

# 2021/22 Senior Honours Project

Due to my notes being in a scanned format, turn it in  
requires me to have 20 words of text within the PDF,  
hence this ramble.



THE UNIVERSITY *of* EDINBURGH  
School of Physics  
and Astronomy

## Workshop Week 2

Experience a realistic research project.

Project Performance: 35% - Supervisor

Project Report: 55% - Supervisor / second marker

Poster: 10% - Supervisor / second marker.

Record notes during Meeting & doing project.  
must be able to submit as a pdf.

Use this week to understand the project  
(LAAMPS).

### Report

15-20 A4 (5000-7000)

Understandable to other STI students

Clear & concise third person or first - keep consistent

Figures & diagrams - how many?

PDF file

Latex/word either is fine

Code? - Not necessary

Write as we go along - 2 weeks to  
polish up the report.

Title page: 1 page

Abstract: 100-200 words  
what is project about  
what was achieved

Introduction: 20% - 25% of page count (4-5 pages)

set the scene

context & motivation - why care?

objectives - key aims

Short overview of background theory

literature survey

Methods:

Reproducibility: describe what I did in great detail

Details: data manipulation: software used, parameters.  
↳ not much on the code but what calculated

discuss algorithms written - Ask supervisor.

Results & Analysis

comprehensible

Plots/diagrams: refer to intent, Explain what things are.  
include a caption, properly cite everything  
label axis, appropriate fonts

Think about uncertainties

units?

Appendix for code - Not necessary.

## Discussion & conclusion:

may be one or two sections

discussion: critical assessment of own work  
How do results compare  
How well did you meet objectives  
Could the methods have been improved  
Are there assumptions / errors

conclusion:

## References:

Harvard or IEEE - choose

consistent format.  
Avoid websites

## Help

Can get written feedback on 5 pages by 29/10

## Poster

Content - summary of the project

Design - Not too many words  
Use plots & figures  
Digestable within 3-5 weeks.

commonly use powerpoint  
template on wiki page.

Roughly A2 but widescreen 16:9.

**Submission**

December 3<sup>rd</sup> @ NOON

PDF report

PDF Poster

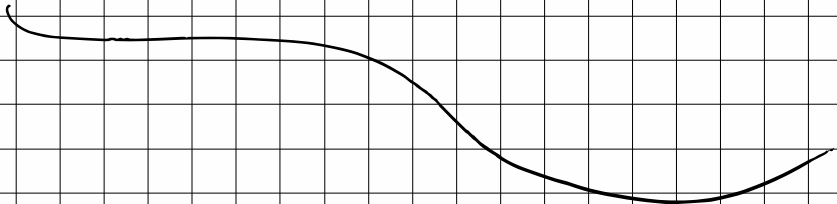
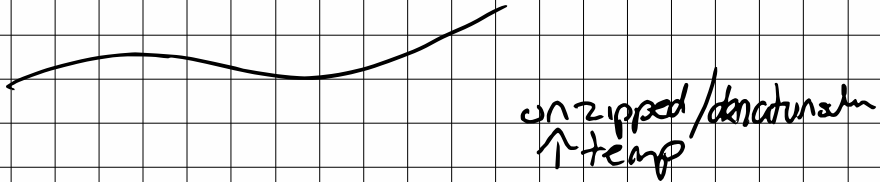
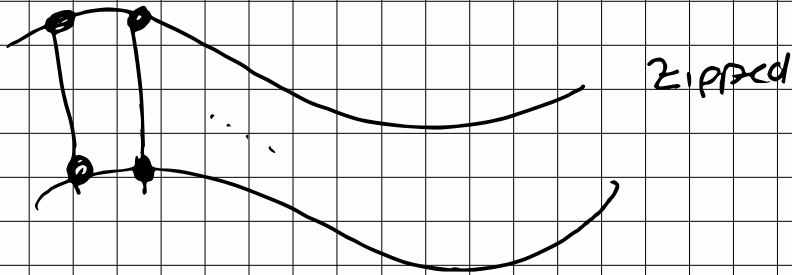
PDF Notes

**Questions**

LAAMPS code cite in methods sections  
say about extending.

# Meeting 27/09

- ① Create txt file for initial conditions
- ② use bumps to take conditions 3 similar
- ③ use vda to visual data.



using Poland-Scheraga model

Main ideas:

- DNA denaturation phase transition @ high temps with more entropy and more configurations as 2 separate strands
- Low temp, H<sub>b</sub> binding (energy) more important to determine state.

step ① output txt file

Questions:

Path length?  
separate strands? 2 or 1 or?

05/10/21 Meeting

## Running Coamps

input < calibrate.lam

take testat file - render C.S. result.

then

input < Full.Lam

## Inputs

100 - 200 each strand.

## Columns

200 types

1 type for 1<sup>st</sup> of each strand

step size = 1

S.F.  $\Rightarrow$  doubles.

## Tutorials



Meeting 12/10

change epsilon to find the write input.

For lamps a few times

change epsilon to find epsilon where  
DNA unzips

19/10

Take large simulations

last line add on extra 0.

Kymograph

time bead o/i  $\rightarrow$  denominator or not.

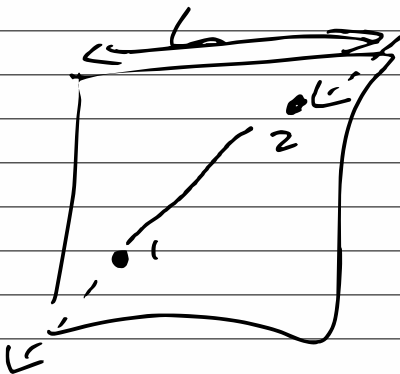
read dump file  
for each pair  $< 2.5$  then give 0.

gnuplot. distances

distance between 2 & 202 1 & 101 etc

$$L_x = -50 \rightarrow 50 \\ = 100$$

the distance



$$x_{1,2} = \sqrt{|x_2 - x_1|}$$

if  $(x_{1,2} > \frac{L_x}{2})$

$$\text{then } x_{1,2} = L_x - x_{1,2}$$

$\rightarrow x_{1,2}$

angles

number of timestep. goes  $\uparrow$  in 1000s

4001000 max

lines per time = 409 sets from 0.

Get Kamographs printed

Get average of time & no. of 1's ✓

Get average 1's with epsilon. ?

COSINE  $\rightarrow$  change to 10

have a look at 1.5 kmo.

Start writing

Karyographs & VMD. - regions of  
black within  
yellow

→

Analysis

Add SD of average

---

Reels COS 20

Introduction - DNA, Poland-Scheraga Model,  
entropy vs enthalpy.

low T en

\* There is a transition

\* diffusion

\* flexibility (cosine)

\* Larger simulation

\* double struts

\* Defect DNA strand,

## Results

Images first

Start w/ 20 - Realistic DNA Flexibility.

show transition

Discuss

→ 10

Discuss

## Wording

I did this instead of this was done.

cos = persistence length - looking more  
↳ how stiff polymers are.  
filter → less entropy  
→ easier to melt.

→ sent out on Monday

→ No coding.

Results → kramograph  
snapshot  
average pairs 1

demonstrated here is a transition  
E is basically temperature.

dependence on flexibility.  
↓  
kramograph

15-20 references.

↓  
3-4 → DNA  
2 → LAARS  
=1

Poster



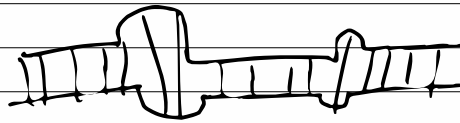
What I could have done with more time

\* larger chains

\* look at the dynamics

figure for PS model

- 10 page ✓



Methods

need first 5 equations

equation of motion

then

$U_{LS}$

$U_{bend}$

$U_{ext}$  - polymer together

initialisation

Results - 2/3/4 pages

system 20

then system 10.