Research Project

Mathematical Modelling of Cell Membrane Dynamics

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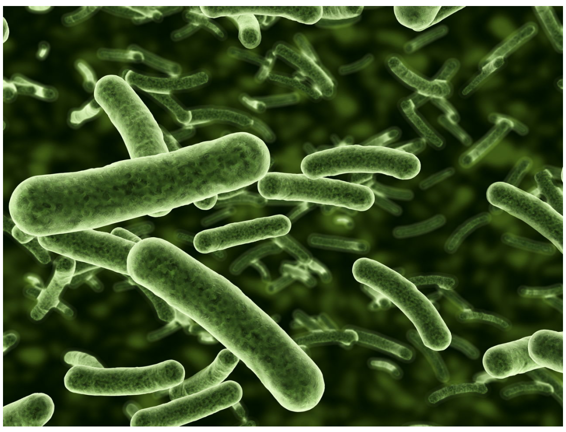

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1 Introduction

First can we detect deceases such as Alzheimer's disease, cancer cells and develop new methods and vaccines [1]. One of the primary components of the cell membranes are lipids which serve many different functions. A key function is that it is consisting of a bilayer of lipids which controls the structural rigidity and the fluidity of the membrane [2]. It also turns out that the lipids often accumulate into so-called lipid rafts which serves as a rigid platform for proteins with special properties such as intracellular trafficking of lipids and lipid-anchored proteins [3].

Modelling of lipid rafts formation can be modelled as a two-phase separation problem based on minimization of the Ginzburg-Landau energy functional [4]

$$\mathcal{E}_{ch}\left(\Gamma\right) = \int_{\Gamma} \Psi\left(c\right) + \frac{\gamma}{2}\left|\nabla c\right|^{2},$$

which is describing the chemical energy for a concentration $c : \Gamma \times [0, T] \mapsto [0, 1]$ over a surface membrane Γ. Several authors have solved this problem often results by deriving variants of Cahn Hilliard Equation or Allen Cahn Equation if the concentration is not conserved both standstill and evolving domains [4–8] .

Assuming that the system is a single-phase system can the elastic bending energy be modelled using the Canham Helrich energy functional [5, 9]

$$\mathcal{E}_{e}\left(\Gamma\right) = \int_{\Gamma} c_b H^2 + c_k K$$

.

Here is $H = \frac{\kappa_1+\kappa_2}{2}$ denoted as the mean curvature and $K = \kappa_1\kappa_2$ as the gaussian curvature with respectively c_b and c_k as tuning parameters and κ_1 and κ_2 as principal curvatures. Using the Gauss-Bonnet theorem can it be shown that the problem above is equivalent to the so-called Willmore energy functional [10, 11]

$$\mathcal{E}\left(\Gamma\right) = \int_{\Gamma} H^2. \tag{1}$$

This is a well known problem in the mathematical community [12, 13]. In fact, it is a mathematical tool used to study the geometry of surfaces because it can be used to study the properties of minimal surfaces, which are surfaces with the least possible area for a given boundary. This is important in many areas of mathematics, including differential geometry, topology and mathematical physics [14–16].

In this report will we establish a numerical scheme on minimization on this functional. However, we will first establish notation by including a section for definitions and important results from differential geometry. We will then derive the underlying PDE's for this equation. Lastly we will establish the model for the problem and discretize the problem using evolationary parametric FEM methods.

2 Background Theory

The section is highly inspired by the notation used in [17]. Let some initial surface $\Gamma^0 \subset \mathbb{R}^3$ smooth compact and oriented surface with no boundary where we can assign a unique point $p \in \Gamma^0$. We define define the time evolutionary surface to be on the form,

$$\begin{aligned}\Gamma = \Gamma\left(t\right) &= \Gamma\left(\chi\left(p,t\right)\right)\\ &= \left\{\chi\left(p,t\right) : \ p \in \Gamma^0\right\}\end{aligned}$$

transformed via the smooth mapping

$$\chi : \Gamma^0 \times [0, T] \mapsto \mathbb{R}^3.$$

We will define a unique evolutionary point $x \in \Gamma\left(t\right)$ based on the smooth mapping $\chi\left(p,t\right) = x$. A way to imagine this is to have a initial point in Γ^0 and the mapping χ describes how this point will deform over time. The outer unit normal vector field of $\Gamma\left(t\right)$ is defined as the mapping $\nu : \Gamma \mapsto \mathbb{R}^3$. The velocity v for a point $x = \chi\left(p,t\right)$ can be defined as

$$\frac{\partial}{\partial t}\chi\left(p,t\right) = v\left(x,t\right).. \tag{2}$$

Given a model of the velocity v can we solve the differential equation (2) and determine the evolution of a point on the surface Γ Assume we have a function $f : \Gamma \mapsto \mathbb{R}$. We can then denote the material derivative as,

$$\begin{aligned}\frac{D}{Dt}f\left(x,t\right) &= \frac{d}{dt}f\left(\chi\left(p,t\right),t\right)\\ &= \frac{\partial f\left(x,t\right)}{\partial t} + \frac{\partial f\left(x,t\right)}{\partial x}\frac{\partial \chi\left(p,t\right)}{\partial t}\end{aligned}$$

for $x \in \Gamma\left(t\right)$.

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We can then finally define the tangential gradient mapping (project gradient) $\nabla_\Gamma f : \Gamma \mapsto \mathbb{R}^3$ and the divergence mapping $\nabla_\Gamma \cdot f : \Gamma \mapsto \mathbb{R}$ s.t.

$$\begin{aligned}\nabla_\Gamma f &= \nabla f - \langle \nu, \nabla f\rangle\,\nu.\\ \nabla_\Gamma \cdot f &= \text{TODO}\end{aligned}$$

and the Laplace-Beltrami operator $\Delta_\Gamma f : \Gamma \mapsto \mathbb{R}$ s.t. $\Delta_\Gamma f = \nabla_\Gamma \cdot \nabla_\Gamma f$.

A method to compute the mean curvature and the so-called Frobenius norm of matrix A involves applying the extended Weingarten map, $A\left(x\right) = \nabla\nu\left(x\right)$, s.t. these identities holds [17],

$$\begin{aligned}H &= tr(A) = k_1 + k_2\\ \left|A\right|^2 &= k_1^2 + k_2^2\end{aligned}.$$

Now, let some arbitrary energy functional have the form

$$\mathcal{J} = \int_{\Gamma} \varphi, .$$

For instance, the case in (1) is $\varphi = H^2$. Using the definition from [18, 19] can we define the shape derivative of some energy functional $\mathcal{J}(\Gamma(t))$ towards any directions $w \forall w \in \mathcal{V}$ to be the limit

$$\begin{aligned} d\mathcal{J}(\Gamma(t);w) &= \lim_{t\to 0} \frac{\mathcal{J}(\Gamma(t)) - \mathcal{J}(\Gamma(0))}{t} \\ &= (\varphi, w)_{\Gamma(t)} \end{aligned}.$$

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The notation used here is $(v,w)_\Gamma = \int_\Gamma vw$ for some $v, w \in L^2(\Gamma)$.

Our goal is to develop the evolutionary dynamics by minimizing the energy functional (1).

To minimize our energy functional (1) of the surface dynamics will we utilize a method called gradient flows. Gradient flows in surface partial differential equation (PDE) are used to solve physical problems where the surface is changing due to some external force. The PDE describes how the surface changes over time in response to this force, thus allowing us to model real-world phenomena such as fluid and heat flow. The gradient of the surface PDE determines the direction and magnitude of the change over time, while the PDE itself may contain additional terms that modify or influence the solution. [20] An alternative approach would be to solve the problem using standard shape optimization techniques using Γ as a variable surface [21]. We say that the L^2 gradient flow is defined as

$$(\dot{\chi}, w)_{\Gamma(t)} = -d\mathcal{J}(\Gamma(t);w).$$

3 The Willmore flow

Lemma 3.1. *The shape derivative of* (1) *has the form*

$$\begin{aligned} d\mathcal{E}(\Gamma;w) = &\int_{\Gamma(t)} \nabla_\Gamma H \nabla_\Gamma w \\ &- \int_\Gamma H|\nabla_\Gamma w|^2 w \\ &+ \frac{1}{2}\int_\Gamma H^3 w \end{aligned}$$

Proof. Proof can be found in [11] □

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