Pourna Sengupta
CSCI 4314: Dynamic Models in Biology
Homework Set 1
February 9, 2021

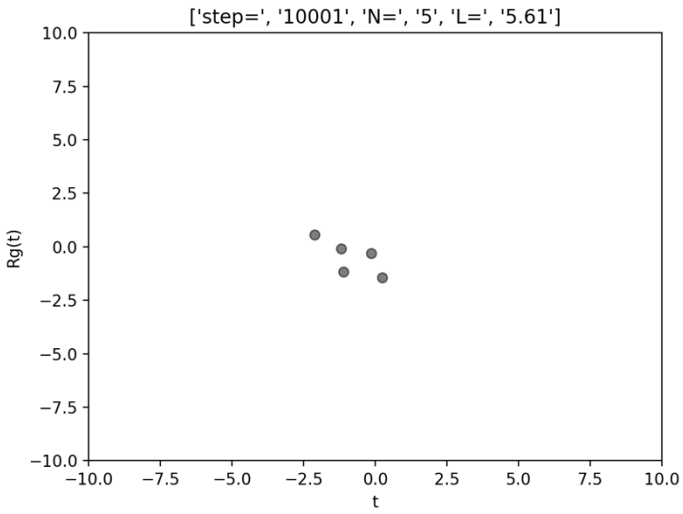
Coarse Grained Simulation of a Protein

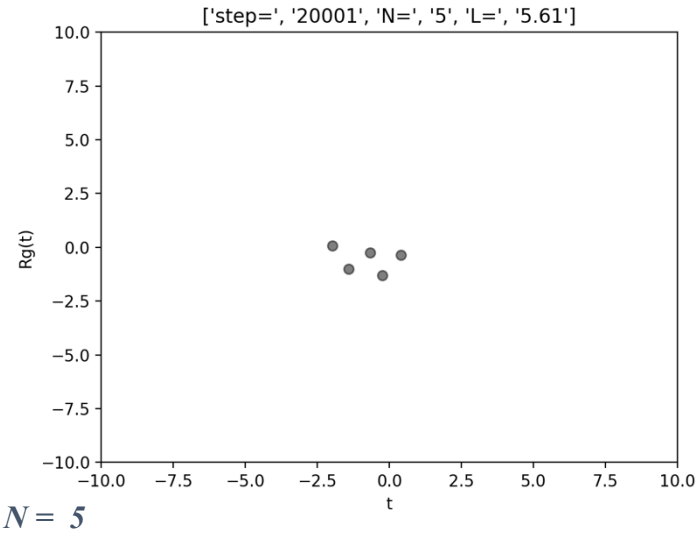
(1) Plot of the $R_g(t)$ (Radius of Gyration)

a. **N = 5**
b. **N = 10**
c. **N = 25**

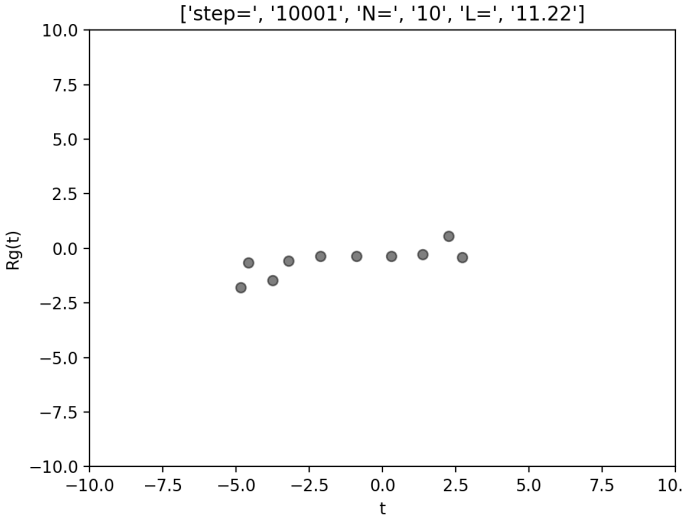
(2) Plot of the $R_g(t)$ (Radius of Gyration)

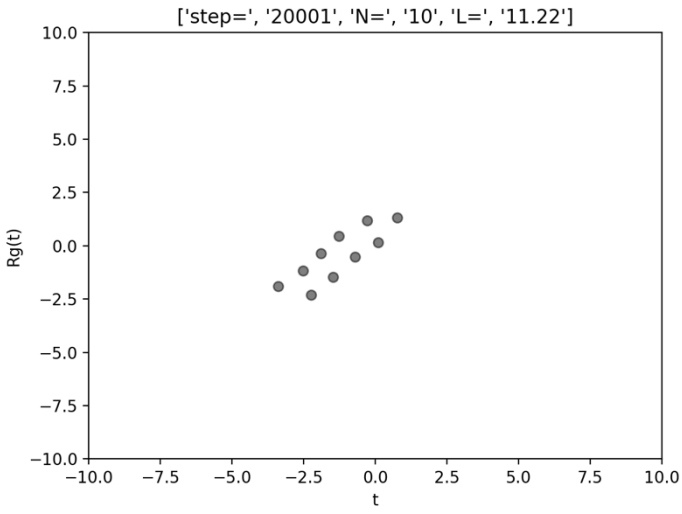
a. $\in = 0$
b. $\in = 0.5$
c. $\in = 1$





N = 5





N = 10

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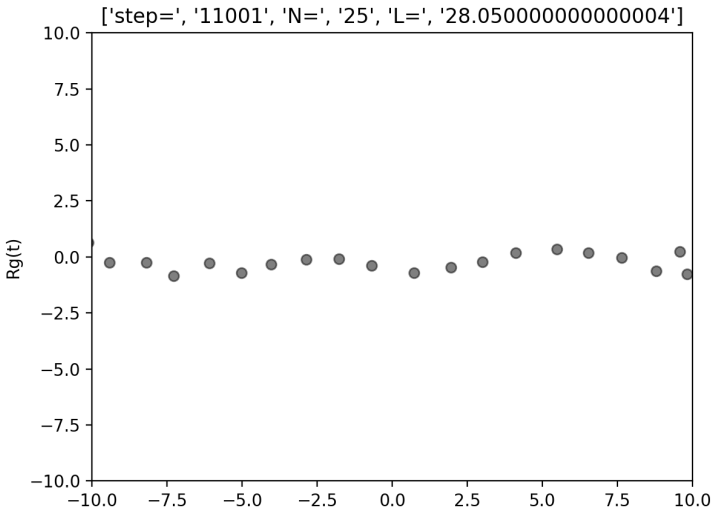
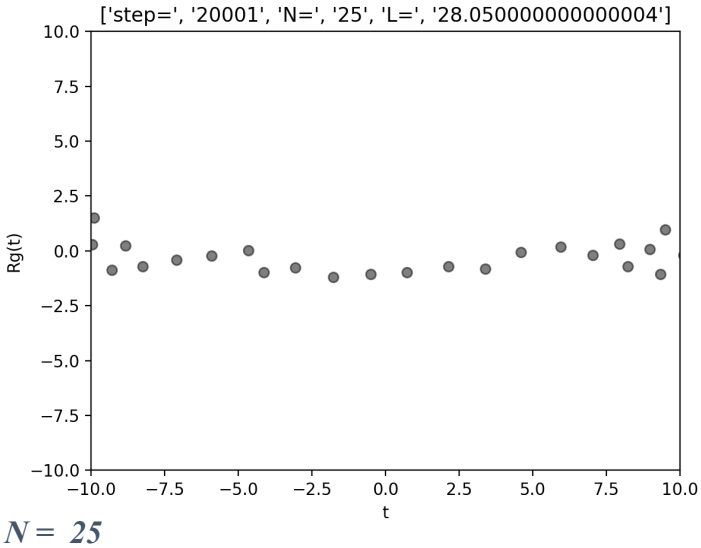
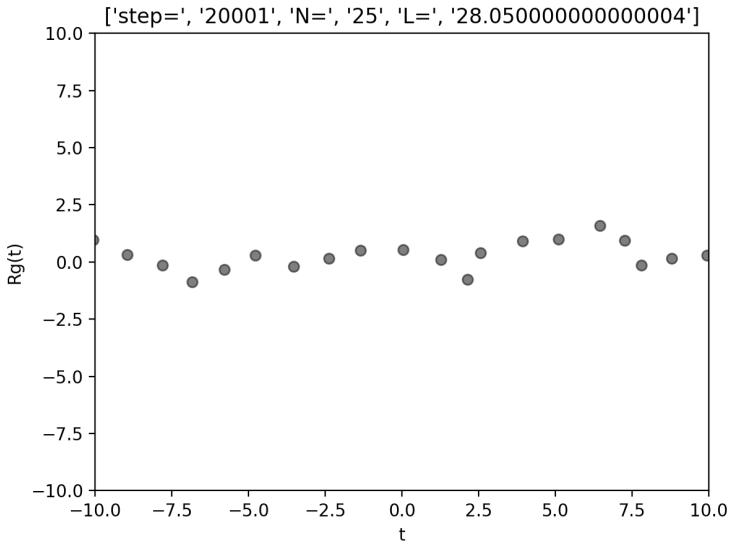
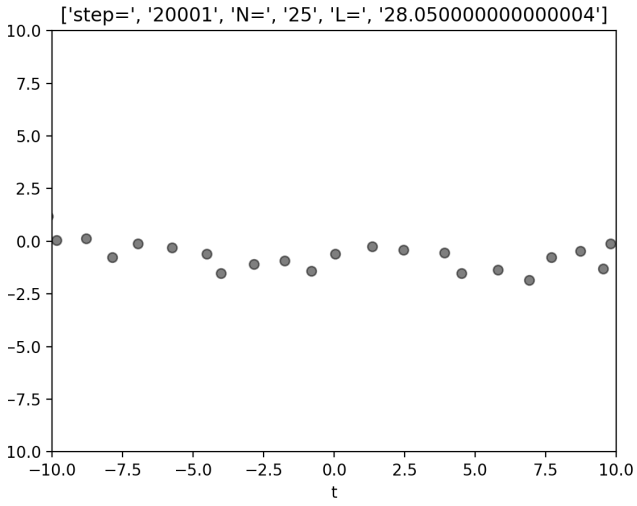




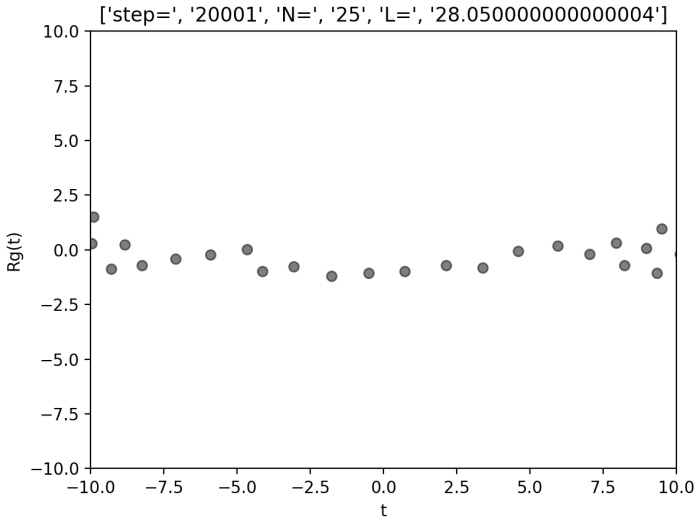
$N = 25$



$\epsilon = 0$



$\epsilon = 0.5$



$\epsilon = 1$

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Paper Review

(1) What do you feel the main contribution of this paper is?
    a. The paper outlines the results of the experiment, focusing on the obviously demonstrated "potential of using DNA to create self-assembling periodic nanostructures". Nanotechnology and nanomedicine are two examples of fields that greatly benefit and grow from research regarding nanostructures and nanoparticles. DNA self-assembly is revolutionary, and therefore moves research and findings withing these important fields forward. Nanomedicine such as Doxil is a great example of how further research into DNA self-assembly can help save the lives of many in time. This paper proves that we must continue to fund research into nanostructures to further medicine and technology and expand our knowledge into them, such as the "parameters that characterize DNA self-assembly" as the paper suggested.
(2) What's the essential principle that the paper exploits?
    a. The paper exploits essential principles of atomic bonding in Molecular Dynamics. In theory, bonds cannot be created. The molecular structure of the DNA crystal self-assembles, creating covalent bonds to join adjacent nucleotide in order to produce a striped lattice. This is to create a "'woven fabric' of DNA strands" from self-assembly of the strands of the DX units.
(3) Describe one major strength of the paper.
    a. The paper provides a very detailed and in-depth explanation and discussion of the conducted experiment and findings. The diagrams/figures included are extensively described, with each step discussed in detail in the paper itself and relative captions to assist in displaying findings. Something I found quite interesting was their discussion of methods at the end of the paper rather than in the middle (before a discussion of their conclusions). This strayed from the typical research paper, which I found beneficial in my understanding. Instead, the paper begins with an explanation of the crystal design using tiling. They clearly discuss how using 2 or 4 DX unit types allows them to produce a two-unit lattice of "woven DNA strands".
(4) Describe one weakness of the paper.
    a. A weakness I found in the paper was their lack of discussion regarding the use of their findings in further research and future experiments. They lightly touch on a few paths of further research and experimentation including "parameters that characterize DNA self-assembly" and "error reduction and purification methods". I believe their discussion of the relevance of their findings could be expanded on to include possible experiments or examples of real world applications of their findings that can be identified in current medicine/technology.
(5) Describe one future work direction you think should be followed.
    a. I agree with the writers in that similar research into aperiodic structures should be conducted. Being able to design self-assembling molecular Wang tiles while meeting algorithmic rules could break barriers in nanostructure research that may allow us to discover revolutionary medicines and technology. One-dimensional aperiodic structures can be applied to optical devices and other 2-D photonic

technology. Further research in photonics can allow us to further the capabilities of laser technology, which could improve medical technology in laser surgery.