THE UNIVERSITY of EDINBURGH
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DNA Unzipping & Overstretching

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Introduction:

DNA consists of two long separate strands that are in a helix or screw-like shape around each other with opposite nucleotides being connected with hydrogen bonds. There are four 'flavours' of nucleotide within a strand of DNA. They are referred to as cytosine, guanine, adenine and thymine[1]. In this project I have used the Poland-Scheraga model of DNA which allows it to be 2 flat strands.

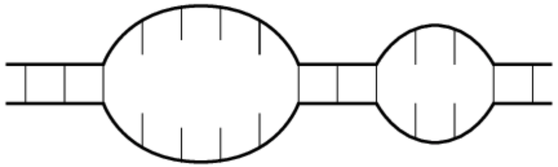

Figure 1: Poland-Scheraga model of DNA[2]

Methods:

A simulation was run using LAMMPS with the persistence length set by an angle of 20 degrees. The simulation was then run for all ε (the only variable to determine temperature) values from 1.0 to 1.7. Base pairs where then measured to determine whether they are open or not and a kymograph is produced for each simulation. The entire method is repeated for an angle of 10 degrees and results compared.

Results:

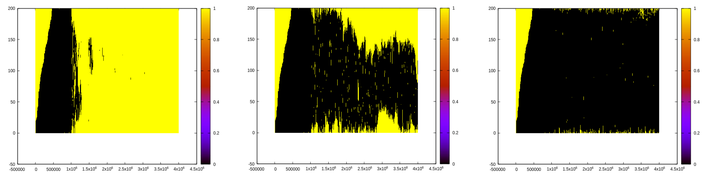

Figure 2: Kymographs of ε = 1.0, 1.3, 1.7

The kymograph above show the average number of open base pairs within the simulation of θ = 20. This shows from that the transition point occurs between 1.0 and 1.7. By looking at all kymographs, 1.3 is the first to show the start of denaturalisation.

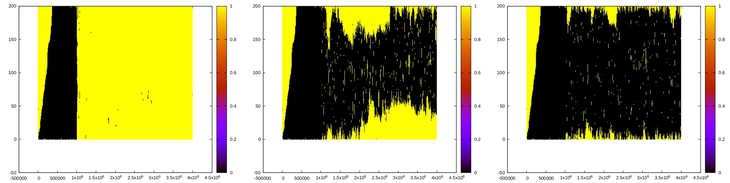

Figure 3: Kymographs of ε = 1.0, 1.6, 1.7

As above these kymographs show when θ = 10. The graph of 1.6 was also the first to show an opening of the DNA strand so it can be said that 1.6 is the transition point for persistence length 10.

From these results we can therefore see that the transition point of the polymer is only affected by the persistence length defined by θ.

Conclusions:

From the results it is clear to see that the only factor that resulted in the change of transition point is the persistence length. This shows that the potential that is produced in the bending of the DNA is strong enough to overcome the entropy levels at different temperatures.

If given more time to do the project, using more values for the persistence length could give some more interesting data points. As well as this, by increasing the length of the simulation there may be some different concepts.

References

[1] C. Richard, et. al. “Poland–Scheraga Models and the DNA Denaturation Transition”. Journal of Statistical Physics 115, (2004).

[2] Q. Berger, et. al. “Disorder and denaturation transition in the generalized Poland–Scheraga model”. arXiv 1807.11397, (2018).

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