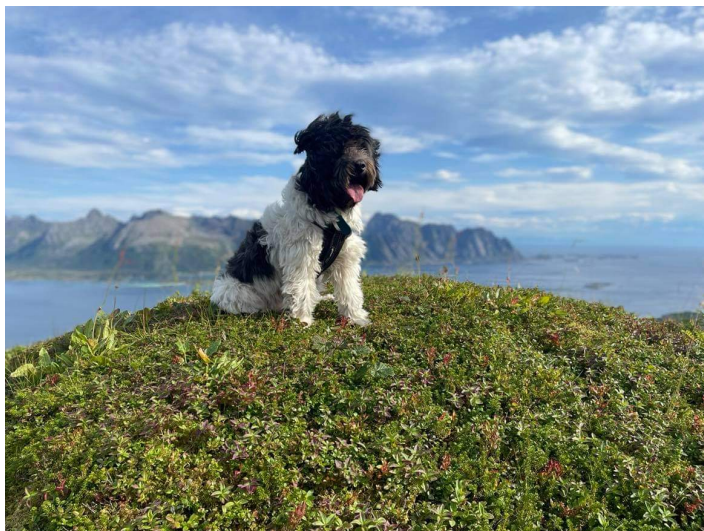


Project Thesis

Solving Cahn Hilliard Equation

Isak Hammer

March 25, 2022



1 Introduction

PLAN FOR REPORT

1) Introduction

2) DG for poission problem

- classical DG
- (Sability/ apriori error analysis)
- (numerical experiments)
- HDG for Possion Equation

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- (CIP for biharmonic equation)
- Hybridized CIP for biharmonic equation
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- Numerical Experiments
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4) Cahn-Hilliard Equation

- Combine CIP Biharmonic with Cahn Hilliard

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2 DG for Possion Problem

2.1 Possion Problem

Lets define the problem

$$\begin{aligned} -\varepsilon \nabla u &= f && \text{in } \Omega \\ u &= u_D && \text{on } \Gamma_D \\ \partial_n u &= g && \text{on } \Gamma_N \\ \partial_n u + \beta u &= h && \text{on } \Gamma_R \end{aligned}$$

Here is $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$.

2.2 Classical DG

2.3 Hybrid DG Method

We want to write this on a weak form. Let the spaces we work on be

$$H^1(\mathcal{T}_h) = \{u \in L^2(\Omega), u \in H^1(T) \forall T \in \mathcal{T}_h\}$$

For the problem to be discontinuous do we define the trial and test function to be $u \in H^1(\Omega)$ and $v \in H^1(\mathcal{T}_h)$. Thus,

$$-\sum_{T \in \mathcal{T}_h} \int_T \varepsilon \nabla^2 u \cdot v dx = \sum_{T \in \mathcal{T}_h} \left\{ \int_T \varepsilon \nabla u \nabla v dx - \int_{\partial T} \varepsilon \cdot \partial_n u \cdot v ds \right\} = \sum_{T \in \mathcal{T}_h} \int_T f \cdot v dx. \quad (1)$$

But we want to introduce the shorter notation equivalently such that

$$\sum_{T \in \mathcal{T}_h} \{ \varepsilon (\nabla u, \nabla v)_T - \varepsilon \langle \partial_n u, v \rangle_{\partial T} \} = \sum_{T \in \mathcal{T}_h} (f, v). \quad (2)$$

Where $\langle \cdot, \cdot \rangle$ is the surface integral operator. Before we continue do we want to introduce an alternative method to integrate using edges. Let $v_F \in L^2(\mathcal{F}_h)$ for the set of all facets \mathcal{F}_h . Now the surface integral can be rewritten such that

$$\sum_{T \in \mathcal{T}_h} \varepsilon \langle \partial_n u, v_F \rangle = \sum_{E \in \mathcal{F}^{int}} \varepsilon \langle \partial_{n^+} u, v_F \rangle_E + \varepsilon \langle \partial_{n^-} u, v_F \rangle_E + \sum_{E \in \mathcal{F}^{ext}} \varepsilon \langle \partial_n u, v_F \rangle. \quad (3)$$

Here we are using the definitions n^+ and n^- illustrated using figure 1. Let's define some crucial spaces for the DG method

$$V = \{(u, u_F) : u \in H^2(\mathcal{T}_h) \cap H^1(\Omega), u_F \in L^2(\mathcal{F}_h)\}$$

$$V_h = \{(u, u_F) : u \in \mathcal{P}^k(T) \forall T \in \mathcal{T}_h, u_F \in \mathcal{P}^k(E) \forall E \in \mathcal{F}_h\}$$

What is the intuition of a polynomial $\mathcal{P}^k(E)$ along an edge?

and now including Dirichlet conditions using the previous definition

$$V_D = \{(u, u_F) \in V, u_F = u_D \text{ on } \Gamma_D\} \quad V_{h,D} = \{(u, u_F) \in V_h, u_F = u_D \text{ on } \Gamma_D\}$$

$$V_0 = \{(u, u_F) \in V, u_F = 0 \text{ on } \Gamma_D\} \quad V_{h,0} = \{(u, u_F) \in V_h, u_F = 0 \text{ on } \Gamma_D\}$$

Defining $(u, u_F) \in V_D$ and $(v, v_F) \in V_0$. Now adding (2) and (3) can we easily see that

$$\sum_{T \in \mathcal{T}_h} \{\varepsilon (\nabla u, \nabla v)_T\} = \sum_{T \in \mathcal{T}_h} (f, v)_T + \sum_{E \in \mathcal{F}^{int}} \varepsilon \langle \partial_{n^+} u, v_F \rangle_E + \varepsilon \langle \partial_{n^-} u, v_F \rangle_E + \sum_{E \in \mathcal{F}^{ext}} \varepsilon \langle \partial_n u, v_F \rangle. \quad (4)$$

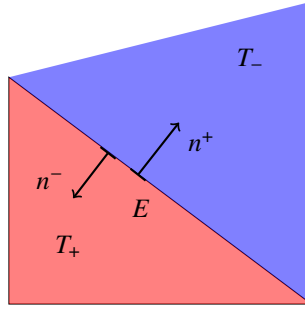


Figure 1: Edge E shared by the triangles T_- and T_+ and the normal unit vectors n^+ and n^- .

Applying the Neumann conditions on Γ_N and Γ_R , can the condition on the exterior facets be rewritten such that

$$\sum_{E \in \mathcal{F}^{ext}} \varepsilon \langle \partial_n u, v_F \rangle = \varepsilon \langle g, v_F \rangle_{\Gamma_N} + \varepsilon \langle h - \beta u, v_F \rangle_{\Gamma_R}$$

Keep in mind that we on the exterior boundaries define the integral so $\langle f, v_F \rangle_\Gamma = \int_\Gamma f \cdot v_F \cdot n ds$ for an arbitrary Neumann boundary function f on some surface Γ . Hence (4) ends up being

$$\sum_{T \in \mathcal{T}_h} \varepsilon (\nabla u, \nabla v)_T - \sum_{E \in \mathcal{F}^{int}} (\varepsilon \langle \partial_{n^+} u, v_F \rangle_E + \varepsilon \langle \partial_{n^-} u, v_F \rangle_E) + \beta \langle \varepsilon u, v_F \rangle_{\Gamma_R} = \sum_{T \in \mathcal{T}_h} (f, v)_T + \langle g, v_F \rangle_{\Gamma_N} + \langle h, v_F \rangle_{\Gamma_R}. \quad (5)$$

According to Lehrenfeld 2010 [1] at page 13 on equation (1.2.7) is (5) equivalent to

$$\sum_{T \in \mathcal{T}_h} (\varepsilon \nabla u, \nabla v)_T - \sum_{T \in \mathcal{T}_h} \langle \varepsilon \partial_n u, [v] \rangle_{\partial T} + \beta \langle \varepsilon u, v_F \rangle_{\Gamma_R} = \sum_{T \in \mathcal{T}_h} (f, v)_T + \langle \varepsilon g, v_F \rangle_{\Gamma_N} + \langle \varepsilon h, v_F \rangle_{\Gamma_R} \quad (6)$$

Where, $u, u_F \in V_D$ and $v, v_F \in V_h$. Here is the jump defined simply as $[v] = v - v_F$. Remember that $v_F = \text{tr}_{\partial T}(v)$. What we see is for (5) and (6) to be equivalent must this be true.

$$\sum_{T \in \mathcal{T}_h} \langle \varepsilon \partial_n u, [v] \rangle_{\partial T} = \sum_{T \in \mathcal{T}_h} \langle \varepsilon \partial_n u, v \rangle_{\partial T} - \langle \varepsilon \partial_n u, v_F \rangle_{\partial T} = \sum_{E \in \mathcal{F}^{int}} \varepsilon (\langle \partial_{n^+} u, v_F \rangle_E + \langle \partial_{n^-} u, v_F \rangle_E). \quad (7)$$

why is it true?

Since $(u, u_F) \in V$ is has to be continious, hence the jump is $\llbracket u \rrbracket = 0$ for the correct solution. Hence, adding $-\langle \varepsilon \partial_n v, \llbracket u \rrbracket \rangle_{\partial T}$ for symmetry and $\tau_h \langle \varepsilon \llbracket u \rrbracket, \llbracket v \rrbracket \rangle_{\partial T}$ for stability with some stabilization parameter τ_h for each $T \in \mathcal{T}_h$. This can be added to lhs on (6) such that,

$$\begin{aligned} & \sum_{T \in \mathcal{T}_h} (\varepsilon \nabla u, \nabla v)_T - \sum_{T \in \mathcal{T}_h} \{ \langle \varepsilon \partial_n u, \llbracket v \rrbracket \rangle_{\partial T} - \langle \varepsilon \partial_n v, \llbracket u \rrbracket \rangle_{\partial T} + \tau_h \langle \varepsilon \llbracket u \rrbracket, \llbracket v \rrbracket \rangle_{\partial T} \} \\ & + \beta \langle \varepsilon u, v_f \rangle_{\Gamma_R} \\ & = \sum_{T \in \mathcal{T}_h} (f, v) + \langle \varepsilon g, v_F \rangle_{\Gamma_N} + \langle \varepsilon h, v_F \rangle_{\Gamma_R} \end{aligned} \quad (8)$$

Finally, we can now construct the discrete system. Let now $u, u_F \in V_{h,D}$ and $v, v_F \in V_{h,0}$ be the discretized spaces. Using what we have in (6) can we define

$$\begin{aligned} F(v, v_F) &= \sum_{T \in \mathcal{T}_h} (f, v) + \langle \varepsilon g, v_F \rangle_{\Gamma_N} + \langle \varepsilon h, v_F \rangle_{\Gamma_R} \\ B(u, u_F, v, v_F) &= \sum_{T \in \mathcal{T}_h} (\varepsilon \nabla u, \nabla v)_T - \sum_{T \in \mathcal{T}_h} \{ \langle \varepsilon \partial_n u, \llbracket v \rrbracket \rangle_{\partial T} - \langle \varepsilon \partial_n \llbracket u \rrbracket \rangle_{\partial T} + \tau_h \langle \varepsilon \llbracket u \rrbracket, \llbracket v \rrbracket \rangle_{\partial T} \} + \beta \langle \varepsilon u, v_F \rangle_{\Gamma_R} \\ B(u, u_F, v, v_F) &= F(v, v_F). \end{aligned} \quad (9)$$

z

3 C^0 Interior Penalty Method for Biharmonic Equation

3.1 Introduction of the Boundary Value Problem

In this section do we want to establish a numerical method to fourth order equations. Instead of embarking on the special case of surface PDE described in (14) can we establish a general numerical theory on \mathbb{R}^2 , which we later can generalize on closed surface later. Assume that we restrict ourself to a compact surface $\Omega \in \mathbb{R}^2$ and let $f \in L^2(\Omega)$ as defined in 5.1. Let say we want to solve the equation on the form.

$$\begin{aligned} \Delta^2 u - \beta \Delta u + \gamma u &= f \quad \beta, \gamma \geq 0 \\ \frac{\partial u}{\partial n} &= 0 \quad \text{on } \Omega \\ \frac{\partial \Delta u}{\partial n} &= q \quad \text{on } \partial \Omega \end{aligned} \quad (10)$$

For convenience are the boundary condition q chosen to be defined via a $\phi \in H^4(\Omega)$ such that $q = \frac{\partial \Delta \phi}{\partial n}$ so $\frac{\partial \phi}{\partial n} = 0$. $\partial \Omega$.

3.2 Weak Formulation

We want to rewrite (10) on weak formulation. Now define the Hilbert space

$$V = \left\{ v \in H^2(\Omega) : \frac{\partial v}{\partial n} = 0 \quad \text{on } \partial \Omega \right\}.$$

It can be shown [2] that a convinient form is to write it as

$$\begin{aligned} a(u, v) &= (f, v)_{L^2(\Omega)} - (q, v)_{L^2(\partial \Omega)} \\ &= \int_{\Omega} D^2 w : D^2 v \, dx + \int_{\Omega} \nabla w \nabla v \, dx + \int_{\Omega} \gamma w \cdot v \, dx. \end{aligned} \quad (11)$$

For all $\forall v \in V$, where

$$D^2 w : D^2 v = \sum_{i,j=1}^2 \frac{\partial^2 w}{\partial x_i \partial x_j} \cdot \frac{\partial^2 v}{\partial x_i \partial x_j}.$$

In fact, according to [2] can it be shown that the problem has a unique solution if and only if $\gamma > 0$. However, in the case where $\gamma = 0$ can we provoke a unique solution by introducing the condition

$$\int_{\Omega} f dx = \int_{\partial\Omega} q ds$$

Taking this into account can we expand the solution space such that

$$V^* = \begin{cases} V, & \text{if } \gamma > 0 \\ \{v \in V : v(p^*) = 0\}, & \text{if } \gamma = 0 \end{cases}$$

Where p^* is a corner in Ω . In fact, now all solutions of (11) exists in V^* .

3.3 Construction of C^0 Interior Penalty Method

We want to construct a C^0 interior penalty method based on C^0 Lagrange elements. Assume \mathcal{T}_h be a triangulation of Ω and V_h be the \mathcal{P}_2 Lagrange finite element space associated with \mathcal{T}_h

$$V_h = \left\{ v \in C(\overline{\Omega}) : v_T = v|_T \in \mathcal{P}_2(T) \quad \forall T \in \mathcal{T}_h \right\}$$

So that we can earn a similar space for the approximated solution space ,

$$V_h^* = \begin{cases} V_h, & \text{for } \gamma > 0 \\ \{v \in V_h : v(p^*) = 0\} & \text{for } \gamma = 0. \end{cases}$$

Here is p^* again a corner in Ω . Let us now generalize the Hilbert space as well to the approximated solution space by defining

$$H^k(\Omega, \mathcal{T}_h) = \{H^1(\Omega) : v_T \in H^k(T) \quad \forall T \in \mathcal{T}_h\}.$$

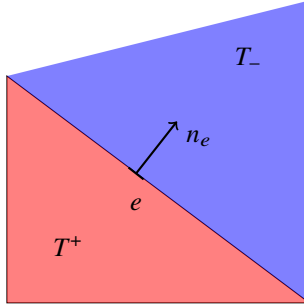


Figure 2: Edge e shared by the triangles T_- and T_+ and the normal unit vector n_e .

Now assume that that $e \in \mathcal{E}_h^i$ is shared between two triangles $T_-, T_+ \in \mathcal{T}_h$. Then we can assume that the unit normal from T_- to T_+ is described as n_e as illustrated in figure 2. Finally, we now want to define jumps internally,

$$\begin{aligned} \left\llbracket \frac{\partial v_h}{\partial n_e} \right\rrbracket &= \frac{\partial v_{T_+}}{\partial n_e}|_e - \frac{\partial v_{T_-}}{\partial n_e}|_e, \quad \forall v \in H^2(\Omega, \mathcal{T}_h) \\ \left\llbracket \frac{\partial^2 v_h}{\partial n_e^2} \right\rrbracket &= \frac{\partial^2 v_{T_+}}{\partial n_e^2}|_e - \frac{\partial^2 v_{T_-}}{\partial n_e^2}|_e \quad \forall v \in H^3(\Omega, \mathcal{T}_h). \end{aligned}$$

And similarly for means internally,

$$\begin{aligned} \left\{ \left\{ \frac{\partial v_{T_-}}{\partial n_e} \right\} \right\} &= \frac{1}{2} \left(\frac{\partial v_{T_+}}{\partial n_e}|_e + \frac{\partial v_{T_-}}{\partial n_e}|_e \right) \quad \forall v \in H^2(\Omega, \mathcal{T}_h) \\ \left\{ \left\{ \frac{\partial^2 v_h}{\partial n_e^2} \right\} \right\} &= \frac{1}{2} \left(\frac{\partial^2 v_{T_+}}{\partial n_e^2}|_e + \frac{\partial^2 v_{T_-}}{\partial n_e^2}|_e \right) \quad \forall v \in H^3(\Omega, \mathcal{T}_h), \end{aligned}$$

Let the edges along the boundary be defined as $e \in \mathcal{E}_h^b$ along a some boundary triangle \mathcal{T}_h . We can then define the jump and mean as

$$\begin{aligned} \left[\left[\frac{\partial v_h}{\partial n_e} \right] \right] &= -\frac{\partial v_T}{\partial n_e}|_e \quad \forall v \in H^2(\Omega, \mathcal{T}_h) \\ \left\{ \left\{ \frac{\partial^2 v_h}{\partial n_e^2} \right\} \right\} &= \frac{\partial v_T}{\partial n_e}|_e \quad \forall v \in H^3(\Omega, \mathcal{T}_h) \end{aligned}$$

Using the results from [2] can we formulate the discrete formulation the boundary value problem (10) using C^0 interior penalty method. Our goals is to find a $u_h \in V_h^*$ such that this is true,

$$\mathcal{A}(u_h, v_h) = (f, v_h)_{L^2(\Omega)} - (q, v_h)_{L^2(\partial\Omega)} \quad \forall v_h \in V_h^*. \quad (12)$$

Where $w_h, v_h \in V_h$ and

$$\begin{aligned} \mathcal{A}(w_h, v_h) &= \sum_{T \in \mathcal{T}_h} \int_T D^2 w_h : D^2 v_h \\ &+ \sum_{e \in \mathcal{E}_h} \int_e \left\{ \left\{ \frac{\partial^2 w_h}{\partial n_e^2} \right\} \right\} \left[\left[\frac{\partial v_h}{\partial n_e} \right] \right] ds \\ &+ \sum_{e \in \mathcal{E}_h} \left\{ \left\{ \frac{\partial^2 v_h}{\partial n_e^2} \right\} \right\} \left[\left[\frac{\partial w_h}{\partial n_e} \right] \right] ds \\ &+ \sum_{e \in \mathcal{E}_h} \frac{\sigma}{|e|} \int_e \left[\left[\frac{\partial w_h}{\partial n_e} \right] \right] \left[\left[\frac{\partial v_h}{\partial n_e} \right] \right] ds \\ &+ \int_{\Omega} \beta \nabla w_h \cdot \nabla v_h dx + \int_{\Omega} \gamma w_h v_h dx. \end{aligned} \quad (13)$$

The notation $|e|$ is to describe the length of the edge e and $\sigma \geq 1$ is a penalty parameter.

4 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 $c_0(\mathbf{x}, t) : \Omega \times [0, \infty] \rightarrow [0, 1]$ and similarly $c_1(\mathbf{x}, t) : \Omega \times [0, \infty] \rightarrow [0, 1]$, where \mathbf{x} is a element of some surface Ω and t is time. However, in the 2 phase problem 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 $c(\mathbf{x}, t) : \Omega \times [0, \infty] \rightarrow [0, 1]$. It has been shown that 2 phase system if thermodynamically unstabl can be evolve into a phase separation described by a evolutionary differential equation [3] 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-seperation on a closed membrane surface Γ , so that $c(\mathbf{x}, t) : \Gamma \times [0, T] \rightarrow [0, 1]$. Then is the surface Cahn Hilliard equation described such that

$$\rho \frac{\partial c}{\partial t} - \nabla_\Gamma (M \nabla_\Gamma (f'_0 - \varepsilon^2 \nabla_\Gamma^2 c)) = 0 \quad \text{on } \Gamma. \quad (14)$$

We define here the tangential gradient operator to be $\nabla_\Gamma c = \nabla c - (\mathbf{n} \cdot \nabla c) \mathbf{n}$ 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 nonconvex and nonlinear.

A important observation is that equation (14) 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.

5 Appendix

5.1 The Space $L^2(\Omega)$

Using the definition from [5] and we let Ω be an open set in \mathbb{R}^d and $p \in \mathbb{R}$ such that $p \geq 1$. Then we denote $L^p(\Omega)$ to be the set of measurable function $u : \Omega \rightarrow \mathbb{R}$ such that it is equipped in a finite Banach space

$$\|u\|_{L^p(\Omega)} = \left(\int_{\Omega} |u|^p \right)^{\frac{1}{p}}.$$

Now let $u, v : \Omega \rightarrow \mathbb{R}$. Then is $L^2(\Omega)$ a Hilbert space when the inner product is finite such that this exists

$$(u, v)_{L^2(\Omega)} = \int_{\Omega} uv.$$

If the integral is finite do we say that $u, v \in L^2(\Omega)$.

5.2 The Space $H^m(\Omega)$, $m > 1$

Again using the definition from [5]. Let $\alpha = (\alpha_1, \dots, \alpha_d)$, $\alpha \geq 0$, such that $|\alpha| = \sum_{i=1}^d \alpha_i$. Now we define the space

$$H^m(\Omega) = \{u \in L^2(\Omega) : D^\alpha u \in L^2(\Omega) \quad \forall \alpha : |\alpha| \leq m\}.$$

Suppose that u, v is measurable functions. We can now define $u \in H^m(\Omega)$ the Banach space is finite.

$$\|u\|_{H^m(\Omega)} = \left(\|u\|_{L^2(\Omega)}^2 + \sum_{k=1}^m \|u\|_{H^k(\Omega)}^2 \right)^{\frac{1}{2}}, \quad \|u\|_{H^k(\Omega)} = \sqrt{\sum_{|\alpha|=k} \|D^\alpha u\|_{L^2(\Omega)}^2}$$

Similarly for the finite Hilbert space

$$(u, v)_{H^m(\Omega)} = \sum_{|\alpha| \leq m} \int_{\Omega} D^\alpha u D^\alpha v$$

References

- [1] Christoph Lehrenfeld. “Hybrid Discontinuous Galerkin methods for solving incompressible flow problems”. PhD thesis. May 2010.
- [2] S. Gu and La.). Department of Mathematics Louisiana State University (Baton Rouge. *C0 Interior Penalty Methods for Cahn-Hilliard Equations*. Dissertation (Louisiana State University (Baton Rouge, La.)) Louisiana State University, 2012. URL: <https://books.google.no/books?id=eKP1xQEACAAJ>.
- [3] 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](https://doi.org/10.1063/1.1744102). eprint: <https://doi.org/10.1063/1.1744102>. URL: <https://doi.org/10.1063/1.1744102>.
- [4] 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>.
- [5] A. Manzoni, A. Quarteroni, and S. Salsa. *Optimal Control of Partial Differential Equations: Analysis, Approximation, and Applications*. Applied Mathematical Sciences. Springer International Publishing, 2021. ISBN: 9783030772253. URL: <https://books.google.no/books?id=V3NpzgEACAAJ>.