Programming Exercise #3

1. *Reference Code Exercise*

Using RefCode (in MD_NP or MD), evaluate the following properties

a) *Scaling Law Verification.*

In later lectures, you will learn about polymer physics. One key concept in polymer physics is the **scaling law**.

The Flory theory predicts that the size of the polymer chains in good solvents scales with N^{ν}, where $\nu = 3/5$ for good solvents. More sophisticated theories predict the value of $\nu = 0.588$. Using the RefCode, by varying the chain length (by varying ELL), try to verify the scaling laws:

$$R = bN^{0.588}$$
$$R_g \sim N^{0.588}$$

where R is the end-to-end distance of the polymer, b is the Kuhn length, and R_g is the radius of gyration of the polymer.

During the course, please also check the **equilibrium time** (the time for the properties of interest approach a stable value).

* Note: you may need several ensembles. Learn to use scripts to control jobs. A sample script is in /home/2015sm0/Script, it might help you.

b) *Excluded volume effect.*

The excluded volume v of interacting particles is defined as

$$v = -\int f(r) d^3r$$

where $f(r)$ is the Mayer *f*-function defined as

$$f(r) = \exp\left[-\frac{U(r)}{kT}\right] - 1$$

with $U(r)$ the inter-particle interaction potential. For good solvents, since particles tend to repel each other, $v > 0$, and the scaling law of a polymer chain consisted of such particles is described in part (a).

Please vary the cutoff radius (r_c) of the Lennard-Jones potential (originally set to 1.12sigma in *ener_wca()* in *ener_ev.c*) and observe the effect of excluded volume. Larger cutoff radius will allow an attractive interaction, lowering the excluded volume. Beware to also shift the truncated potential so that $U(r_c) = 0$ so that the potential is physical.

* Note: The usual cutoff radius of L-J potential is set to 1.12 for purely repulsive potential, and 2.5 for the attractive part.

c) *Bending rigidity effect.*

The parameter *KB* in *input.dat* defines the bending rigidity of the polymer chain. Please vary the value of *KB* and observe the effect of the stiffness of a polymer

chain on the radius of gyration R_g.

In addition, in previous session, I told you that to correspond the simulation to real physical systems, the persistence length of the simulated polymer and that of a real polymer are compared. The persistence length l_p is defined as the characteristic length of the autocorrelation of tangential vector along the chain

$$\langle \vec{t}(s) \cdot \vec{t}(0) \rangle = \exp\left(-\frac{s}{l_p}\right)$$

Please verify that for *KB*=5, $l_p = 5$. In addition, if you are interested, try also to find the dependence of l_p on KB.

(It should be almost linear for 5<*KB*<25, with $5 < l_p < 25$.)

d) *Using RefCode to model colloid system.*

If you wish to simulate granular system or colloidal suspension, it can also be done by RefCode. Change *KB* and *KV* to 0, and *ELL* will become the number of monomer particles with L-J (or other) interactions. If you use MD_NP, you can also simulate binary composition systems, where the number of particles of the second type is controlled with *NPNUM*.