Lipid Bilayer Bending Due to Membrane-Protein Interactions: A Computational Investigation

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Every single cell in an organism has a membrane that, in addition to being a compartmental barrier, plays a role in maintaining cell shape and function. For example, sickle cell anemia is a very deadly disease that is caused when the cell membrane deforms in an irregular manner. Additionally, cells cannot survive with processes that bend the cell membrane like endo/exocytosis. Therefore, maintaining the desired cell shape is vital for living organisms. To understand more about how membranes bend, in this project, we extended an existing model of membrane dynamics called MEM3dg. This model accounted for only one protein, so we were able to incorporate another protein to increase the capabilities of the model. We first derived the equations for the new protein using Discrete Differential Geometry (DDG), and then implemented these equations into software in order to use a computer to perform the calculations. With the code implemented, we were ready to test different scenarios in our model. The first test we did was testing the symmetry of the proteins. That is, we looked to see if turning on protein 1 and turning off protein 2 produced the same results, or membrane shape, as turning off protein 1 and turning on protein 2. Next we demonstrated what this new model can do by experimenting with proteins with different adsorption coefficients and opposing spontaneous curvatures. We varied the ratio of the adsorption coefficient to see when the effects of one protein overtook the effects of the other protein. As we did this, we were able to see how the proteins interacted with each other through the membrane shape but more generally, we were able to see how the improved version of MEM3dg was able to handle the effects of two proteins.