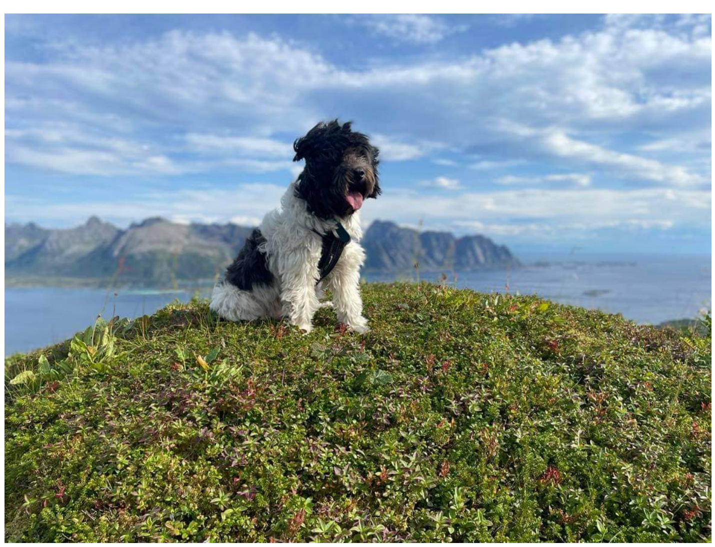
Project Thesis
Solving Cahn Hilliard Equation

Isak Hammer

March 24, 2022



1 Introduction

Introduction

2 Cahn Hilliard Equation on a Closed Membrane

Let c_0 and c_1 indicate the concentration profile of the substances in a a 2 -phase system such that $c_0(\mathbf{x}, t) : \mathbf{\Omega} \times [0, \infty] \to [0, 1]$ and similarly $c_1(\mathbf{x}, t) : \mathbf{\Omega} \times [0, \infty] \to [0, 1]$, where $\mathbf{x}$ is a element of some surface $\mathbf{\Omega}$ 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 $c(\mathbf{x}, t) : \mathbf{\Omega} \times [0, \infty] \to [0, 1]$. It has been shown that 2 phase system if thermodynamically unstabl can be evolve into a phase seperation 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-seperation 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 divaded 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 coarsering 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 nonconvex 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 Hybrid Symmetric Interior Penalty DG Method on Heat Equation

Lets define the problem

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

Here is $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$. We want to write this on a weak form. Let the spaces we work on be

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

.

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,

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

But we want to introduce the shorter notation equivalently such that

$$
\sum_{T\in\mathcal{T}_h} \{\varepsilon (\nabla u, \nabla v)_T - \varepsilon \langle \partial_n u, v\rangle_{\partial T}\} = \sum_{T\in\mathcal{T}_h} (f, v). \tag{3}
$$

Where $\langle\cdot,\cdot\rangle$ is the surface integral operator. Before we contitinue do we want to introduce a 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

$$
\sum_{T\in\mathcal{T}_h} \varepsilon \langle \partial_n u, v_F\rangle = \sum_{E\in\mathcal{F}^{int}} \varepsilon \langle \partial_{n^+} u, v_F\rangle_E + \varepsilon \langle \partial_{n^-} u, v_F\rangle_E + \sum_{E\in\mathcal{F}^{ext}} \varepsilon \langle \partial_n u, v_F\rangle. \tag{4}
$$

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

$$
\begin{aligned}
V &= \left\{ (u, u_F) : u \in H^2(\mathcal{T}_h) \cap H^1(\Omega), u_F \in L^2(\mathcal{F}_h) \right\} \\
V_h &= \left\{ (u, u_F) : u \in \mathcal{P}^k(T)\, \forall T \in \mathcal{T}_h, \quad u_F \in \mathcal{P}^k(E)\, \forall E \in \mathcal{F}_h \right\}
\end{aligned}
$$

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

and now including drichlet conditions using the previous definition

$$
\begin{aligned}
V_D &= \{(u, u_F) \in V, u_F = u_D \quad \text{on } \Gamma_D\} \quad V_{h,D} = \{(u, u_F) \in V_h, u_F = u_D \quad \text{on } \Gamma_D\} \\
V_0 &= \{(u, u_F) \in V, u_F = 0 \quad \text{on } \Gamma_D\} \quad V_{h,0} = \{(u, u_F) \in V_h, u_F = 0 \quad \text{on } \Gamma_D\}
\end{aligned}
$$

Defining $(u, u_F) \in V_D$ and $(v, v_F) \in V_0$. Now adding (3) and (4) can we easily see that

$$
\sum_{T\in\mathcal{T}_h} \{\varepsilon (\nabla u, \nabla v)_T\} = \sum_{T\in\mathcal{T}_h} (f, v)_T + \sum_{E\in\mathcal{F}^{int}} \varepsilon \langle \partial_{n^+} u, v_F\rangle_E + \varepsilon \langle \partial_{n^-} u, v_F\rangle_E + \sum_{E\in\mathcal{F}^{ext}} \varepsilon \langle \partial_n u, v_F\rangle. \tag{5}
$$

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 a arbitary neumann boundary function f on some surface Γ. Hence (5) ends up being

$$
\sum_{T\in\mathcal{T}_h} \varepsilon (\nabla u, \nabla v) - \sum_{E\in F^{int}} (\varepsilon \langle \partial_{n^+} u, v_F\rangle_E + \varepsilon \langle \partial_{n^-} u, v_F\rangle_E) + \beta \langle \varepsilon u, v_F\rangle_{\Gamma_R} = \sum_{T\in T_h} (f, v)_T + \langle g, v_F\rangle_{\Gamma_N} + \langle h, v_F\rangle_{\Gamma_R}. \tag{6}
$$

According to Lehrenfeld 2010 [3] at page 13 on equation (1.2.7) is (6) equivalent to

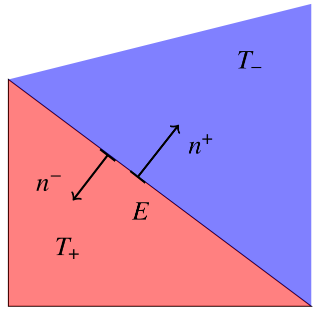


Figure 1: Edge E shared by the triangles T_- and T_+ and the normal unit vectors n^+ and n^-.

$$\sum_{T\in\mathcal{T}_h}(\varepsilon\nabla u,\nabla v)_T-\sum_{T\in\mathcal{T}_h}\langle\varepsilon\partial_n u,[\![v]\!]\rangle_{\partial T}+\beta\langle\varepsilon u,v_F\rangle_{\Gamma_R}=\sum_{T\in\mathcal{T}_h}(f,v)+\langle\varepsilon g,v_F\rangle_{\Gamma_N}+\langle\varepsilon h,v_F\rangle_{\Gamma_R} \tag{7}$$

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 $v_F=tr_{\partial T}(v)$. What we see is for (6) and (7) to be equivalent must this be true.

$$\sum_{T\in\mathcal{T}_h}\langle\varepsilon\partial_n u,[\![v]\!]\rangle_{\partial T}=\sum_{T\in\mathcal{T}_h}\langle\varepsilon\partial_n u,v\rangle_{\partial T}-\langle\varepsilon\partial_n u,v_F\rangle_{\partial T}=\sum_{E\in\mathcal{F}^{int}}\varepsilon\left(\langle\partial_{n^+}u,v_F\rangle_E+\langle\partial_{n^-}u,v_F\rangle\right). \tag{8}$$

why is it true?

Since $(u,u_F)\in V$ is has to be continious, hence the jump is $[\![u]\!]=0$ for the correct solution. Hence, adding $-\langle\varepsilon\partial_n v,[\![u]\!]\rangle_{\partial T}$ for symmetry and $\tau_h\langle\varepsilon[\![u]\!],[\![v]\!]\rangle_{\partial T}$ for stability with some stabilization parameter τ_h for each $T\in\mathcal{T}_h$. This can be added to lhs on (7) such that,

$$\begin{aligned}\sum_{T\in\mathcal{T}_h}(\varepsilon\nabla u,\nabla v)_t&-\sum_{T\in\mathcal{T}_h}\{\langle\varepsilon\partial_n u,[\![v]\!]\rangle_{\partial T}-\langle\varepsilon\partial_n v,[\![u]\!]\rangle_{\partial T}+\tau_h\langle\varepsilon[\![u]\!],[\![v]\!]\rangle_{\partial T}\}\\&+\beta\left\langle\varepsilon u,v_f\right\rangle_{\Gamma_R}\\&=\sum_{T\in\mathcal{T}_h}(f,v)+\langle\varepsilon g,v_F\rangle_{\Gamma_N}+\langle\varepsilon h,v_F\rangle_{\Gamma_R}\end{aligned} \tag{9}$$

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 (7) can we define

$$F(v,v_F)=\sum_{T\in\mathcal{T}_h}(f,v)+\langle\varepsilon g,v_F\rangle_{\Gamma_N}+\langle\varepsilon h,v_F\rangle_{\Gamma_R}$$

$$B(u,u_F,v,v_F)=\sum_{T\in\mathcal{T}_h}(\varepsilon\nabla u,\nabla v)_t-\sum_{T\in\mathcal{T}_h}\{\langle\varepsilon\partial_n u,[\![v]\!]\rangle_{\partial T}-\langle\varepsilon\partial_n[\![u]\!]\rangle_{\partial T}+\tau_h\langle\varepsilon[\![u]\!],[\![v]\!]\rangle_{\partial T}\}+\beta\langle\varepsilon u,v_F\rangle_{\Gamma_R}$$

$$B(u,u_F,v,v_F)=F(v,v_F). \tag{10}$$

4 C^0 Interior Penalty Method

4.1 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 (1) 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 5.2. Let say we want to solve the equation on the form.

$$\begin{aligned}\Delta^2u-\beta\Delta u+\gamma u&=f\quad\beta,\gamma\geq0\\\frac{\partial u}{\partial n}&=0\quad\text{on }\Omega\\\frac{\partial\Delta u}{\partial n}&=q\quad\text{on }\partial\Omega\end{aligned}. \tag{11}$$

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 $\frac{\partial \phi}{\partial n} = 0$. $\partial\Omega$.

4.2 Weak Formulation

We want to rewrite (11) 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 [4] that a convinient form is to write it as

$$\begin{aligned} a(u, v) &= (f, v)_{L^2(\Omega)} - (q, v)_{L^2(\partial\Omega)} \\ &= \int_\Omega D^2 w : D^2 v dx + \int_\Omega \nabla w \nabla v dx + \int_\Omega \gamma w \cdot v dx. \end{aligned} \tag{12}$$

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 [4] 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 (12) exists in V^*.

4.3 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 à $\mathcal{P}_2$ Lagrange finite element space associated with $\mathcal{T}_h$

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

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

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

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,

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

And similarly for means internally,

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

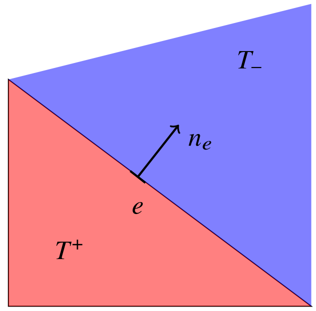


Figure 2: Edge e shared by the triangles T_- and T_+ and the normal unit vector n_e.

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

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

Using the results from [4] can we formulate the discrete formulation the boundary value problem (11) using C^0 interior penalty method. Our goals is to find a $u_h \in V_h^*$ such that this is true,

$$\mathcal{A}\left(u_h, v_h\right) = \left(f, v_h\right)_{L^2(\Omega)} - \left(q, v_h\right)_{L^2(\partial\Omega)} \quad \forall v_h \in V_h^*. \tag{13}$$

Where $w_h, v_h \in V_h$ and

$$\begin{aligned} \mathcal{A}\left(w_h, v_h\right) = &\sum_{T \in \mathcal{T}_h} \int_T D^2 w_h : D^2 v_h \\ &+ \sum_{e \in \mathcal{E}_h} \int_e \left\{\!\!\left\{ \frac{\partial^2 w_h}{\partial n_e^2} \right\}\!\!\right\} \left[\!\left[\frac{\partial v_h}{\partial n_e} \right]\!\right] ds \\ &+ \sum_{e \in \mathcal{E}_h} \left\{\!\!\left\{ \frac{\partial^2 v_h}{\partial n_e^2} \right\}\!\!\right\} \left[\!\left[\frac{\partial w_h}{\partial n_e} \right]\!\right] ds \\ &+ \sum_{e \in \mathcal{E}_h} \frac{\sigma}{|e|} \int_e \left[\!\left[\frac{\partial w_h}{\partial n_e} \right]\!\right] \left[\!\left[\frac{\partial v_h}{\partial n_e} \right]\!\right] ds \\ &+ \int_\Omega \beta \nabla w_h \cdot \nabla v_h dx + \int_\Omega \gamma w_h v_h dx. \end{aligned} \quad . \tag{14}$$

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

5 Appendix

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

Using the definition from [5] and we let Ω be a 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 $u : \Omega \to \mathbb{R}$ 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 $u, v : \Omega \to \mathbb{R}$. Then is $L^2(\Omega)$ a Hilbert space when the inner product is finite such that this exists

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

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

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

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

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

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

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

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] 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.

[3] Christoph Lehrenfeld. "Hybrid Discontinuous Galerkin methods for solving incompressible flow problems". PhD thesis. May 2010.

[4] 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.

[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.