Research Project

Mathematical Modelling of Cell Membrane Dynamics

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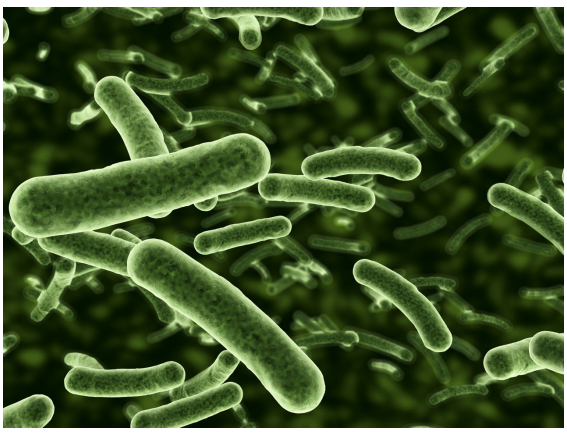

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1 Introduction

The value of understanding the basic underlying mechanics of the cell membrane dynamics has quite a lot of application. 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]

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

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 [4–7] .

Assuming that the system is a single-phase system can the elastic bending energy be modelled using the Canham Helrich energy functional [8]

$$\mathcal{E}_e(\Gamma) = \int_{\Gamma} 2c_b H^2 + c_k K \, dx$$

.

Here is H denoted as the mean curvature and K as the gaussian curvature with respectively c_b and c_k as tuning parameters.

2 Cahn Hilliard Equation on a Closed Membrane

Let c_0 and c_1 indicate the concentration profile of the substances in a 2 -phase system such that $c_0(\mathbf{x},t) : \Omega \times [0,\infty] \to [0,1]$ and similarly $c_1(\mathbf{x},t) : \Omega \times [0,\infty] \to [0,1]$, where $\mathbf{x}$ is a element of some surface Ω and t is time. However, in the 2 phase problem will we will restrict ourself so that $c_0(t,\mathbf{x}) + c_1(t,\mathbf{x}) = 1$ at any $\mathbf{x}$ at time t. A property of the restriction is that we now can express c_0 using c_1, with no loss of information. Hence, let us now define $c = c_0$ so $c(\mathbf{x},t) : \Omega \times [0,\infty] \to [0,1]$. It has been shown that 2 phase system if thermodynamically unstable can be evolve into a phase separation described by a evolutional differential equation [9] using a model based on chemical energy of the substances. However, further development has been done [4] to solve this equation on surfaces. Now assume model that we want to describe is a phase-separation on a closed membrane surface Γ, so that $c(\mathbf{x},t) : \Gamma \times [0,T] \to [0,1]$. Then is the surface Cahn Hilliard equation described such that

$$\rho \frac{\partial c}{\partial t} - \nabla_\Gamma \left(M \nabla_\Gamma \left(f_0' - \varepsilon^2 \nabla_\Gamma^2 c \right) \right) = 0 \quad \text{on } \Gamma. \tag{1}$$

We define here the tangential gradient operator to be $\nabla_\Gamma c = \nabla c - (\mathbf{n}\nabla c)\,\mathbf{n}$ applied on the surface Γ restricted to $\mathbf{n} \cdot \nabla_\Gamma c = 0$.

Lets define ε to be the size of the layer between the substances c_1 and c_2. The density ρ is simply defined such that $\rho = \frac{m}{S_\Gamma}$ is a constant based on the total mass divided by the total surface area of Γ. Here is the mobility M often derived such that is is dependent on c and is crucial for the result during a possible coarsening event [4]. However, the free energy per unit surface $f_0 = f_0(c)$ is derived based on the thermodynamical model and should according to [4] be non convex and nonlinear.

A important observation is that equation (1) is a fourth order equation which makes it more challenging to solve using conventional FEM methods. This clear when writing the equation on the equivalent weak form and second order equations arise.

3 Energy Functionals

Let $c(x,t) : \Gamma \times [0,T] \mapsto [0,1]$. From [4] can we observe the energy functionals

$$E_1(c) = \int_\Gamma f(c).$$

where

$$f(c) = f_0(c) + \frac{1}{2}\varepsilon^2 |\nabla_\Gamma c|^2$$

and the conservation law $\rho\frac{\partial c}{\partial t} + div_\Gamma \mathbf{j} = 0$ for the evolution of c, derived from the Ficks Law $\mathbf{j} = -M\nabla_\Gamma \mu$ for the chemical potential derived by the functional derivative $\mu = \frac{\delta f}{\delta c}$. The double well function is denoted as

$$f_0(c) = \frac{\zeta}{4}c^2(1-c)^2$$

References

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