NDnano
Center for Nano Science and Technology

NDnano Summer Undergraduate Research 2017 Project Summary

1. Student name & university: Nishi Kashyap, Indian Institute of Technology, Delhi

2. ND faculty name & department: Prof. Jonathan Whitmer, Department of Chemical Engg

3. Project title: **Predicting material elastic responses from Molecular Dynamics Simulations**

4. Briefly describe new skills you acquired during your summer research:
The amount of technical growth I had in these 2 summers, surpasses any past project's exposure. Not only did I learn multiple softwares but also how to use or learn them more efficiently. I came across new commands, built-in programmes and most importantly explored them to greater depths. Although I had to sit in front of a screen for long hours but that was completely worth it. I got comfortable using Linux operating system, Gromacs, VMD and further enhanced my coding skills. Now I feel very confident about my software skills which for me is a big achievement. I have gained respect for the time and effort that goes into research. I could not have asked for a better exposure.

5. Briefly share a practical application/end use of your research:

With the knowledge of equilibrium properties of the biological membranes, we can modulate them as per our needs. Since they are defining factors for the functioning of membranes, determination of elastic behavior by determining bending modulus would escalate the existing applications.

6. 50- to 75-word abstract of your project:
Biological membranes play a very important role especially when it comes to functioning of living cells. They experience fluctuating properties like undulation of surface due to excitation at physiological temperatures which has a serious impact on their functioning. Clearly, being able to monitor their elastic properties holds a lot of significance. For studying these undulations in membranes, like, local protrusions and variable thickness, Helfrich-type continuum model,one of the most reliable method, has been applied using fourier transformation. All the results have been obtained on 1,2-dimyristoyl-*sn*-glycero-3-phosphocholine (DMPC).The study further includes analysis on multiple mixtures of Dipalmitoylphosphatidylcholine (DPPC), 1,2-(cis-cis-9,12-octadecadienoyl)-sn-glycero-3-phosphatidylcholine (DUPC) and Cholestrol.

7. References for papers, posters, or presentations of your research:

- Brandt EG, Braun AR, Sachs JN, Nagle JF, Edholm O. Interpretation of Fluctuation Spectra in Lipid Bilayer Simulations. *Biophysical Journal*. 2011
- Schmid, F., 2013. Fluctuations in lipid bilayers: Are they understood?. *Biophysical Reviews and Letters*, *8*(01n02), pp.1-20.
- Bessonov, K. and Harauz, G., 2010. Molecular dynamics investigation of myelin basic protein stability on lipid membranes. *Studies by Undergraduate Researchers at Guelph*, *4*(1), pp.79-86.

One-page project summary that describes problem, project goal and your activities / results:

The biological membranes experience a lot of fluctuations due to thermal excitation at physiological temperatures. These include undulations, thickness modulation or local protrusions. It is these factors that have a major influence on the properties and functioning of membranes. It is important to study these factors to have a control on the bilayer functions. In the study, we prepare multiple such bilayers and determine their bending modulus by applying Helfrich type continuum model.

It was pretty interesting yet complex in the start. I started with preparation of lipid bilayers using GROMACS and Coarse Graining model, as represented in figure 1. The choice of CG is due to the complexity of length and time scales of other counterparts. This was integrated with Martini force-field, which is very well known for proteins. I tried many different lipids but finally chose DMPC for working. No specific reason for choice, only that literature data for DMPC was quite easily accessible.

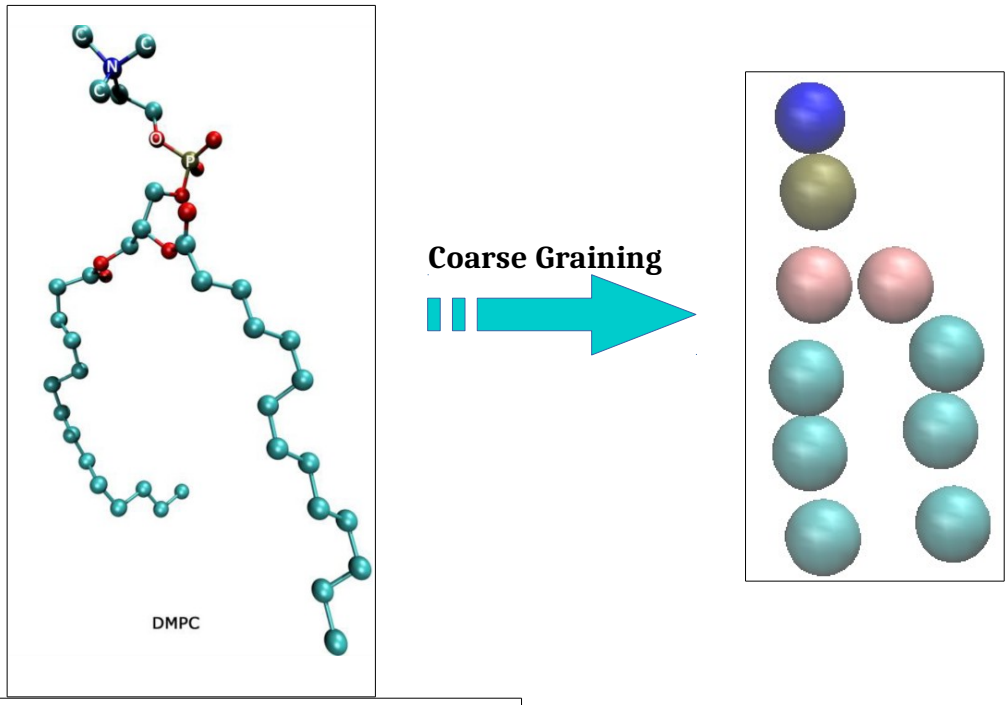

Figure1: AA representation of DMPC

Bessonov, K. and Harauz, G., 2010. Molecular dynamics investigation of myelin basic protein stability on lipid membranes

Starting with these lipids and arranging them in form of bilayer they were set to a stabilization run for 120ns initially and extended to 2-3microseconds later on. After this we finally obtain a properly equilibrated system, shown in figure 2, to perform further analysis on. Some of the samples for the bilayers:

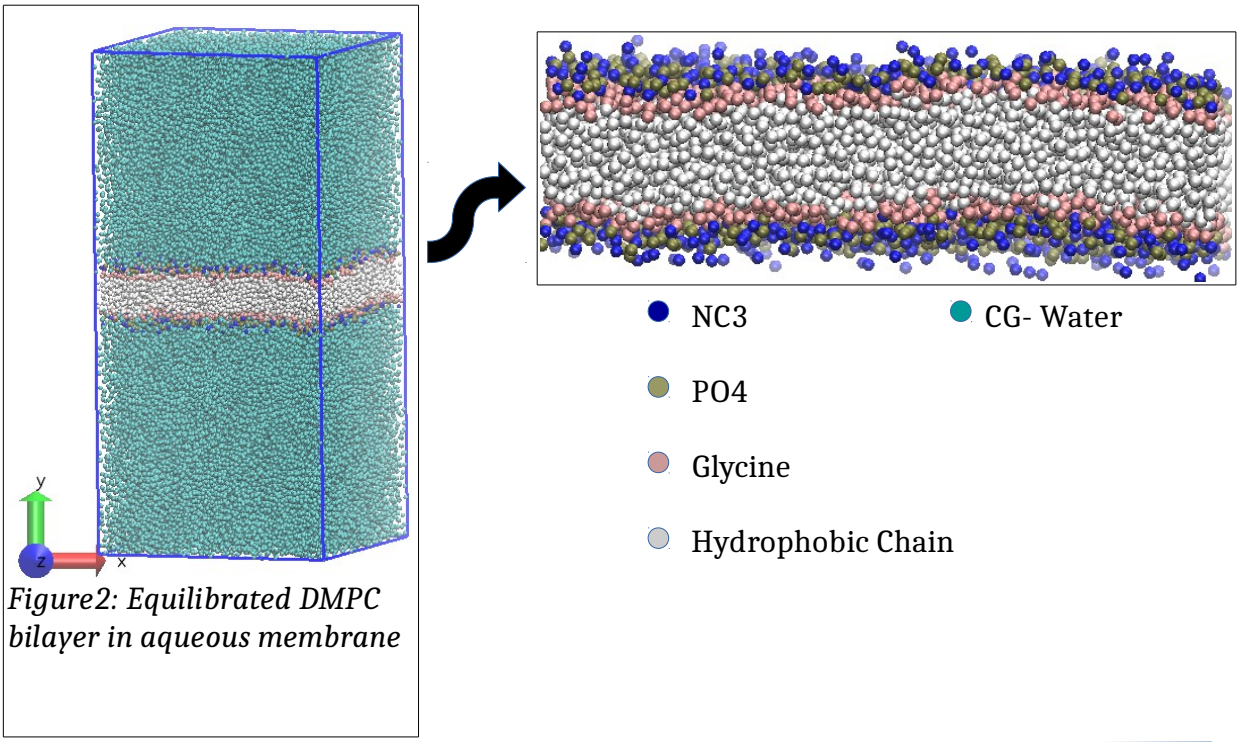

Figure2: Equilibrated DMPC bilayer in aqueous membrane

We were interested in determining the bending modulus for these DMPC membranes. For the determination of equilibrium properties of these membranes, Helfrich-type continuum model, has been in use since long. It is based on the prediction that the undulation has a fluctuation spectrum which follows a power law behavior. The structure factor, defined as the mean square fourier component of the membrane surface, is proportional to inverse fourth power of wave vector and thus diverges at small vectors. The work involved following a complete fourier based method to obtain the property of interest.

We could see a good correlation between literature and simulated value, as explained in figure 3. Although at some part it is very noisy but to improve that, further simulations are running. Probably the equilibration time was not long enough to not have any discrepancy.

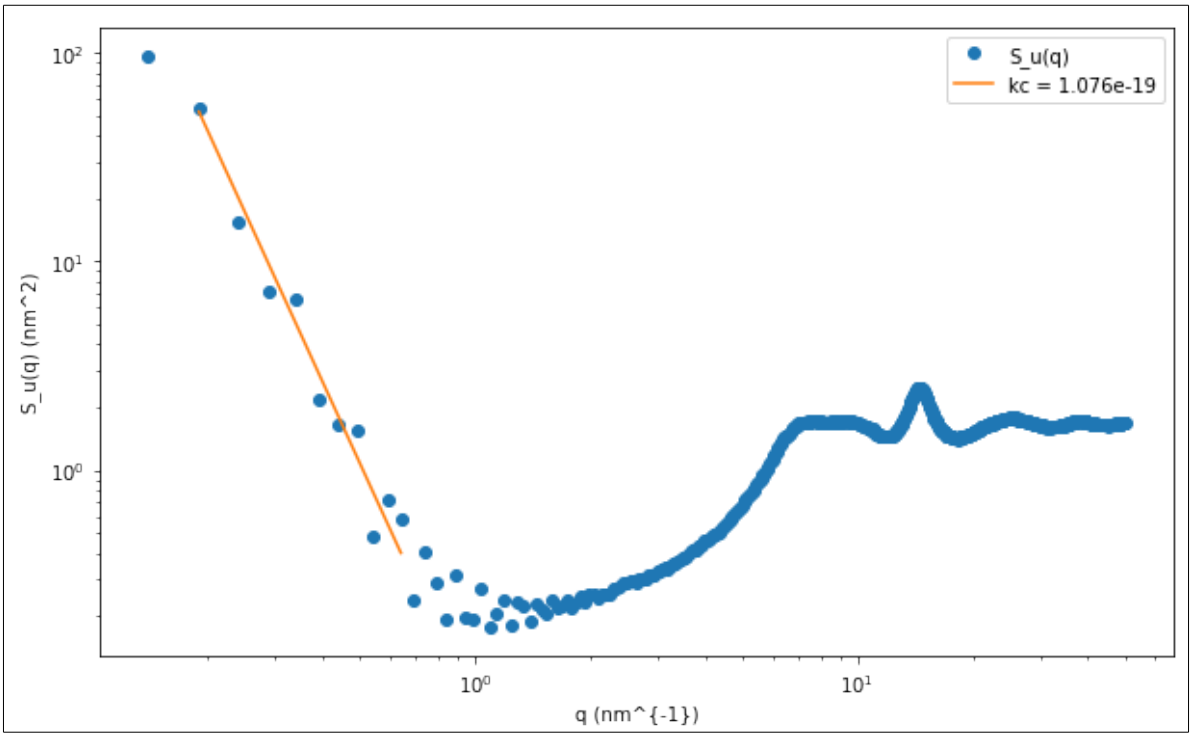

Figure3: Variation of structure factor with wave vector

Apart from lipid bilayers, I also worked on a couple of mixtures to get more clarity on the subject and to see how they deviate in the presence of other lipids.

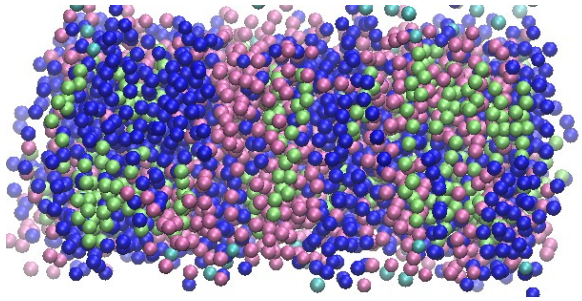

Figure4: Mixture composed of DPPC, DUPC and CHOl

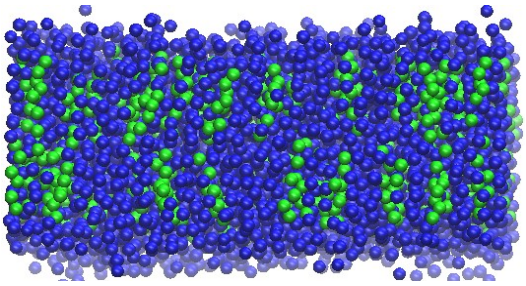

Figure5: Mixture composed of DPPC and CHOl

- DPPC
- DUPC
- CHOL

Analyzing these were pretty interesting since they did show some deviations from expectations. But this would be a good project in itself to work on.