

# Research Statement

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Our research is at the intersection of applied mathematics, continuum mechanics, and biophysics, aiming to develop theories and numerical schemes that capture the interplay between geometry and energetics governing the equilibrium solutions at a continuum level. We explore the potential of unstretchable surfaces for innovative deployable structures, delve into the biomechanics of lipoproteins and viral dynamics, and investigate the interplay between elastic boundaries and surface tension in constrained minimal surfaces. Complementing these areas, we enhance computational simulations through refined numerical methods. Our work aims to bridge theoretical and practical realms, contributing to materials science and biophysics advancements.

## 1 Folding and Mobility of Unstretchable Surfaces and linkages

Research on folding unstretchable materials is crucial, finding applications in wearable technologies for creating adaptable and comfortable smart textiles [1], and in aerospace for designing reliable deployable structures [2]. Inspired by origami, this field has led to innovative solutions such as foldable emergency shelters and medical devices that navigate the human body's complexities [3]. Additionally, it plays a significant role in soft robotics [4], enabling the creation of robots that mimic biological flexibility [5]. These diverse applications showcase the practical relevance of this research and its potential to advance industries and improve quality of life. Below is a summary of our work in this direction:

### 1.1 Folding of helicoids into Möbius bands

Recently, we proposed a variational framework to determine shape of Möbius bands obtained from folding of unstrechtable, elastic helicoids [6]. The Möbius bands obtained have

nonplanar midlines of uniform torsion, distinctly different from the previously discovered Möbius bands. Depending on the single input parameter, the pitch of the reference helicoid, we determined Möbius bands with optimum symmetry and asymmetry, unknotted and knotted topology.

**Key finding:** Our study provides a guideline to design reference helicoid templates which can be folded, without stretching or contraction, into Möbius bands with given  $n$  half twists and  $n$ -fold rotational symmetry (optimal symmetry): the pitch of the reference helicoid of axis length  $\ell$  is given by

$$p = \frac{n}{2\ell} - \frac{2}{\pi\ell} \sin^{-1} \frac{1}{n}, \quad n = 3, 5, 7, \dots \quad (1)$$

These unique bands have minimal ring strains desired in synthesizing ring compounds such as Möbius annulenes [7] and DNA origami [8].

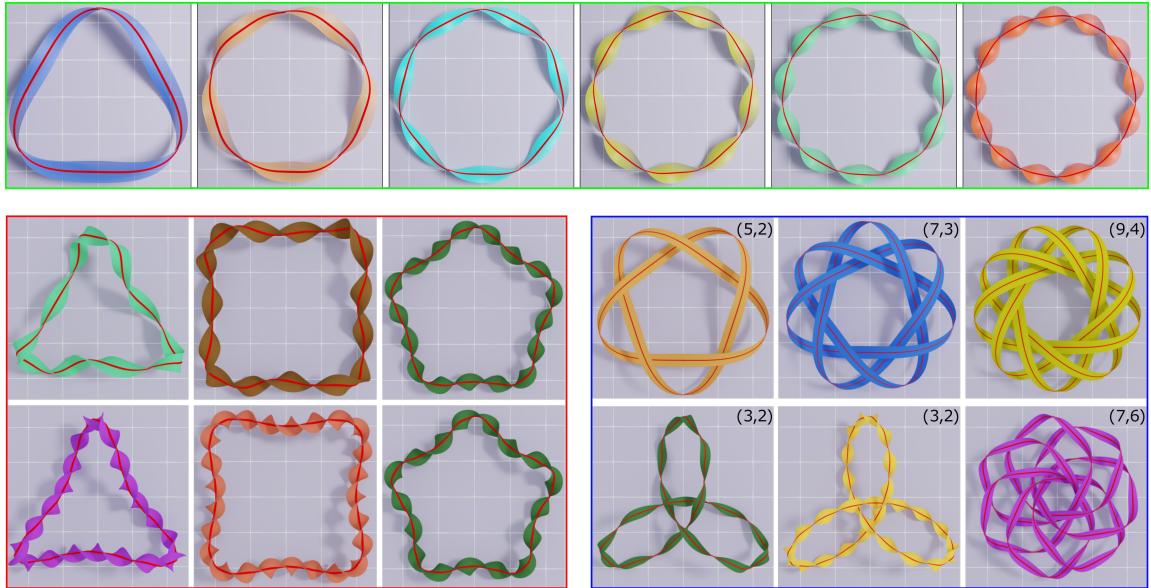


Figure 1: Representative bands with optimal symmetry (top-panel), non-optimal symmetry (bottom-left), and knotted topology (bottom-right) obtained from folding of unstrechable helicoids.

## 1.2 Everting motion of surfaces and linkages

We found that the Möbius bands constructed from folding of unstrechable helicoids, described in subsection ??above possess an internal degree of freedom. To explore that, we developed a kinematically consistent evolution equation and derived an analytical solution

that yields the bands' continuous inside-out (everting) periodic motion. During the everting motion, the bands remain unstretched, and their bending energy remains constant. Such everting motion could help design functional möbius bands with desired properties. Please see the application of our eversion framework in the interactive visualization of Möbius and orientable binormal scrolls.

It is well known that a linkage with an internal degree of freedom can move, but the governing equation of that mobility needs to be better understood. We formulated a discretized version of the above evolution equation and applied it to linkages. Solving that evolution equation numerically yields a continuous everting motion of the linkages. Our work can be used to design mechanisms with precise control and usability.

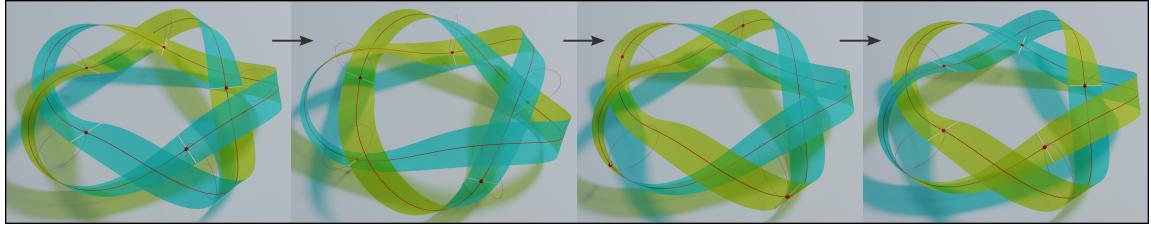


Figure 2: Everting motion of a (5,2) Möbius knot.

## 2 Biophysics

Be it the engulfing of foreign particles during endocytosis, expansion of ion channels in neurons for passing of ions, or the repulsive interaction between apolipoproteins in high-density cholesterol molecules, the competition between the electrostatic interactions, elastic energies, and geometric constraints are prevalent in nature. Understanding the equilibrium and non-equilibrium shapes that emerge from such competitions is crucial in understanding biological phenomena, cell shaping, curvature sorting, or topological changes. Below is a summary of our work in this direction:

### 2.1 Reverse Cholesterol Transport

High-density lipoprotein (HDL) particles, crucial for transporting cholesterol to the liver, comprise a spherical core with charged Apo-I and Apo-II protein loops attached to its surface. These proteins' shapes are vital for HDL functionality. My Ph.D. research studied the equilibrium shapes of charged, elastic curves confined to spherical surfaces. I explored the balance between elastic energy, favoring circular shapes, and electrostatic repulsion, pushing these curves apart. This interplay leads to complex equilibrium shapes in the proteins, offering insights into the structural principles of HDL particles.

**Key findings:** For the given charge, length, and bending rigidity of the proteins, our framework yields the precise equilibrium shape of the proteins confined to a core. We provide a detailed stability analysis of the circular configuration of the proteins. Depending on the parameters, the first unstable mode could be 1, 2, 3, and so on, as shown in our publication [12].

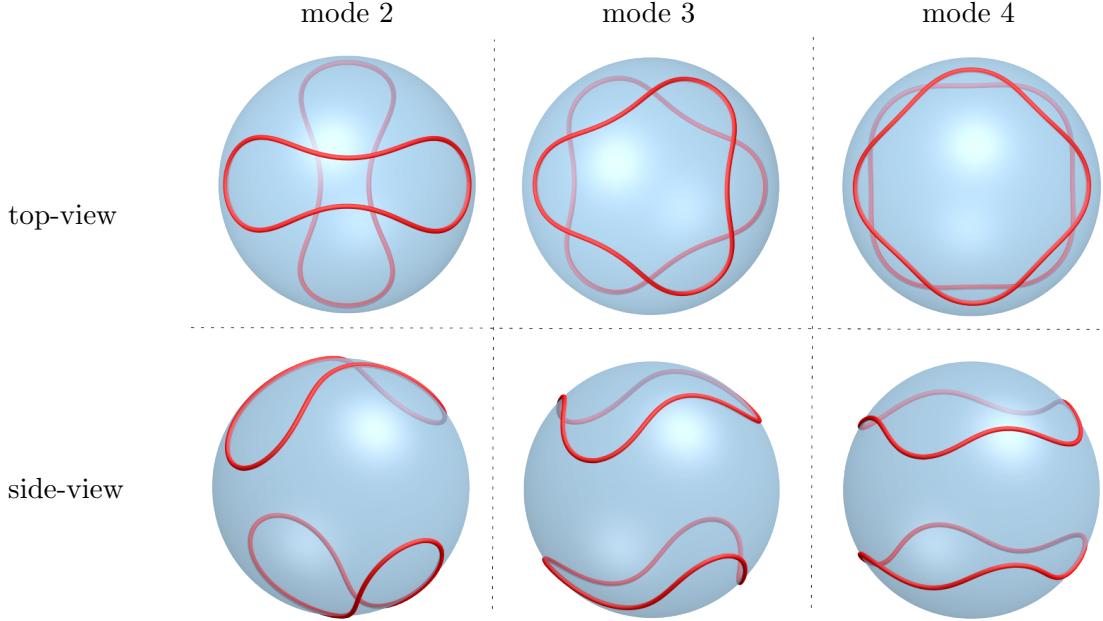


Figure 3: A few possible arrangements of charged proteins, shown with red colored curves, on a sphere.

## 2.2 Virus modeling via energy minimization

Understanding the rheological properties of viruses, closely related to their shapes, is crucial for unraveling their behavior and interactions within the human body. Our research employs energy minimization to determine shapes of viruses, and thus, their rheological properties. This approach has provided valuable insights into viruses' functionality and hydrodynamic behavior. In particular, we have identified the significant impact of spike protein geometry [9], core shape [10], and charge distribution [11] on the rheological properties of Covid-19 virus. These findings mainly highlight the critical influence of spike proteins on viral behavior, setting the stage for more detailed future studies. Our future goal is to expand our research to include a broader spectrum of viruses. We plan to incorporate more intricate features into our models, allowing us to delve into the diversity of viral shapes and their implications for biological functions and disease mechanisms. Ultimately,

these deeper insights can potentially guide the development of innovative therapeutic approaches, enhancing our capacity to tackle viral infections effectively.

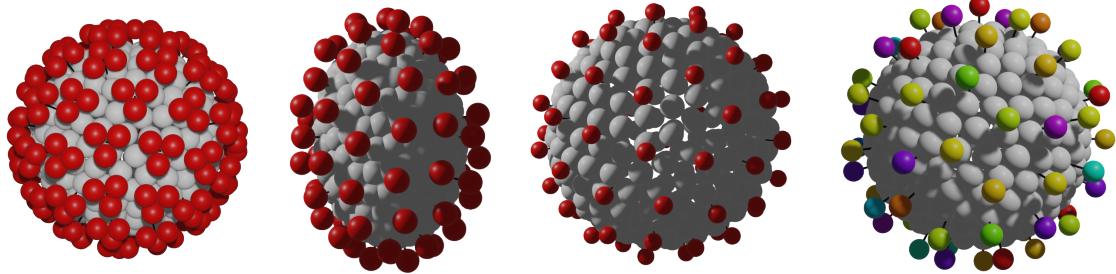


Figure 4: Left-to-right:Covid particles with triangular spike proteins [9], oblate core, prolate core [10], and charge heterogeneity [11]. We studied the effect of these features on the rheological properties of Covid-19 particles.

### 2.3 Surface tension mediated shapes

Surface tension, a critical interfacial phenomenon, significantly influences natural and engineered systems. Its role extends beyond shaping films and liquid interfaces; it is crucial in phenomena like Marangoni propulsion, observed in water-walking insects such as the rove beetle (*Stenus comma*). These insects exploit surface tension imbalances for locomotion by releasing surfactants at water-air interfaces. Our research models the impact of surface tension on fluid-interface objects using the beetle’s leg as a prototype. We also generalized the model to arbitrarily shaped floating objects [13]. This modeling helps estimate propulsion forces, torques, and load capacities, with broader implications for understanding fluid dynamics across various contexts, from robotic design to microgravity fluid behavior.

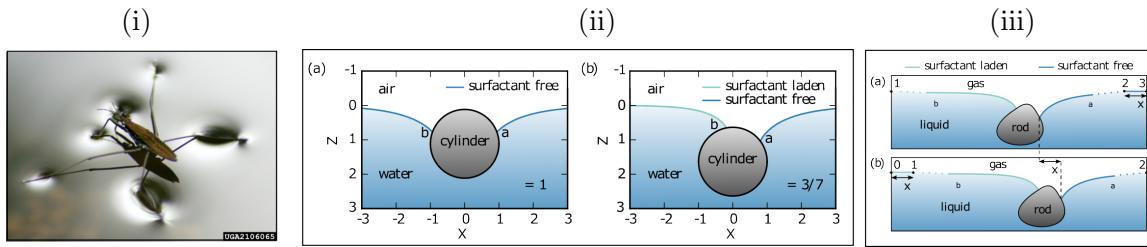


Figure 5: (i) picture of a rove beetle showing deformation of the water surface around its legs. (ii) effect of surface tension imbalance on a floating cylinder. (iii) generalization of our model to arbitrary shaped floating objects.)

## **2.4 Electro-mechanical coupling in Voltage-gated ion channels**

Voltage-gated ion channels, crucial transmembrane proteins, selectively regulate ion transport, playing a pivotal role in cellular function. These proteins have charged domains responsive to transmembrane electrostatic potential changes, initiating their opening and subsequent ion transport. However, this opening process is not straightforward; it necessitates overcoming the mechanical stiffness of the embedding lipid membrane, resulting in a complex interplay between electrostatic interactions and mechanical forces.

In our research, we utilize a continuum modeling approach to elucidate the effects of charged lipid membranes, which alter electrostatic interactions, and cholesterol molecules, which modify the membrane's mechanical stiffness, on the ion channels' opening dynamics. Our work [14] deepens our understanding of ion channel mechanisms and has broader implications for cellular biology and medical science.

**Below are some of the additional themes I plan to work on in the future.**

## **A Constrained Minimal Surfaces**

My interest in the intricate world of minimal surfaces has led me to explore constrained minimal surfaces, specifically fluid membranes with finite surface tension bounded by elastic curves. This research is at the intersection of mathematics and biology, unraveling the complexities of shapes dictated by the interplay of elastic boundaries and surface tension. My ongoing work aims to shed light on the role of surface tension in the buckling of blood platelets, a phenomenon yet to be fully understood. While I have not published papers in this area yet, my research is poised to make significant contributions to the field in the near future.

## **B Transition pathway between local minima**

Gaussian process regression, a pivotal tool in theoretical chemistry for identifying minimum energy paths in reactions, remains underutilized in mechanics. This method, essential for revealing transition states in chemical processes, is ripe for application in mechanical deformation studies.

My research seeks to bridge this gap by employing Gaussian process regression to analyze the equilibrium shapes of elastic curves and surfaces. A key focus is tracing the minimum energy path between distinct equilibrium states, such as transitioning between various configurations of unknotted and knotted elastic bands or the unfolding of an elastic band into its reference configuration. By adapting and refining techniques from theoretical chemistry, my goal is to forge a novel framework for dissecting mechanical energy landscapes.

This innovative approach promises not only to enhance our understanding of the dynamics of mechanical shape transformations but also to revolutionize the design of materials and structures with programmable shape-changing capabilities, using optimized Gaussian process codes. This research represents a significant stride towards redefining our approach to mechanical design and material science.

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