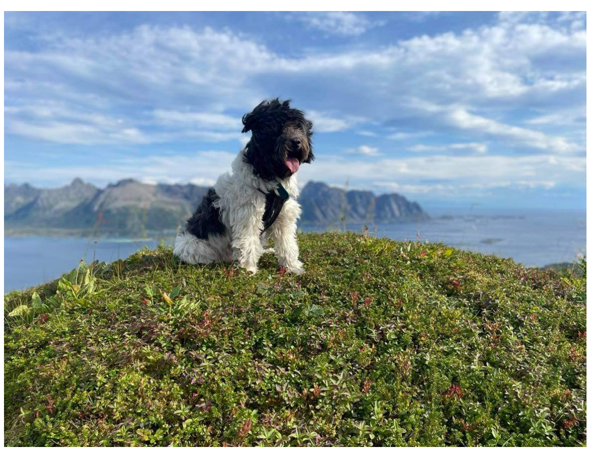
Master Thesis

Mathematical Modelling of Cell Membrane Dynamics

Isak Hammer

Supervisor: André Massing



Department of Mathematical Sciences

Norwegian University of Science and Technology

1 Introduction

The goal of the thesis implement modern FEM methods to solve the Cahn-Hilliard equation. The plan is to first understand the methods we want to use for the Poisson equation and then implement and do a thoughtful analysis for the method for the fourth order Biharmonic equation. Once this framework is established will we aim for solving the Chan-Hilliard equation using well known techniques for time-discretization and nonlinear problems.

The thesis is planned to have the following structure:

(a) Understand and implement a discontinuous Galerkin method for the Poisson equation.

(b) Derive an unfitted continuous interior penalty method for the biharmonic equation and show that the method is well-posed.

(c) Implement a time discretization scheme of an linear Cahn-Hilliard equation

(d) Implement nonlinear iteration methods for the (nonlinear) Cahn-Hilliard Equation

2 Elliptic

3 Biharmonic equation

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 [1] using a model based on chemical energy of the substances. However, further development has been done [2] 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 [2]. However, the free energy per unit surface $f_0 = f_0(c)$ is derived based on the thermodynamical model and should according to [2] 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.

4 Energy Functionals

Let $c(x,t) : \Gamma \times [0,T] \mapsto [0,1]$. From [2] can we observe the energy functionals

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

where

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

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

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

5 Linear Cahn-Hilliard equation

6 Cahn Hilliard equation

References

[1] John W. Cahn and John E. Hilliard. "Free Energy of a Nonuniform System. I. Interfacial Free Energy". In: *The Journal of Chemical Physics* 28.2 (1958), pp. 258–267. DOI: 10.1063/1.1744102. eprint: https://doi.org/10.1063/1.1744102. URL: https://doi.org/10.1063/1.1744102.

[2] Vladimir Yushutin et al. "A computational study of lateral phase separation in biological membranes". In: *International Journal for Numerical Methods in Biomedical Engineering* 35.3 (2019). e3181 cnm.3181, e3181. DOI: https://doi.org/10.1002/cnm.3181. eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/cnm.3181. URL: https://onlinelibrary.wiley.com/doi/abs/10.1002/cnm.3181.