1 Reproduce the result from paper using LAMMPS

Step 1 requires (in LJ units):

Interaction between molecules (ϵ) mimicked by harmonic oscillator vanished off at 3σ. NVE with langevin. Thermostat without thinking about the on/off states and force.

Parameters: N=10, R=2, L=2, dt=0.02 in thermostat, r_0=0.5 for the bond length, s_s =2 for spring constant (bonds) ϵ=2.5, ϵ_w=0.3 for the LJ constant between monomers and between wall particles, f_{hr}=5 within region 1 and only acting on the first monomer, f_{pull}=1.0 is acting on the first monomer iff in region 2, 200^3 3D box, ignore $k_{on} = 10$ and $k_{off} = 1$ for now.

Problems:

Lost atom

"Walls" are generated by repulsion, original method can cause diffusion

The positions and momentum of all atoms should be defined in data file

Force design: set center of region 1 as point A, position of polymer B, distance $r = \sqrt{\delta x^2 + \delta y^2 + \delta z^2}$, $fx = 5 \times \delta x/r$, $fy = 5 \times \delta y/r$, $fz = 5 \times \delta z/r$

2 Revise the model into 3D

3 Try models in different attraction forces besides harmonic approximation

Hydrogen bonding, fene and electrostatics

4 Heterogeneous monomers

5 Design initial structures for peptides