

Senthil Mudaliar (smm96@cornell.edu)

M&AE 715 , Prof. Zabaras

Final Project – Proposal Abstract

Abstract:

I wish to use the Final project as an opportunity to learn about Molecular Dynamics simulations and its applications to biology. I wish to use GROMACS to study membrane-protein MD simulation [1]. Two types of membrane proteins will be simulated – one is a potassium channel, the other is an outer-membrane protein. Various system properties will be analyzed. We will measure fluctuations in temperature, pressure and number of particles. Furthermore, we will examine the various contributions to the total energy (which is held constant). We will also analyze the Lipid Bilayer – we will analyze mass densities of various components of the system, specifically the density of the lipid headgroups, lipid tails, protein and water. Finally we will analyze some protein specific properties. These include root mean square deviation (RMSD) and root mean square fluctuation (RMSF). We will also chart the motion of ions in the KcsA ion channel (selective for potassium ion). This will mark the end of the final project.

However, if time is available once this project is over, I wish to go through another GROMACS exercise that investigates the behavior of the Ribonuclease S-peptide [2]. This will be done purely for “fun”.

References:

[1]: http://www.dddc.ac.cn/embo04/practicals/9_16.htm

[2]: <http://www.gromacs.org/documentation/reference/online/speptide.html>