BT2042: Fundamentals of Biophysical Chemistry
Assignment I
March 9, 2020

Deadline for Submission: 4 pm on March 26, 2020

Instructions The code employed to simulate the system, details of the calculations and a write-up should be sent to my email athi@iitm.ac.in (**as one zipped file with the title Name1_Name2.zip or Name1.zip**). This will account for 40% of the total points. Late submissions will NOT be entertained.

The submission will not be evaluated without the code employed – each group should write their own code. **Any kind of plagiarism or copying will not be accepted and will be reported to the Disciplinary Committee followed by a U grade**.

Questions

Consider a short polymer of 4 beads floating around in a lattice which is 10 times larger than the polymer itself (similar to the lattice protein described in the class).

You can think of this polymer to be a precursor of longer polymer in pre-biotic times. The polymer can undergo both the end-move and the corner move (I had mistakenly referred to the latter as crankshaft) as discussed in the class. Consider that there are 5 other such polymers in the lattice (at some distance from each other). Given the six polymers in the lattice and assuming $k_bT=1$, simulate the following:

1. If no intra-molecular interactions are allowed, and if the bead *a* of one polymer can interact only with the bead *a* of another polymer (inter-molecular interactions; similarly, *b* can interact only with *b* in another molecule and so on), what kind of different molecular assemblies due to observe after 10^6 Monte Carlo moves employing the Metropolis criterion? Two beads can be assumed to interact when they are separated by a single lattice length. Note that a molecule can interact with more than one molecule as long as the distance criterion is satisfied.

   The simulations need to be repeated 10 times (at least) to say if the same set of structures are observed on every realization. This simulation would be equivalent to simulating aggregation. The simulations can also be run for different bead-bead inter-molecular interaction energies of -1, -2 and -5 (in relative units).

2. Extending on question 1, what kind of assemblies are observed for the different interaction energies provided, when any bead of one molecule can interact with any bead of another molecule?

3. What structures do you observe when only *a* and *b* can interact with *a* and *b* of another molecule? In other words, *c* and *d* do not contribute to any inter-molecular interaction energies.