



MECH 493 project:

Nonlinear mechanics of biological membranes:

A computational tool to understand cellular processes, virus replication and evolution, and to design the next generation drug delivery system based on nanomedicine

Project type

Computational

Background

Most cellular/viral processes, like drug uptake, phagocytosis, and virus infection and replication, are mediated by lipid membranes. Their mechanical reconfiguration is controlled by a multitude of biophysical processes, such as chemical reactions and long-range specie diffusion. Despite the extensive literature on the subject, only recently we acknowledged the importance of computational tools and the central role of mechanics in these processes. Thus, a general tool is currently missing. In this project, we will work with the student toward the development of computational tools capable of generating simple solution to understand (i) reaction-mediated (short-range) and (ii) diffusion-mediated (long-range) intra and intercellular processes. These will be based on the minimization of energy functionals via the solution of Euler-Lagrange equations. The student will be instructed on the fundamentals required and on how to develop the codes.

Research objective

The objective is the development of a code, preferably in Matlab (optionally in Python or C), that can generate the configuration of a membrane based on the boundary conditions, following energy minimization principles. This will first solve quasi-static problems, and then can be developed to solve dynamic problems.

Project goals

The following lists the projected milestones for the project:

1. Familiarization with the basic concepts of membrane mechanics, starting from the Helfrich free energy functional. Next, the energy integral will be written in polar coordinate for axisymmetric problems, as well in Cartesian coordinates for planar problems. Optionally, the equations can be formulated for generic 3D problems.
2. Implementation of the Euler-Lagrange equations to minimize the free energy integral.
3. Development of a Matlab code to solve the above equations numerically, for quasi-static problems
4. Development of a Matlab code to solve the equations for dynamic problems.

Facilities and team

The student can work on their laptop or can be provided a desktop to work on, either in person or to be used remotely to launch simulations. The student will interact with the research group of the PI, and possibly attend the weekly group meetings.