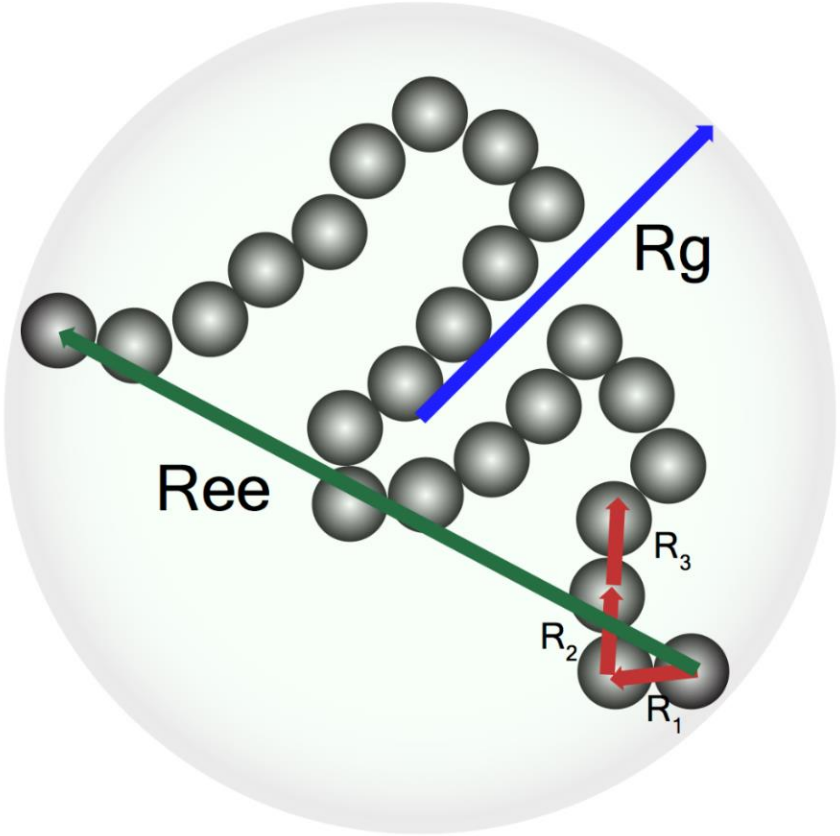
Tutorial 2: short analysis on one polymer chain and build polymer melt

Questions for this tutorial

1. Calculate system potential, and evaluate system state

2. Dependence of the radius of gyration (***Rg***) on the end-to-end distance (***Ree***)

$$Rg^2 = \frac{1}{N}\sum_{i=1}^{N}(\boldsymbol{r}_i - \boldsymbol{r}_{mean})^2$$



Units

Quantity	Reduced unit	SI unit
Energy	ε^*	1.9665 kJ/mol = 0.47 kcal/mol
Length	σ^*	0.45 nm
Mass	m^*	56.11 amu = $93.173 \cdot 10^{-27}$ kg
Charge	q^*	1 e = $1.602 \cdot 10^{-19}$ C
Time	$\tau^* = \sigma^* \sqrt{(m^*/\varepsilon^*)}$	2.4037 ps
Temperature	$T^* = \varepsilon^*/k_B$	236.51 K
Pressure	$P^* = \varepsilon^*/\sigma^{*3}$	358.35 bar = $3.5835 \cdot 10^{7}$ Pa
Mass density	$\rho^* = m^*/\sigma^{*3}$	1022.5 kg/m^3
Number density	$n^* = 1/\sigma^{*3}$	10.974 nm^{-3}
Permittivity	$\varepsilon_0^* = N_A \cdot q^{*2}/(\sigma^* \varepsilon^*)$	$1.7469 \cdot 10^{-8}$ C^2/Nm^2

Print out system information

commands:

thermo_style custom step pe ke press vol etotal ….

http://lammps.sandia.gov/doc/thermo_style.html

thermo 50

http://lammps.sandia.gov/doc/thermo_style.html

```
# 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
```

Write out data and restart files

commands:

write_data datafile

https://lammps.sandia.gov/doc/write_data.html

write_restart restart_file

https://lammps.sandia.gov/doc/write_restart.html

restart 1000 system.restart

https://lammps.sandia.gov/doc/restart.html

What is in the restart file:

System unit, atom style,

simulation box information,

boundary condition,

group definition,

atom type and properties,

force field parameters,

bonding information among atoms.

Restart a simulation from a restart file

Read in restart file:

read_restart restart_file

https://lammps.sandia.gov/doc/read_restart.html

Comment out not required information from your input file and run.

What is in the restart file:

System unit, atom style,

simulation box information,

boundary condition,

group definition,

atom type and properties,

force field parameters,

bonding information among atoms.

Calculate end-to-end distance

commands:

variable a1 equal x[1]-x[20]

variable a2 equal y[1]-y[20]

variable a3 equal z[1]-z[20]

*variable dist_sq equal v_a1*v_a1+v_a2*v_a2+v_a3*v_a3*

variable dist equal sqrt(v_dist_sq)

Using thermos_style to print it out

thermo_style custom step v_dist

```
# 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
```

Define variables and out put

Calculation end-to-end distance

variable a1 equal x[1]-x[20]

variable a2 equal y[1]-y[20]

variable a3 equal z[1]-z[20]

*variable dist_sq equal v_a1*v_a1+v_a2*v_a2+v_a3*v_a3*

variable dist equal sqrt(v_dist_sq)

Output to an individual file

variable r1 equal step

variable r2 equal v_dist

fix extra all print 100 "${r1} ${r2}" file distance.xvg screen no

Calculate radius of gyration

commands:

Compute gyr all gyration

Using thermos_style to print it out

thermo_style custom step c_gyr

Group concept in Lammps

http://lammps.sandia.gov/doc/group.html

Question:

Calculate end-to-end distances (***l***) and radius of gyration (***r***) of polymer chains of :

5 beads

10 beads

40 beads

50 beads

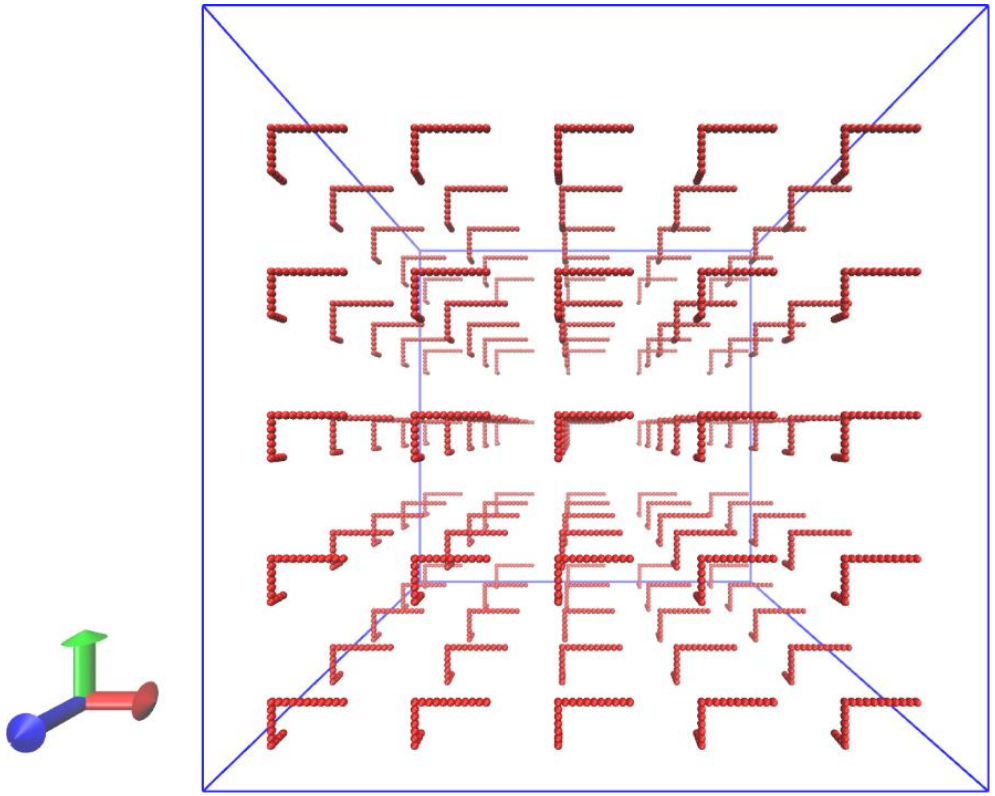
and try to find the relationship between ***r*** and ***l***.

Polymer data files:

http://folk.ntnu.no/senbox/polymer/

Making bigger systems

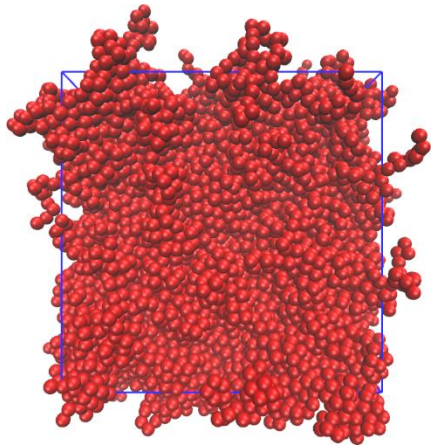
replicate command in Lammps: *replicate 2 2 2*



Manipulate simulation system

Rescale simulation box: change_box

```
Variable  i  in  loop  40
lable  loop
    change_box  all  x  scale 1.02  remap
    change_box  all y  scale 1.02  remap
   change_box  all z  scale  1.02 remap
   run 1000
next i
jump  input loop
```



Question:

Print out system density during the simulation,

And try to make the system density to be 0.85