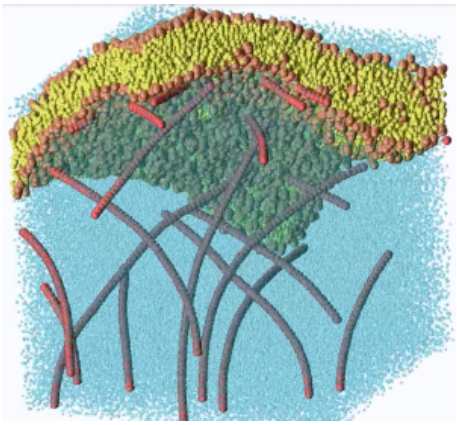
DPD Simulation of a Membrane



Description: This project will work toward the simulation of a cell membrane using a type of molecular dynamics known as Dissipative Particle Dynamics (DPD). In the first week, we will implement a basic molecular dynamics simulator in C++, probably in 2D, to learn about the inner workings of particle-based simulators. In the second week, we will learn about the DPD method and how to implement it in LAMMPS, a DOE-funded software package for molecular dynamics. We will use LAMMPS to simulate a cell membrane and get some nice 3D visuals. Time permitting, we can explore some more involved things like how the membrane moves when subject to a force from polymerization of a rigid polymer network, or how it flexes if the membrane is pinned at certain points. You can see what these sorts of simulations look like in this YouTube video.

Prerequisites: While we will make our basic MD simulator in C++, basic programming background in any language and the ability to Google things are probably sufficient. LAMMPS uses its own scripting language which is very easy to learn and no prior background with LAMMPS is assumed. We will not be focusing on the high performance computing aspects like how to optimize and parallelize code (LAMMPS is already highly optimized), so this project is suited to beginner or intermediate programmers who are more interested in learning how to approach the simulation of some biophysical problems.