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=0.01 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 (solved by discretizing the time in more detail). (Solved)

"Walls" are generated by repulsion, original method can cause diffusion. (Solved)

The positions and momentum of all atoms should be defined in data file. (Solved)

Force design: parameter x_{lo} and x_{hi} as the range of action, Δ as scaling, f_{max} as maximum force added, ω as frequency and t as time. $F = \frac{tanh(\frac{x-x_{lo}}{\Delta})-tanh(\frac{x-x_{hi}}{\Delta})}{2} f_{max} cos(\omega t)$

FFS for different ω: initial flux estimated by diffusion constant 0.00245 via curve fitting.

step 2: cut the LJ pairing between polymers and wall atoms at 1.12 instead of 3 to avoid overlapping around the corner; calculating the free energy change from the wall to anywhere left by $-k_B T ln(P)$ where P is subtracted from the spring we fixes by umbrella sampling.

2 Revise the model into 3D

(solved)

3 Try models in different attraction forces besides harmonic approximation

Hydrogen bonding, fene and electrostatics

4 Heterogeneous monomers

5 Design initial structures for peptides