A Computational Application of Subdivision Surfaces to Biophysics

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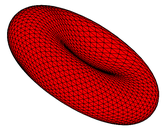
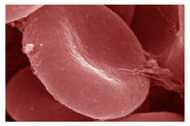
Motivation

A problem in biophysics is to explain the shape of membranous structures, such as a red blood cell. The currently acccepted model for this purpose is due to Wolfgang Helfrich. While we may observe membranes in a laboratory, it would be advantageous to simulate them on a computer. Thus, our goal is to develop the numerical tools necessary to allow for an accurate simulation of membranes and numerical exploration of the Helfrich model.





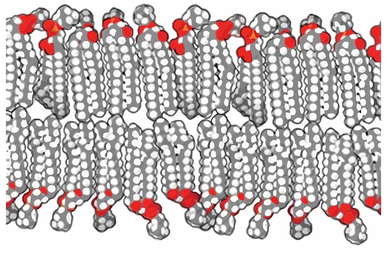
The Problem

The Helfrich model proposes that the membrane shape is determined by minimizing a curvature quantity known as the *bending energy*, subject to a few physical constraints. More formally, the problem is

$$\begin{aligned} \min_S \ & \int_S \alpha H^2 + \beta K \, dA \\ \text{s.t. } A &= \int_S 1 \, dA = a_0, \\ V &= \frac{1}{3}\int_S [x\hat{\mathbf{i}} + y\hat{\mathbf{j}} + z\hat{\mathbf{k}}] \cdot n \, dA = v_0 \\ M &= \int_S H \, dA = m_0. \end{aligned}$$

where a_0 and v_0 are the area and volume constraints, m_0 is the lipid bilayer constraint, H is the mean curvature, K is the Gaussian curvature, dA is the area element of the surface, and both α and β are due to the physical environment.

While the area and volume constraints are natural, the total mean curvature (M) constraint deserves an explanation. It is due to the area difference created by the lipid bilayer structure.



$$M = \int_S H \, dA = \lim_{\varepsilon \to 0} \frac{S_{+\varepsilon} - S_{-\varepsilon}}{2\varepsilon}$$

Computational Challenge

A smooth surface is an infinite dimensional object, not to mention that it may have nontrivial topology. This naturally leads to the questions:

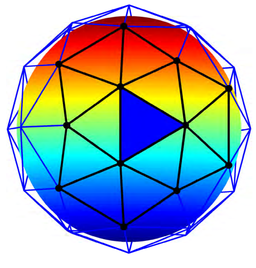
- How could one accurately represent a surface on a computer, which has finite memory?
- How could one faithfully compute all the relevant attributes (area, volume, mean curvature, bending energy)?
- How would one solve the optimization problem computationally required by the Helfrich Model?

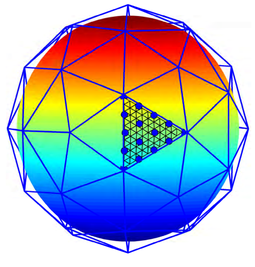
Our Approach

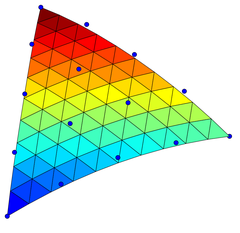
We explore the Helfrich model computationally using *subdivision surfaces*, which are traditionally used in the computer aided design industry (i.e. Pixar). We use these to approximate the cell membrane surface, and then we solve the optimization problem numerically, allowing us to accurately simulate the Helfrich model.

How Do We Do This?

For each subdivision surface, there is an associated *control mesh*. The control mesh is a finite set of vertices and associated edges; this structure captures the topology of the cell. Using this data, we can calculate the local polynomial patches that form the whole surface. From the polynomials, we calculate the quantities we need for the Helfrich model: area, volume, total mean curvature, bending energy and their rates of change with respect to the vertices. We can then find the surface of minimal energy by solving the constrained minimization problem using standard optimization tools.







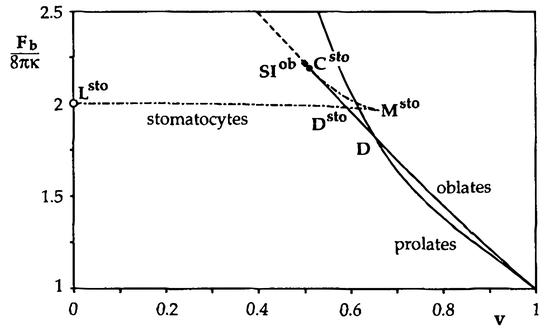
$$\begin{aligned} P &= \sum_\nu C_\nu \Phi_\nu \\ &= \sum_\nu C_\nu \textstyle\sum_\eta d_{\nu\eta} B_\eta \\ &= \sum_{\eta,\nu} C_\nu d_{\nu\eta} B_\eta \\ &= \sum_\eta \bar{C}_\eta B_\eta \end{aligned}$$

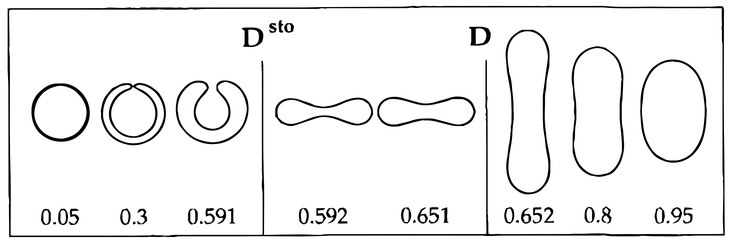
$$D_{C_\nu} W = D_{C_\nu}\bar{C}_\eta \times D_{\bar{C}_\eta} W$$

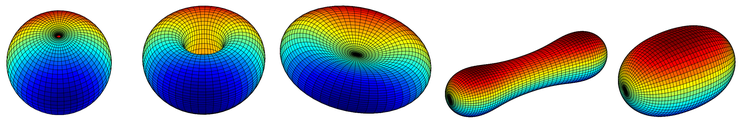
linear nonlinear

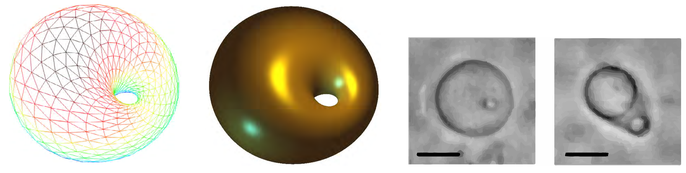
Results

Our figures generated from numerical simulation agree with previous theoretical and experimental results from the biophysics community.









Future Work

- Numerical exploration of uniqueness
- Numerical analysis of proposed approach
- Implementation in C++

Acknowledgements

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