Calculus of Variations: Theory and Applications to Solid Mechanics

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Outline

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Motivation and Origins

Definition (Continuum Mechanics)

Continuum mechanics is a classical differential equation model used to describe the interaction and movement of particles in a material

Features:

- Comprises both solid and fluid mechanics
- Assumes materials fill the entire body
- Same makeup if material is divided into pieces
- Adheres to Newton's Second law (resulting in a PDE)
- Prevalent in the 20th century study of solid mechanics

Motivation and Origins (continued)

Definition (Peridynamics)

Peridynamics (PD) is a nonlocal model for elasticity of solids that uses integrals over derivatives, attributed to Stewart A. Silling

Features:

- “Peri" means “near;" “dyna" means "force"
- Exchanges derivatives in continuum models for integrals (helps address crack formation)
- Treats particles as having a bond between them
- Range of interaction parameterized by δ, called **horizon**
- Material parameters represented by $h(x)$ (e.g., density)

Fundamental Equations of PD

Notation (Silling 2000)

- L_u: *force per unit of reference volume*
- u: *displacement [vector field]*
- f: *particle interaction function*
- Ω: *range of possible interactions*

Then for all $t \geq 0$, $x \in \Omega$,

$$L_u(x,t) = \int_\Omega f(u(x',t) - u(x,t), x' - x)dx'$$

If $b \in \mathbb{R}^n$ *is the loading force density of an external force then*

$$L_u(x,t) + b = 0$$

Motivation and Origins

For our problem the nonlocal operator is

$$Lu(x) \;=\; \frac{1}{2}\int_{\Omega_\delta} H(x,y)\frac{k_\delta(x-y)}{|x-y|^2}Du(x,y)dy$$

Nonlocal equations [or systems] take the form

$$\begin{cases} Lu \;=\; f, x \in \Omega \\ u \;=\; 0, x \in \Omega_\delta \setminus \Omega \end{cases}$$

Common in solid state mechanics, including peridynamics

Outline

Banach and Hilbert Spaces

Definition (Banach Space)

A **Banach space** is a normed space $(X, \|\cdot\|_X)$ that is **complete** (where all Cauchy sequences have limits)

Definition (Hilbert Space)

A **Hilbert space** is a Banach space $(H, \|\cdot\|_H)$ whose norm is induced by an inner product $\langle\cdot,\cdot\rangle$, i.e., $\|u\|_H^2 = \langle u, u\rangle$.

Example

The space $(L^2(0,1), \|\cdot\|_{L^2(0,1)})$ is a Hilbert space with inner product $\langle u, v\rangle = \int_0^1 u(x)v(x)dx$.

Coercivity and Boundedness

Definition (Bi-linear form)

A function $b : H \times H \to \mathbb{R}$ is a **bi-linear form** if it is linear in both arguments.

Definition (Coercivity)

A bi-linear form b is **coercive** if $\exists \alpha > 0$ such that $b(u, u) \geq \alpha \|u\|_H^2$ for all $u \in H$.

Definition (Boundedness)

A linear form $a : H \to \mathbb{R}$ is **bounded** (or continuous) if $\exists C_a > 0$ such that $|a(u)| \leq C_a \|u\|_H$ for all $u \in H$. A bi-linear form b is **bounded** (or continuous) if $\exists C > 0$ such that $|b(u, v)| \leq C \|u\|_H \|v\|_H$ for all $u, v \in H$.

Lax-Milgram and Riesz Representation

Theorem (Riesz Representation Theorem)

If x^* is a bounded linear functional on $(H, \|\cdot\|_H)$ with $x^* \in H^*$, then $\exists! z \in H$ such that

$$x^*(x) = \langle x, z \rangle \qquad \forall x \in H$$

Corollary (Lax-Milgram Theorem)

Assume $b : H \times H \to \mathbb{R}$ is a bounded, coercive, bi-linear form. Then for any $\varphi \in H^*$, then $\exists! u \in H$ such that

$$b(u, v) = \langle \varphi, v \rangle \qquad \forall v \in H$$

Uniqueness

Theorem (Classical Poisson Equation, c.f. Evans text)

Let $f \in C(\Omega)$. There exists at most one solution $u \in C^2(\Omega)$ of

$$\begin{cases} -\triangle u(x) = f(x), x \in \Omega \\ u(x) = 0, \qquad x \in \partial\Omega \end{cases}$$

Outline

What is an Integral Equation?

Definition (Integral Equation)

An **integral equation** is an equation that involves integral operators rather than differential operators to measure [physical] quantities.

Example (Volterra Equations)

Volterra Equation of First Kind:

$$f(x) = \int_a^x K(x,t)\varphi(t)dt$$

Volterra Equation of Second Kind:

$$\varphi(x) = f(x) + \lambda \int_a^x K(x,t)\varphi(t)dt$$

Stochastic variants appear in actuarial science, namely in **ruin theory**

What is the Fractional Laplacian?

Definition (Fractional Laplacian)

For $s \in (0, 1)$, define

$$(-\triangle)^s u(x) := c(n, s) \int_{\mathbb{R}^n} \frac{2u(x) - u(x+y) - u(x-y)}{|y|^{n+2s}} dy$$

Definition (Classical Laplacian)

$$\triangle u := \sum_{i=1}^{n} \frac{\partial^2 u}{\partial x_i^2}, u \in C^2(\Omega)$$

What are Fractional Sobolev Spaces?

Definition (Fractional Sobolev Space)

For $p \in [1, \infty)$, $s \in (0, 1)$, we define

$$W^{s,p}(\Omega) = \left\{ u \in L^p(\Omega), \frac{|u(x) - u(y)|}{|x - y|^{\frac{n}{p}+s}} \in L^p(\Omega \times \Omega) \right\}$$

with norm

$$\|u\|_{W^{s,p}(\Omega)} = \left(\int_\Omega |u|^p dx + \int_\Omega \int_\Omega \frac{|u(x) - u(y)|}{|x - y|^{\frac{n}{p}+s}} dxdy \right)^{\frac{1}{p}}$$

These are designed as Banach Spaces “between" $L^p(\Omega)$ and $W^{1,p}(\Omega)$.

Classical Results: Fractional Sobolev Spaces

Proposition (Continuous Embedding)

Let $p \in [1, \infty)$, $0 < s \leq s' < 1$, $\Omega \subset \mathbb{R}^n$ be open, then $\exists C = C(n, s, p) \geq 1$ such that

$$\|u\|_{W^{s,p}(\Omega)} \leq C\|u\|_{W^{s',p}(\Omega)}$$

Proposition (Extension)

Let $\Omega \subset \mathbb{R}^n$ be open, $u \in W^{s,p}(\Omega)$. If there is a compact $K \subset \Omega$ such that $u = 0$ in $\Omega \setminus K$, then the extension $\widetilde{u}$ of u by zero on $\mathbb{R}^n \setminus \Omega$ satisfies

$$\|\widetilde{u}\|_{W^{s,p}(\mathbb{R}^n)} \leq C\|u\|_{W^{s,p}(\Omega)}$$

NOTE: There are other domains where extensions take place, but finding a characterization is an open problem!

Uniqueness

Theorem (Uniqueness for Fractional Laplace Equation)

Let $f \in L^2(\Omega)$. There exists a unique solution $u \in H_0^s(\Omega)$ of

$$\int_\Omega \int_\Omega \frac{(u(x)-u(y))(w(x)-w(y))}{|x-y|^{n+2s}} dxdy = \int_\Omega f(x)w(x)dx$$

for all $w \in H_0^s(\Omega)$.

NOTE: $H_0^s(\Omega) = W_0^{s,2}(\Omega)$, zero boundary data!

Regularity Result

Theorem (Grubb 2015)

Let $\Omega \subset \mathbb{R}^n$ be a domain for which $\partial\Omega \in C^\infty$. If $g \in H^r(\Omega)$ for some $r \geq -s$, then the solution to

$$\begin{cases} (-\triangle)^s u(x) = g(x), x \in \Omega \\ u(x) = 0, \qquad\qquad x \in \mathbb{R}^n \setminus \Omega \end{cases}$$

belongs to $H^{s+\theta}(\Omega)$, where $\theta := \min\left\{s + r, \frac{1}{2} - \epsilon\right\}$ for $\epsilon > 0$ arbitrarily small. In fact, $\exists C > 0$ such that

$$\|u\|_{H^{s+\theta}(\Omega)} \leq C\|g\|_{H^r(\Omega)}.$$

NOTE: $H^r(\Omega) = W^{r,2}(\Omega)$

Generalizations of Singularities

The Fractional Laplacian is just one type of nonlocal operator!

$$(-\triangle)^s u(x) \;=\; c(n,s)\int_{\mathbb{R}^n} \frac{2u(x)-u(x+y)-u(x-y)}{|y|^{n+2s}}dy$$

Key aspects to carry over:

- Possesses a singularity near origin
- Singularity is radial and non-negative
- Finiteness not dependent on [strong] differentiability of u

Outline

What is the Calculus of Variations?

Definition (Calculus of Variations)

The field of **calculus of variations** is the study of minimizing (or maximizing) integral functionals over a certain function space.

Canonical example: let $\Omega \subset \mathbb{R}^n$ be a bounded domain, find $u \in W^{1,1}(\Omega; \mathbb{R}^m)$ that minimizes an **objective functional**

$$\mathcal{F}[u] := \int_\Omega f(x, u(x), \triangledown u(x))dx.$$

Sample questions:

- What types of conditions do we want to assume on f?
- When do minimizers exist, and when are they unique?
- What is the regularity of minimizers (when they exist)?

Case Study: The Isoperimetric/Isovolumetric Problem

Let $\alpha, \beta > 0$, find $u : [0, 1] \to \mathbb{R}$ with $u(0) = \alpha$ and $u(1) = \beta$ that minimizes

$$\mathcal{F}[u] := \int_0^1 \sqrt{1 + (u'(t))^2} dt$$

while having the iso-perimeter constraint

$$\int_0^1 u(t) dt = A$$

for some fixed $A > 0$.

Sample Objective Functionals

Example

Object Fitting:

$$I(u) := \int_\Omega (u(x) - u_{des}(x))^2 dx$$

where u_{des} is the optimal shaping of a material in $\mathbb{R}^3$ to fit in a hole

Example

Work: $W = Fd$ from physics

$$I(u,g) := \int_\Omega u(x) \cdot g(x) dx$$

What is the Direct Method?

Let X be a complete metric space, $\mathcal{F} : X \to \mathbb{R} \cup \{+\infty\}$ be the objective functional satisfying two conditions:

1. **Coercivity:** If $\mathcal{F}[u_j] \leq \Lambda$ for some sequence $\{u_j\}_{j=1}^{\infty} \subset X$ and a $\Lambda \in \mathbb{R}$, then $\{u_j\}_{j=1}^{\infty}$ has a sub-sequence converging to some $\bar{u} \in X$.
2. **Lower semi-continuity:** If $\{u_j\}_{j=1}^{\infty} \subset X$ is a sequence where $u_j \to \bar{u}$ in X, then $\mathcal{F}[\bar{u}] \leq \liminf_{j\to\infty} \mathcal{F}[u_j]$.

Any functional $\mathcal{F}$ satisfying these conditions has a minimizer in X!

How to use/prove the Direct Method

- Show objective functional is bounded from below
- Pick a sequence of functions approaching the infimum
- Use compactness properties to obtain suitable sub-sequence
- Show limit of sub-sequence actually attains the infimum
- Uniqueness: contradiction/convexity argument

Abstract Minimization Result

Theorem

Let Z_{ad} be a nonempty, closed, bounded, and convex subset of Z. Let $S : Z \to Y$ be a compact operator, and $G : Y \to \mathbb{R}$ be lower semi-continuous. Then the Banach Space optimization problem

$$\min_{g \in Z_{ad}} \left\{ f(g) \;:=\; G(Sg) + \frac{\lambda}{2} \|g\|_Z^2 \right\}$$

has an optimal solution $\bar{g}$. Furthermore, if $\lambda > 0$, and G and S are linear on their respective domains, then there is a unique minimizer.

A Mountain Pass Theorem

Application of calculus of variations: prove existence of [non-trivial] solutions to PDEs
Denote $C\Omega := \mathbb{R}^n \setminus \Omega$

Theorem (Nonlocal Mountain Pass (Servadei-Valdinoci 2012))

Let K be a kernel so that if $\gamma(x) := \min\{|x|^2, 1\}$, then $\gamma K \in L^1(\mathbb{R}^n)$. Denote

$$Y_0 := \{(g(x) - g(y))\sqrt{K(x-y)} \in L^2(\mathbb{R}^{2n} \setminus (C\Omega \times C\Omega)), g = 0 \text{ on } C\Omega\}.$$

Then the following problem has a non-trivial solution on $u \in Y_0$:

$$\int_{\mathbb{R}^n} \int_{\mathbb{R}^n} (u(x) - u(y))(\varphi(x) - \varphi(y))K(x-y)dxdy = \int_\Omega f(x, u(x))\varphi(x)dx$$

for all $\varphi \in Y_0$.

What is Optimal Design?

Definition

Optimal design is a variational problem where a material is chosen to adhere to a specific force-displacement behavior as closely as possible

Prototypical design (scalar-valued):

$$\begin{cases} \min_{(h,u)\in\mathcal{H}\times X_0} \int_{\Omega_\delta}\int_{\Omega_\delta} F(x',x,h,u)dx'dx \\ L_\delta(u) = f(x) \text{ in } \Omega, \quad u = 0 \text{ in } \Omega_\delta \setminus \Omega \end{cases}$$

where L_δ is a nonlocal operator (e.g., Fractional Laplacian over $\Omega_\delta \times \Omega_\delta$)

Outline

Γ-Convergence

Definition

We say that the family $E_\delta : L^2(\Omega;\mathbb{R}^n) \to \mathbb{R} \cup \{+\infty\}$ **Γ-converges** strongly in $L^2(\Omega;\mathbb{R}^n)$ to $E_0 : L^2(\Omega;\mathbb{R}^n) \to \mathbb{R} \cup \{+\infty\}$ (denoted $E_\delta \xrightarrow{\Gamma} E_0$) if:

i) **The liminf inequality:** Assume $u_\delta \to u$ strongly in $L^2(\Omega;\mathbb{R}^n)$. Then

$$E_0(u) \leq \text{liminf}_{\delta \to 0^+} E_\delta(u_\delta)$$

ii) **Recovery sequence property:** For each $u \in L^2(\Omega;\mathbb{R}^n)$, there exists a sequence $\{u_\delta\}_{\delta>0}$ where $u_\delta \to u$ strongly in $L^2(\Omega;\mathbb{R}^n)$ and

$$\text{limsup}_{\delta \to 0^+} E_\delta(u_\delta) \leq E_0(u)$$

Why Γ-Convergence?

Proposition

If $E_\delta \xrightarrow{\Gamma} E_0$ and $\{u_\delta\}_{\delta>0} \subset L^2(\Omega;\mathbb{R}^n)$ is a recovery sequence such that $u_\delta \to u$ strongly in $L^2(\Omega;\mathbb{R}^n)$, then

$$\lim_{\delta\to 0^+} E_\delta(u_\delta) = E_0(u).$$

- Considers convergence of certain sequences
- Direct method produces bounded sequences
- Compactness results used to get convergent sub-sequences
- Connects nonlocal problems to local problems (e.g. those on Sobolev Spaces)

Example: Γ-Convergence vs. Pointwise Convergence

Example

Let $F_h(x) := hxe^{-2h^2x^2}$. Then $F_h \xrightarrow{\Gamma} F$ in $\mathbb{R}$, defined as

$$F(x) = \begin{cases} -\frac{1}{2}e^{-\frac{1}{2}}, & x = 0 \\ 0, & x \neq 0 \end{cases}$$

However, $\{F_h\}_{h>0}$ converges pointwise on $\mathbb{R}$ to the zero function.

Case Study: Phase Transitions

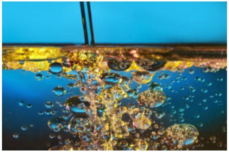

Figure: Image courtesy of wonderopolis.com

Let $\rho : \Omega \to [0,1]$ represent a mixing of Fluid A and Fluid B in some vessel ($\Omega \subset \mathbb{R}^n$, $n = 2$ or $n = 3$), 0 representing Fluid A only; 1 representing Fluid B only This constraint indicates proportion of fluids:

$$\int_\Omega \rho(x)dx = \gamma \in (0, |\Omega|)$$

We look to find an equilibrium by minimizing a **Gibbs energy**

$$\mathcal{G}[\rho] = \int_\Omega W_0(\rho(x))dx$$

Case Study: Phase Transitions (continued)

Definition (Double-well potential)

A **double-well potential** is an energy potential [function] that has two minima.

If W_0 is a double-well, denote its minima as α and β, want $\gamma \in (\alpha|\Omega|, \beta|\Omega|)$. For well-posedness, we try to minimize the surface area between the two phases $E_\alpha := \{x \in \Omega, \rho(x) = \alpha\}$, $E_\beta := \{x \in \Omega, \rho(x) = \beta\}$. So we look to minimize the rescaled penalty functional

$$\mathcal{F}_\epsilon[u] \;:=\; \int_\Omega \frac{1}{\epsilon} W(u(x)) + \epsilon |\bigtriangledown u(x)|^2 dx,\; u : \Omega \to [-1, 1]$$

Case Study: Phase Transitions (continued)

Definition (Perimeter)

The **perimeter** of a set is

$$\mathrm{Per}_\Omega(E) := \sup\left\{ \int_E \mathrm{div}\varphi dx, \varphi \in C_C^1(\Omega; \mathbb{R}^d), \|\varphi\|_{L^\infty(\Omega)} \leq 1 \right\}$$

Theorem (Modica-Mortola 1977)

We have $\mathcal{F}_\epsilon \xrightarrow{\Gamma} \mathcal{F}_0$ in the strong $L^1(\Omega)$-topology, where

$$\mathcal{F}_0[u] = \begin{cases} 2Per_\Omega(\{x \in \Omega, u(x) = \alpha\}) \int_\alpha^\beta \sqrt{W(s)}ds, \\ u \in BV(\Omega; \{\alpha, \beta\}), \int_\Omega udx = \gamma; \\ +\infty \text{ otherwise} \end{cases}$$

Outline

Notation

- Let $\Omega \subset \mathbb{R}^n$ be a bounded domain
- Projected difference: $Du(x, y) := \frac{(u(x)-u(y))\cdot(x-y)}{|x-y|}$, nonlocal linearized strain (for vector-valued functions)
- Kernel sequence $\{k_\delta\}_{\delta>0}$ radial, integrable, non-negative, supported in $B(0, \delta)$, $k_\delta(r)r^{-2}$ is non-increasing, and $\int_{\mathbb{R}^n} k_\delta(\xi)d\xi = 1$
- Design function: $H(x, y) := \frac{h(x)+h(y)}{2}$, $h \in L^\infty(\Omega), h > 0$

Notation (continued)

For fixed $\delta > 0$:

$$B(u,v) \ := \ \int_{\Omega_\delta}\int_{\Omega_\delta} k_\delta(x-y)\frac{Du(x,y)Dv(x,y)}{|x-y|^2}dxdy$$

$$B_h(u,v) \ := \ \int_{\Omega_\delta}\int_{\Omega_\delta} H(x,y)k_\delta(x-y)\frac{Du(x,y)Dv(x,y)}{|x-y|^2}dxdy$$

$$X(\Omega_\delta;\mathbb{R}^n) := \{u \in L^2(\Omega_\delta;\mathbb{R}^n), B(u,u) < \infty\}$$

$$X_0(\Omega_\delta;\mathbb{R}^n) := \{u \in X, u = 0 \text{ in } \Omega_\delta \setminus \Omega\}$$

Linear Theory

Lemma

The space $X(\Omega;\mathbb{R}^n)$ equipped with the norm

$$\|u\|_{X(\Omega;\mathbb{R}^n)} := \|u\|_{L^2(\Omega;\mathbb{R}^n)} + [u]_{X(\Omega;\mathbb{R}^n)}$$

is a Hilbert Space, and so is X_0; here $[u]_{X(\Omega;\mathbb{R}^n)} = B(u,u)^{\frac{1}{2}}$

Theorem (Existence and Uniqueness)

For any $u_0 \in \partial X$ and $g \in L^2(\Omega;\mathbb{R}^n)$, there exists a unique $u \in u_0 + X_0$ such that the state system

$$B_h(u,w) = \int_\Omega g(x)\cdot w(x)dx$$

is satisfied for all $w \in X_0$.

Minimization Problem

Goal: find $(\bar{u}, \bar{g}) \in (u_0 + X_0(\Omega_\delta; \mathbb{R}^n)) \times L^2(\Omega; \mathbb{R}^n)$ minimizing

$$I_\delta(u, g) = \int_\Omega F(x, u(x))dx + \frac{\lambda}{2}\|g\|^2_{L^2(\Omega;\mathbb{R}^n)}$$

subject to: $\lambda > 0$, $g \in Z_{ad} \subset L^2(\Omega; \mathbb{R}^n)$ and $u \in u_0 + X_0$ solving

$$B_h(u, v) = \int_\Omega g(x) \cdot v(x)dx \quad \forall v \in X_0$$

Here $\bar{g}$ is an external force and $\bar{u}$ represents displacement

Minimization Problem (continued)

Take Z_{ad} to be a nonempty, closed, convex, and bounded subset of $L^2(\Omega; \mathbb{R}^n)$, typically

$$Z_{ad} \;=\; \{a \leq z_i(x) \leq b, 1 \leq i \leq n\}$$

where $a \leq b$. Also, $\lambda > 0, g \in Z_{ad} \subset L^2(\Omega; \mathbb{R}^n)$, $u \in u_0 + X_0$.
Assumptions on $F : \Omega \times \mathbb{R} \to \mathbb{R}$:

1. For all $v \in \mathbb{R}$, $x \mapsto F(x, v)$ is measurable
2. For all $x \in \Omega$, $v \mapsto F(x, v)$ is continuous

Also need that $X_0(\Omega; \mathbb{R}^n) \subset\subset L^2(\Omega; \mathbb{R}^n)$

Existence and Uniqueness of Minimizers

Theorem (Existence and Uniqueness of Minimizers)

There exists $(\bar{u}, \bar{g}) \in (u_0 + X_0(\Omega_\delta; \mathbb{R}^n)) \times L^2(\Omega; \mathbb{R}^n)$ *minimizing*

$$I_\delta(u, g) = \int_\Omega F(x, u(x))dx + \frac{\lambda}{2}\|g\|^2_{L^2(\Omega;\mathbb{R}^n)},$$

where $u \in u_0 + X_0$ *solves*

$$B_h(u, v) = \int_\Omega g(x) \cdot v(x)dx \quad \forall v \in X_0$$

This minimizer is unique if F *is linear in its second argument:*

$$F(x, \alpha u(x) + \beta v(x)) \;=\; \alpha F(x, u(x)) + \beta F(x, v(x))$$

Convergence of Solutions

Theorem

Suppose $\{(\bar{u}_\delta, \bar{g}_\delta)\}_{\delta>0}$ *denotes the sequence of minimizers for the functionals* $\{I_\delta\}_{\delta>0}$*. If* $\bar{u}_\delta \to \bar{u}$ *strongly in* $L^2(\Omega;\mathbb{R}^n)$ *and* $\bar{g}_\delta \rightharpoonup \bar{g}$ *weakly in* $L^2(\Omega;\mathbb{R}^n)$*, then* $(\bar{u}, \bar{g})$ *is a minimizer to a local optimal control problem on* $W^{1,2}(\Omega;\mathbb{R}^n)$*.*

Notice $\{\bar{u}_\delta\}_{\delta>0}$ have bounded semi-norm so compactness gives a $\bar{u}$
Notice $\{\bar{g}_\delta\}_{\delta>0}$ are bounded in $L^2(\Omega;\mathbb{R}^n)$ so compactness gives a $\bar{g}$

Outline

Selected References

- H. Brezis, *Functional Analysis, Sobolev Spaces, and Partial Differential Equations*, Springer, 2011.
- G.B. Folland, *Real analysis. Modern techniques and their applications.* Wiley, New York, 1984
- T. Mengesha and Q. Du (2014), *The bond-based peridynamic system with Dirichlet-type volume constraint*, Proceedings of the Royal Society of Edinburgh, **144A**, 161–186.

Selected References (continued)

- J. Munoz (2020), Local and nonlocal optimal control in the source, `https://arxiv.org/pdf/2004.02794.pdf`.
- A. C. Ponce (2004), An estimate in the spirit of Poincaré's inequality, *J. Eur. Math. Soc. (JEMS)*, 6:1–15.
- S. Silling, Reformulation of elasticity theory for discontinuities and long-range forces. *J. of Mech. Phys. Solids* **48** (2001), 175–209.
- F. Troltzsch, *Optimal Control of Partial Differential Equations: Theory, Methods, and Applications*, American Mathematical Society, 2010.