Molecular Dynamics

1 MD Concepts

Question 1: What are the atomic masses of calcium, carbon, nitrogen, oxygen, and hydrogen?

Question 2: What approximation do we make in our simulations in Project 3 regarding atomic mass, and how might this affect the simulation?

Question 3: What physical analogy do we use to describe bonds between atoms?

Question 4: Qualitatively, how does the value of kb or kn affect the way paired atoms behave (describe it in terms of the physical analogy from #3)?

Question 5: Usually, which one is larger, kb or kn? Why?

Question 6: What are the types of interaction(s) that kn is representing?

Question 7: How do the different interactions included in kn compare in magnitude/relevance? You don't need to get into a lot of detail, just mention a few and if you think one is (much) greater or less than another.

Question 8: What do we use to measure the overall stability of the structure over time as we are simulating dynamics?

Question 9: What are the different contributors to this measurement (#8)?

2 Simulations of Calmodulin

Question 1: Describe the number and type of secondary structures visible in calmodulin. (Hint: play around with the Representations window in VMD.)

For the next questions, compare the molecule behavior under different parameter settings. Speed will vary, so slow down the visualization slightly - just a millimeter or two off full speed so you can see the movement more clearly - and describe simulations relative to other ones.

Question 2: Which motion is the most dramatic when varying the temperature?

A. Temp = 50K

B. Temp = 350K

C. Temp = 4500K

Question 3: Which motion is wider when varying the spring constants?

A. Kb=1,000, Kn=100

B. Kb=40,000, Kn=400

Question 4: The simulations for the two nbCutoff values (0.25 and 0.75) should look markedly different. Why does changing this parameter result in the observed molecule behaviors?

Question 5: At what size time step does your simulation become completely unstable?

Question 6: In Line representation (the default in VMD), focus on some of the amino acids with ring systems. What do these rings seem to be doing that goes against what realistic chemistry dictates (this is more evident at more extreme parameter settings)?

Question 7: Does the presence of calcium seem to stabilize the binding sites when you compare the same location with and without calcium in the visualization with VMD, using the ”CPK” representation? Why?

Question 8: Does the calcium seem to be well constrained to the binding site in the visualization simulation?

Question 9: Do the calcium binding site feature scores observed over time reflect increased or decreased stability in the binding site or not? Why or why not? Think about the allowed freedom of moving and how this freedom relates to achieving a thermodynamically stable configuration.

Question 10: Do the calcium binding site scores change significantly at the high temperature in contrast with the default temperature? In what way?

Question 11: Compare and contrast the three lines you generated for sitesCa1.euc and sitesCa2.euc. What occurs when you remove calcium? When you mutate the atom interactions?

Question 12: What do your observations in #11 suggest about the importance of calcium and/or amino acids at the calcium binding site for calmodulin?

Question 13: List three ways the simulation could be modified to more accurately represent the interactions taking place? How computationally reasonable are these modifications you propose?