

COEFFICIENT CONTROL OF VARIATIONAL INEQUALITIES

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ABSTRACT. Within this chapter, we discuss control in the coefficients of an obstacle problem. Utilizing tools from H-convergence, we show existence of optimal solutions. First order necessary optimality conditions are obtained after deriving directional differentiability of the coefficient to solution mapping for the obstacle problem. Further, considering a regularized obstacle problem as a constraint yields a limiting optimality system after proving, strong, convergence of the regularized control and state variables. Numerical examples underline convergence with respect to the regularization. Finally, some numerical experiments highlight the possible extension of the results to coefficient control in phase-field fracture.

1. INTRODUCTION

In this chapter, we consider an optimization problem of the form

$$(1.1) \quad \begin{aligned} \min J(q, u) &= j(u) + \frac{\alpha}{2} \|q\|^2 \\ \text{s.t.} \quad &\begin{cases} (q \nabla u, \nabla(v - u)) \geq (f, v - u) & \forall v \in K, \\ u \in K, & q \in Q^{\text{ad}}, \end{cases} \end{aligned}$$

governed by an obstacle problem in a domain $\Omega \subset \mathbb{R}^d$, where d denotes the spatial dimension, for a control q in an admissible set $Q^{\text{ad}} \subset L^2(\Omega; \mathbb{R}_{\text{sym}}^{d \times d})$ that is closed and convex, and a state $u \in K \subset H_0^1(\Omega)$. The precise mathematical problem statement will be presented in Section 2. In the following, let us briefly comment on the control-to-state coupling. For each given fixed, uniformly positive definite, control $q \in Q^{\text{ad}}$ acting as a coefficient function and data f the obstacle problem of finding $u \in K$ solving

$$(q \nabla u, \nabla(v - u)) \geq (f, v - u) \quad \forall v \in K,$$

has a well developed theory providing existence and regularity of solutions u , see, e.g., [35, 52].

Optimization problems similar to (1.1), but with control acting in the right hand side f , rather than the coefficient q , have been investigated over many years. Indeed, even in this case the obstacle problem gives rise to a non-differentiable operator $f \mapsto u$, in general. Early works by [25] provided directional differentiability, and [42, 43] provide necessary optimality conditions for such problems. Similar results for constraints of Signorini rather than obstacle type can be found in [6]. For an overview of these results; see also [7] or [9].

The inherent non-differentiability of the previous problem statement, with control in the right hand side f , motivated the investigation of relaxation approaches for the variational inequality in [8]. A scheme that allows for an efficient solution is

the primal-dual active set method proposed in [31]. A convergence analysis for a similar regularization approach was established in [53].

The lack of differentiability results in the difficulty of asserting suitable necessary optimality conditions for this problem class and different stationarity concepts, such as strong, weak, C-, or M-stationarity need to be considered. Indeed, strong stationarity is a necessary optimality condition if suitable compatibility conditions on the control bound are satisfied and the control space is large enough [59], but in more general situations weaker concepts need to be considered, see, e.g. [60]. We refer also to [26] for a comparison of different stationarity concepts. Recently, [51] characterized the Bouligand generalized differential for the mapping $f \mapsto u$ given by the obstacle problem, and [13] obtained stationarity conditions for time dependent variational inequalities of obstacle type. Moreover, the authors of [2] provided directional differentiability results for quasi-variational inequalities of obstacle type with control in the right hand side f . Further, [15] established sensitivity results for variational inequalities of second kind.

Algorithmic approaches for this problem class can be based on the regularization of the variational inequality [38] coupled with a path-following strategy [37]. The latter can also be coupled with adaptive mesh refinement utilizing a posteriori error estimates [39]. Alternatively, non-smooth optimization techniques such as bundle-methods can be combined with inexact solutions of the sub-problems as proposed in [29]. Based on the observation that real valued Lipschitz functions on Banach spaces are differentiable on a dense subset, if the norm is differentiable away from zero [50], it was proposed by [14] to utilize smooth sub-problems in a trust-region framework whenever differentiability can be asserted and only fall back to the use of non-linear directional derivatives if differentiability fails.

The novelty of this book chapter is the extension of some of the previously mentioned findings to control in the coefficient q rather than the right hand side f . In this context, existence no longer follows from the compactness of the mapping $L^2 \ni f \mapsto u \in H^1$, and H-convergence [45, 46, 58] or G-convergence [57] needs to be considered to analyze well-posedness of the problem. We also refer the reader to [1]. These techniques have been utilized successfully in the context of free-material optimization [27] as well as in the discretization error analysis of matrix identification problems [16, 17].

Furthermore, we provide a proof of concept to extend the coefficient control to phase-field fracture. The variational approach to fracture, known as phase-field nowadays, goes back to [21, 11, 36, 41]. Monographs, recent overviews, and two phase-field benchmark settings are provided in [12, 3, 10, 61, 54, 20, 18]. Our formulation starts from our own prior work [48, 49]. In the current work, the coefficient control acts in the elasticity tensor as it is common in free-material optimization, see, e.g., [27]. A prototype setting is described and investigated in a computational fashion.

The rest of the manuscript is organized as follows. In Section 2, we will state the precise problem under consideration and collect some well known facts on the obstacle problem needed in the upcoming analysis. We will then discuss the well-posedness of our optimization problem. In Section 3, we will discuss directional differentiability of the control to state map, generalizing results of [42] to the case of control in the coefficients, and eventually obtain a first formulation of first order necessary optimality conditions. These results will be detailed in a forthcoming

publication. In Section 4, we discuss recent results concerning optimality conditions for a regularized variational inequality as given in [56]. In Section 5, we show some numerical results for the coefficient control in the obstacle problem highlighting the convergence of the regularized solutions to the limiting VI-solution. Finally, in Section 6, we provide a prototypical extension towards phase-field fracture and provide some illustrating numerical examples. The article closes with an outlook and summary of further project results in Section 7.

2. PROBLEM STATEMENT AND EXISTENCE OF SOLUTIONS

In this section, we start by collecting precise assumptions for our model problem and eventually show existence of at least one global minimizer.

2.1. Notation and Assumptions. Let us first agree on some general notation and underlying assumptions. Let $\Omega \subset \mathbb{R}^d$ be a given Gröger-regular domain, c.f. [23], where $d \in \{1, \dots, 3\}$. We use the notation $Q := L^2(\Omega; \mathbb{R}_{\text{sym}}^{d \times d})$ and $U := H_0^1(\Omega)$, $\|\cdot\|$ and (\cdot, \cdot) denote the $L^2(\Omega)$ -norm and inner product for scalar, vector, and matrix valued functions. The admissible sets for the control and state are defined as

$$Q^{\text{ad}} = \{q \in L^2(\Omega; \mathbb{R}_{\text{sym}}^{d \times d}) \mid 0 < q_{\min} I \leq q(x) \leq q_{\max} I, \text{ a.e.}\} \subset Q,$$

$$K = \{u \in H_0^1(\Omega) \mid u \leq \psi\} \subset U,$$

for given $q_{\min}, q_{\max}, \psi \in \mathbb{R}$ with $q_{\min} < q_{\max}$, $\psi > 0$, and I denoting the identity matrix. Here $<$ and \leq denote the standard ordering of symmetric matrices given by the positive definite and positive semi-definite cone, respectively.

Moreover, let $f \in L^2(\Omega)$ be fixed, $\alpha > 0$ a positive cost parameter, and $j : U \rightarrow \mathbb{R}$ a weakly lower semicontinuous Fréchet-differentiable functional that is bounded from below. Then, we will consider the optimization problem

$$(P) \quad \begin{aligned} \min J(q, u) &= j(u) + \frac{\alpha}{2} \|q\|^2 \\ \text{s.t.} \quad &\begin{cases} (q \nabla u, \nabla(v - u)) \geq (f, v - u) & \forall v \in K, \\ u \in K, & q \in Q^{\text{ad}}. \end{cases} \end{aligned}$$

Within this setup it is known that for any given $q \in Q^{\text{ad}}$, the obstacle problem of finding $u \in K$ solving

$$(2.1) \quad (q \nabla u, \nabla(v - u)) \geq (f, v - u) \quad \forall v \in K$$

admits a unique solution, which follows immediately from the equivalent strictly convex minimization problem

$$u = \operatorname{argmin}_{v \in K} \frac{1}{2} (q \nabla v, \nabla v) - (f, v).$$

This in turn is equivalent to the existence of a Lagrange multiplier $\lambda \in H^{-1}(\Omega)$ such that

$$(q \nabla u, \nabla \varphi) = (f, \varphi) - \langle \lambda, \varphi \rangle \quad \forall \varphi \in H_0^1(\Omega).$$

Since $f \in L^2(\Omega)$ and $\psi \in \mathbb{R}$, [52, Chapter 5, Proposition 2.2] shows that in fact the solution satisfies $\nabla \cdot (q \nabla u) \in L^2(\Omega)$ and thus we can define the multiplier

$$\lambda := \nabla \cdot (q \nabla u) + f \in L^2(\Omega).$$

Here it should be noted that L^∞ -regularity of the coefficient $q \in Q^{\text{ad}}$ is in general not sufficient for $u \in H^2(\Omega)$.

Following [52, Chapter 5, Proposition 2.2], and using that ψ is constant, we find

$$\begin{aligned} \|\nabla \cdot (q \nabla u)\| &\leq 2\|f\|, \\ (2.2) \quad \|\lambda\| &= \|\nabla \cdot (q \nabla u) + f\| \\ &\leq 3\|f\|. \end{aligned}$$

From this, the Lax-Milgram theorem asserts the uniform bound

$$(2.3) \quad \|\nabla u\| \leq c \frac{q_{\max}}{q_{\min}} \|f\|,$$

and eventually the solution u of (2.1) can equivalently be characterized by the complementarity system

$$\begin{aligned} (2.4) \quad & -\nabla \cdot (q \nabla u) + \lambda = f \quad \text{in } L^2(\Omega), \\ & \lambda \geq 0 \quad \text{in } L^2(\Omega), \\ & u \leq \psi, \quad \text{q.e. in } \Omega, \\ & (\lambda, u - \psi) = 0. \end{aligned}$$

For the remainder of this chapter, we define the control-to-state mapping $S: Q^{\text{ad}} \rightarrow U, q \mapsto u$, where u solves the obstacle problem (2.1) for a given coefficient function $q \in Q^{\text{ad}}$.

2.2. Existence of Solutions. In this subsection, we discuss existence of solutions to (P). Due to the appearance of the product $q \nabla u$ in the variational inequality (VI) (2.1), weak* convergence of the control as it is induced by the boundedness of $Q^{\text{ad}} \subset L^\infty(\Omega; \mathbb{R}_{\text{sym}}^{d \times d})$ is not sufficient for passage to the limit in the VI. To circumvent this difficulty we resort to H -convergence, see, e.g., [58, Section 2].

Definition 2.1. A sequence $q_k \in Q^{\text{ad}}$ H -converges to $q \in Q^{\text{ad}}$ (in symbols $q_k \xrightarrow{H} q$) if for any sequence $u_k \in U$ satisfying

$$\begin{aligned} u_k &\rightharpoonup u, & \text{in } U, \\ \nabla \cdot (q_k \nabla u_k) &\rightarrow f, & \text{in } U^* \end{aligned}$$

for some $u \in U$ and $f \in U^*$ it holds

$$q_k \nabla u_k \rightharpoonup q \nabla u, \quad \text{in } L^2(\Omega; \mathbb{R}^d).$$

With the help of this concept we obtain the following existence result:

Theorem 2.2. There exists at least one solution of (P).

Proof. The proof follows the standard line of arguments. Clearly, J is bounded from below, and thus we can select a minimizing sequence $(q_k, u_k) \in Q^{\text{ad}} \times K$, with corresponding Lagrange multiplier λ_k . Due to H -compactness of Q^{ad} , see, e.g., [1, Theorem 1.2.16], we can select an H -convergent subsequence q_k with limit q . Further, by the bound (2.3) $u_k \rightharpoonup u$ in U and by (2.2)

$$\nabla \cdot (q_k \nabla u_k) \rightharpoonup g \quad \text{in } L^2(\Omega)$$

for some $g \in L^2(\Omega)$. By compactness of the embedding $L^2(\Omega) \subset U^*$ the convergence is strong in U^* and the definition of H -convergence asserts

$$q_k \nabla u_k \rightharpoonup q \nabla u, \quad \text{in } L^2(\Omega; \mathbb{R}^d).$$

Further, the bound (2.2) implies weak convergence $\lambda_k \rightharpoonup \lambda$ in $L^2(\Omega)$. Combined, we see that the limit (q, u, λ) satisfies the first equation in (2.4). Clearly, K is closed with respect to weak convergence in U , i.e., $u \leq \psi$ holds, and the complementarity relation $(\lambda, \psi - u) = 0$ follows from strong convergence of u_k in $L^2(\Omega)$. The sign condition on λ follows immediately by Mazur's lemma. Thus, the limit satisfies the system (2.4), which means that the pair (q, u) solves (2.1).

It remains to see the lower-semicontinuity of J . The first term is weakly lower semicontinuous by assumption, while the norm on q is lower-semicontinuous with respect to H -convergence by [16, Lemma 2.1]. This shows the assertion. \square

3. FIRST ORDER NECESSARY OPTIMALITY CONDITIONS

In this section, we first prove directional differentiability of the control-to-state mapping S and eventually derive a first order optimality condition in form a variational inequality, that can be viewed as a first step towards optimality conditions in qualified form.

3.1. Directional Differentiability of S . In order to prove directional differentiability of the control to state map S in the sense of Hadamard, see, e.g., [55, Definition 2.2], we need to show that for a given control $q \in Q^{\text{ad}}$ and direction $d \in Q$ with $q + d \in Q^{\text{ad}}$, the limit

$$S'(q; d) := \lim_{t \downarrow 0} \frac{S(q + td) - S(q)}{t}.$$

exists. Let us proceed in two steps. First, let us define the auxiliary operator

$$\hat{S}_q: H^{-1}(\Omega) \rightarrow H_0^1(\Omega), \quad f \mapsto u,$$

with $u \in K$ such that

$$(q \nabla u, \nabla(\varphi - u)) \geq (f, \varphi - u), \quad \forall \varphi \in K.$$

In other words, in this operator the coefficient matrix $q \in Q^{\text{ad}}$ is fixed, and the right-hand-side $f \in H^{-1}(\Omega)$ is mapped to the solution of the classical obstacle problem with the given coefficient q . Note that then we have

$$u = S(q) = \hat{S}_q(f).$$

As already pointed out in the introduction, the operator S_q acting on a control in the right hand side is well understood. Applying the results of [42] and [59], we obtain:

Lemma 3.1. The operator $\hat{S}_q: H^{-1}(\Omega) \rightarrow H_0^1(\Omega)$ is directionally differentiable at all points $f \in H^{-1}(\Omega)$. Its directional derivative $z := \hat{S}'_q(f; h) \in H_0^1(\Omega)$ in direction $h \in H^{-1}(\Omega)$ is given by the unique solution of the variational inequality

$$(3.1) \quad z \in \mathcal{K}(f), \quad (q \nabla z, \nabla(\varphi - z)) \geq (h, \varphi - z) \quad \forall \varphi \in \mathcal{K}(f),$$

with

$$\mathcal{K}(f) = \{\varphi \in H_0^1(\Omega): \varphi \leq 0 \text{ q.e. on } \{\hat{S}_q(f) = \psi\} \text{ and } \varphi = 0 \text{ q.e. on } q\text{-supp}(\lambda)\},$$

where $u = \hat{S}_q(f)$ and $\lambda = \nabla \cdot (q \nabla u) + f$ is the associated Lagrange multiplier defined in (2.4).

Proof. This is a formulation of [47, Theorem 2.9], cf., [42], applied to \hat{S}_q and adopted to our notation. The concrete form of the critical cone is due to [59]. \square

Now, as pointed out in [47], the operator \hat{S}_q is Lipschitz continuous and therefore even Hadamard differentiable. This yields our desired differentiability result for the operator S :

Theorem 3.2. The operator $S: Q \rightarrow H_0^1(\Omega)$ is directionally differentiable at all points $q \in Q^{\text{ad}}$. Its directional derivative $\tilde{u} := S'(q; d) \in H_0^1(\Omega)$ in direction $d \in Q$ with $q + d \in Q^{\text{ad}}$ is given by the unique solution of the variational inequality

$$(3.2) \quad \tilde{u} \in \mathcal{K}(q), \quad (q \nabla \tilde{u}, \nabla(\varphi - \tilde{u})) \geq (\nabla \cdot (d \nabla u), \varphi - \tilde{u}) \quad \forall \varphi \in \mathcal{K}(q),$$

with $u = S(q)$ and

$$\mathcal{K}(q) = \{\varphi \in H_0^1(\Omega) : \varphi \leq 0 \text{ q.e. on } \{u = \psi\} \text{ and } \varphi = 0 \text{ q.e. on } q\text{-supp}(\lambda)\},$$

Proof. Set $u = S(q)$ and note that $u_{td} = S(q + td)$ fulfills the variational inequality

$$(3.3) \quad u_{td} \in K \quad ((q + td) \nabla u_{td}, \nabla(\varphi - u_{td})) \geq (f, \varphi - u_{td}) \quad \forall \varphi \in K,$$

which is equivalent to

$$u_{td} \in K \quad (q \nabla u_{td}, \nabla(\varphi - u_{td})) \geq (f, \varphi - u_{td}) - t(d \nabla u_{td}, \nabla(\varphi - u_{td})) \quad \forall \varphi \in K.$$

Using integration by parts in the right-hand-side of the last inequality we deduce

$$S(q + td) = u_{td} = \hat{S}_q(f + \nabla \cdot (td \nabla u_{td})),$$

with

$$f + \nabla \cdot (td \nabla u_{td}) \in H^{-1}(\Omega).$$

We note that (3.3) implies that $\nabla \cdot (d \nabla u_{td})$ tends to $\nabla \cdot (d \nabla u)$ in H^{-1} as t tends to zero. Therefore, applying the Hadamard-differentiability of \hat{S}_q , i.e., Lemma 3.1, we observe

$$\frac{(S(q + td) - S(q))}{t} = \frac{\hat{S}_q(f + t \nabla \cdot (d \nabla u_{td})) - \hat{S}_q(f)}{t} \rightarrow \hat{S}'_q(f; \nabla \cdot (d \nabla u))$$

as $t \rightarrow 0$, and hence S is directionally differentiable with $S'(q; d) = \hat{S}'_q(f; \nabla \cdot (d \nabla u))$. \square

Following [59], we obtain an analogue to the complementarity system (2.4), namely that the variational inequality (3.2) is equivalent to the complementarity system

$$(3.4) \quad \begin{aligned} -\nabla \cdot (q \nabla \tilde{u}) + \tilde{\lambda} &= \nabla \cdot (d \nabla u) \quad \text{in } H^{-1}(\Omega), \\ \tilde{\lambda} &\in \mathcal{K}(\tilde{q})^\circ, \\ \tilde{u} &\in \mathcal{K}(\tilde{q}), \\ \langle \tilde{\lambda}, \tilde{u} \rangle_{H^{-1}(\Omega), H_0^1(\Omega)} &= 0. \end{aligned}$$

3.2. Optimality Conditions. To obtain necessary optimality conditions, we rewrite our optimization problem (P) into the, usual, reduced form utilizing the control-to-state mapping S :

$$\min_{q \in Q^{\text{ad}}} f(q) := j(S(q)) + \frac{\alpha}{2} \|q\|^2.$$

Note that the Fréchet differentiability of j and $\|\cdot\|^2$ and the directional differentiability of S thanks to Theorem 3.2 yields directional differentiability of f . The

following primal first order necessary condition is then a straight forward consequence of the convexity of Q^{ad} .

Lemma 3.3. Let $\bar{q} \in Q^{\text{ad}}$ be a locally optimal control for (P) with associated state $\bar{u} = S\bar{q}$. Then the following variational inequality is fulfilled:

$$(j'(\bar{u}), S'(\bar{q}; q - \bar{q})) + \alpha(\bar{q}, q - \bar{q}) \geq 0 \quad \forall q \in Q^{\text{ad}}.$$

Proof. The proof follows by standard arguments. We refer to, e.g., [47, Lemma 3.2] for a similar setting with control in the right-hand-side and additional state constraints. Since $\bar{q} \in Q^{\text{ad}}$ and Q^{ad} is convex, we know that $q_t := \bar{q} + t(q - \bar{q}) \in Q^{\text{ad}}$ for all $q \in Q^{\text{ad}}$. Since \bar{q} is locally optimal, we observe

$$\begin{aligned} 0 &\leq f(q_t) - f(\bar{q}) \\ &= j(S(q_t)) - j(S(\bar{q})) + \frac{\alpha}{2}(\|q_t\|^2 - \|\bar{q}\|^2) \end{aligned}$$

for all $q \in Q^{\text{ad}}$ and t sufficiently small. Since both j and $\|\cdot\|^2$ are Fréchet differentiable, dividing by $t > 0$ and passing to the limit yields

$$0 \leq j'(\bar{u})(S'(\bar{q}; q - \bar{q}) + \alpha(\bar{q}, q - \bar{q})) \quad \forall q \in Q^{\text{ad}}$$

by Theorem 3.2. □

4. OPTIMALITY CONDITIONS FOR A REGULARIZED PROBLEM

In this section, we introduce a set of limiting optimality conditions for (P) on domains $\Omega \subset \mathbb{R}^2$ by utilizing a regularization approach and considering the limit points of stationarity conditions for a series of regularized problems, similar to the approach in, e.g., [39]. To this effect, we introduce a regularized version of the obstacle problem and consider the limits of its optimal solutions. Additional supporting results regarding the regularity estimates used can be found in [56] and a more detailed explanation of the results presented in this section with all pertinent proofs will be provided in a forthcoming paper.

For the regularized problem, we introduce a biquadratic penalization $r : \mathbb{R}^+ \times \mathbb{R} \rightarrow \mathbb{R}$ of the obstacle energy functional into the problem, see, [39]. The resulting problem is given by

$$\begin{aligned} (P_\gamma) \quad \min_{q_\gamma, u_\gamma} \quad & J(q_\gamma, u_\gamma) = \frac{1}{2}\|u_\gamma - u_d\|_2^2 + \frac{\alpha}{2}\|q_\gamma\|_2^2 \\ \text{s.t.} \quad & -\nabla \cdot (q_\gamma \nabla u_\gamma) + r(\gamma; u_\gamma) = f \quad \text{in } H^{-1}(\Omega), \\ & u_\gamma \in H_0^1(\Omega), \quad q_\gamma \in Q^{\text{ad}}, \end{aligned}$$

with

$$r(\gamma; u_\gamma) := \gamma \left[\max((u_\gamma - \psi), 0)^3 \right].$$

Similar to the penalizations in, e.g., [39, 53], the penalization $r(\gamma; u_\gamma)$ describes a locally Lipschitz continuous, monotone Nemyzkii operator. Also note, that the control is a positive definite and symmetric operator. Since, given a control $q_\gamma \in Q^{\text{ad}}$, the left-hand side of the PDE

$$-\nabla \cdot (q_\gamma \nabla u_\gamma) + r(\gamma; u_\gamma) = f$$

is Lipschitz-continuous and monotone, we can apply the Browder-Minty theorem to ensure that for each $q_\gamma \in Q^{\text{ad}}$ a unique solution $u_\gamma \in H_0^1(\Omega)$ exists.

The existence of an optimal solution to the regularized problem can be proven by analogous arguments as in Theorem 2.2 providing:

Theorem 4.1. There exists at least one solution for (P_γ) .

Further, the regularization allows us to formulate a set of optimality conditions for this problem, see, e.g., [16].

Proposition 4.2. Let $(\bar{q}_\gamma, \bar{u}_\gamma) \in Q^{\text{ad}} \times H_0^1(\Omega)$ be a local minimum of (P_γ) . Then there exists $\bar{p}_\gamma \in H_0^1(\Omega)$ such that

$$\begin{aligned} -\nabla \cdot (\bar{q}_\gamma \nabla \bar{u}_\gamma) &= f - r(\gamma, \bar{u}_\gamma) && \text{in } H^{-1}(\Omega), \\ -\nabla \cdot (\bar{q}_\gamma \nabla \bar{p}_\gamma) &= \bar{u}_\gamma - u_d - \partial_u r(\gamma, \bar{u}_\gamma) \bar{p}_\gamma && \text{in } H^{-1}(\Omega), \\ (\alpha \bar{q}_\gamma - \nabla \bar{u}_\gamma \otimes \nabla \bar{p}_\gamma) (q - \bar{q}_\gamma) &\geq 0 && \forall q \in Q^{\text{ad}} \end{aligned}$$

with $\nabla u_\gamma \otimes \nabla p_\gamma$ describing the outer product of ∇u_γ and ∇p_γ .

By passing to the limit with $\gamma \rightarrow \infty$ we can utilize these conditions to formulate optimality conditions for the original problem (P). First we consider limits of the variables corresponding to the solutions of the regularized Problem (P_γ) .

Theorem 4.3. If $\gamma \rightarrow \infty$, then there is a subsequence of solutions $(\bar{q}_\gamma, \bar{u}_\gamma)$ to problem (P_γ) , with corresponding adjoint $p_\gamma \in H_0^1(\Omega)$ as defined in Proposition 4.2, such that

$$\begin{aligned} \bar{q}_\gamma &\rightarrow \bar{q} && \text{in } L^p \left(\Omega, \mathbb{R}_{\text{sym}}^{2 \times 2} \right) \text{ for all } 2 \leq p < \infty, \\ \bar{u}_\gamma &\rightarrow \bar{u} && \text{in } W^{1,p}(\Omega) \text{ for an } 2 < p < \infty, \\ \bar{p}_\gamma &\rightarrow \bar{p} && \text{in } W^{1,p}(\Omega) \text{ for an } 2 < p < \infty, \\ \bar{q}_\gamma \nabla \bar{u}_\gamma &\rightarrow \bar{q} \nabla \bar{u} && \text{in } L^2 \left(\Omega, \mathbb{R}^2 \right), \\ \bar{q}_\gamma \nabla \bar{p}_\gamma &\rightarrow \bar{q} \nabla \bar{p} && \text{in } L^2 \left(\Omega, \mathbb{R}^2 \right), \\ \nabla \bar{u}_\gamma \otimes \nabla \bar{p}_\gamma &\rightarrow \nabla \bar{u} \otimes \nabla \bar{p} && \text{in } L^p \left(\Omega, \mathbb{R}_{\text{sym}}^{2 \times 2} \right) \text{ for an } 1 < p < \infty, \\ r(\gamma, \bar{u}_\gamma) &\rightarrow \bar{\lambda} && \text{in } H^{-1}(\Omega), \\ \partial_u r(\gamma, \bar{u}_\gamma) \bar{p}_\gamma &\rightarrow \bar{\mu} && \text{in } H^{-1}(\Omega) \end{aligned}$$

for some $(\bar{q}, \bar{u}, \bar{p}, \bar{\lambda}, \bar{\mu}) \in Q^{\text{ad}} \times H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega) \times L^2(\Omega)$.

Based on these limits we can formulate a set of limiting optimality conditions for the original problem.

Theorem 4.4. Any limit point $(\bar{q}, \bar{u}, \bar{p}, \bar{\lambda}, \bar{\mu}) \in Q^{\text{ad}} \times H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega) \times L^2(\Omega)$ obtained in Theorem 4.3, fulfills the first order optimality system

$$\begin{aligned}
-\nabla \cdot (\bar{q} \nabla \bar{u}) &= f - \bar{\lambda} && \text{in } H^{-1}(\Omega), \\
\bar{u} &\leq \psi && \text{q.e. in } \Omega, \\
\bar{\lambda} &\geq 0 && \text{in } H^{-1}(\Omega), \\
(\bar{\lambda}, \bar{u} - \psi) &= 0, \\
-\nabla \cdot (\bar{q} \nabla \bar{p}) &= \bar{u} - u_d - \bar{\mu} && \text{in } H^{-1}(\Omega), \\
(\bar{p}, \bar{\lambda}) &= 0, \\
(\bar{\mu}, \bar{u} - \psi) &= 0, \\
(\bar{p}, \bar{\mu}) &\geq 0, \\
(\alpha \bar{q} - \nabla \bar{u} \otimes \nabla \bar{p})(q - \bar{q}) &\geq 0 && \forall q \in Q^{\text{ad}}.
\end{aligned}$$

5. NUMERICAL EXPERIMENTS

In this section, we present numerical results on an obstacle problem with coefficient control and its regularization. As a basis we consider an inverse problem for the estimation of matrix coefficients in an elliptic pde as has been studied in [16]. This is an optimal control problem with coefficient control, which we further modify by introducing an obstacle ψ , adjusting the objective and adding a barrier term to handle the condition $q \in Q^{\text{ad}}$.

5.1. Example 1. The resulting problem on the domain $\Omega = (-1, 1)^2 \subset \mathbb{R}^2$ is then given by

$$\begin{aligned}
&\min_{q \in L^2(\Omega, \mathbb{R}_{\text{sym}}^{2 \times 2}), u \in H_0^1(\Omega)} J(q, u) + \beta B(q) \\
&\text{s.t. } -\nabla \cdot (q \nabla u) = f - \lambda \quad \text{in } H^{-1}(\Omega), \\
&u \leq \psi \quad \text{q.e. in } \Omega, \\
&\lambda \geq 0 \quad \text{in } H^{-1}(\Omega), \\
&(\lambda, u - \psi) = 0,
\end{aligned} \tag{PMEst}$$

with given $\psi > 0$, $\psi \in \mathbb{R}$ and

$$f(x_1, x_2) = (1 - x_2^2) \left(6x_1^2 + 2 \right) + 2(1 - x_1^2). \tag{5.1}$$

To enforce $q \in Q^{\text{ad}}$, we introduce a logarithmic barrier term

$$-B(q) = \int_{\Omega} \log(\det(q - q_{\min} I)) + \log(\det(q_{\max} I - q)) \, dx,$$

with $q_{\min} = 0.5$, $q_{\max} = 10$ into the objective with a, small, barrier parameter $\beta > 0$. While B is clearly a barrier for the admissible control set Q^{ad} during the iterations one must assert that indeed the iterates remain within Q^{ad} as B can be finite outside of Q^{ad} . To do so, the trace of the matrices is monitored as in two dimensions a matrix is positive definite if its determinant and trace are positive.

The objective is given by

$$J(q, u) = \frac{1}{2} \|u - u_d\|_2^2 + \frac{\alpha}{2} \|q - q_d\|_2^2$$

with desired state

$$u_d(x_1, x_2) = (1 - x_1^2)(1 - x_2^2),$$

and desired control

$$q_d(x_1, x_2) = \begin{pmatrix} 1 + x_1^2 & 0 \\ 0 & 1 \end{pmatrix}$$

following [16] with the additional introduction of q_d . This is done so that without the introduction of an obstacle, the desired solution (q_d, u_d) would be the optimal solution of (P^{MEst}) with objective $J(q, u)$.

The problem setting has been implemented in C++ using the DOpElib optimization suite, see [22], which uses the deal.II finite element library, see [5, 4]. For our finite element approximations, we utilize a uniform mesh dependent on refinement level $l \geq 0$ that is constructed of $2^l \times 2^l$ quadratic cells of size h . To compute discretized solutions (q_h, u_h) , we utilize piecewise bilinear finite elements.

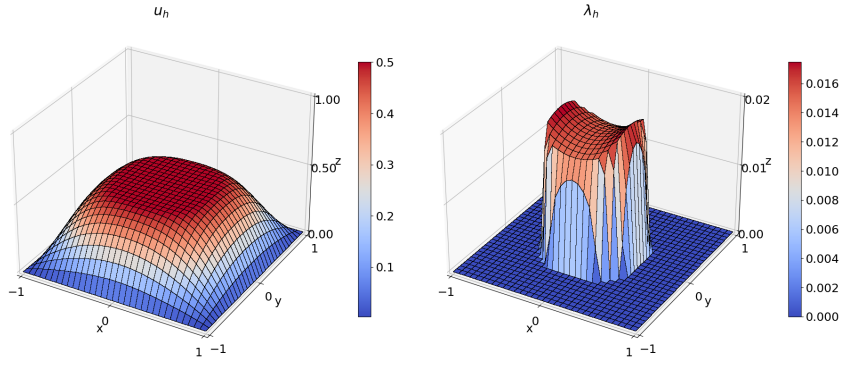


FIGURE 5.1. State solution (u_h, λ_h) for Problem (P^{MEst}) at refinement level $l = 5$

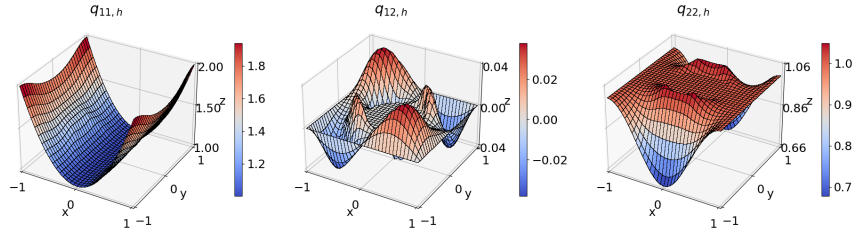


FIGURE 5.2. Control solution q_h for Problem (P^{MEst}) at refinement level $l = 5$

In this first problem, we compute solutions for (P^{MEst}) on $\Omega = (-1, 1)^2$ with obstacle $\psi = 0.5$ at refinement levels $l = 5$. Here we have weighted the Tikhonov term in the objective with $\alpha = 0.1$ and the barrier with $\beta = 0.0001$. We have chosen

$$q^{\text{init}} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

as the initial control. To implement the obstacle we have equivalently reformulated the set of complementarity constraints into

$$\lambda - \max\{0, \lambda + c(u - \psi)\} = 0 \iff u \leq \psi, \lambda \geq 0, (\lambda, u - \psi) = 0,$$

for arbitrary $c > 0$. In the computations, we have chosen this parameter as $c = 1$. Figure 5.1 shows the state solution u_h and the associated Lagrange multiplier λ_h of this problem. We can observe the obstacle acting as a constraint on the state, preventing the state u_h from achieving the desired solution u_d . Note that, since the Lagrange-multiplier λ_h acts as a slack variable, it allows us to observe the area in which the obstacle constraint is active. The effects on the corresponding control solution q_h are illustrated in Figure 5.2.

5.2. Example 2. To study the effects of the regularization, we use the regularized problem formulation. It is given by

$$(P_\gamma^{\text{MEst}}) \quad \min_{q_\gamma \in L^2(\Omega), u_\gamma \in H_0^1(\Omega)} J(q_\gamma, u_\gamma) \\ \text{s.t.} \quad -\nabla \cdot (q_\gamma \nabla u_\gamma) + \gamma \max(u_\gamma - \psi, 0)^3 = f \quad \text{in } H^{-1}(\Omega)$$

with penalty parameter $\gamma > 0$. All other quantities as the domain Ω , the parameters α, β , and the obstacle ψ are chosen as in Problem (P^{MEst}) .

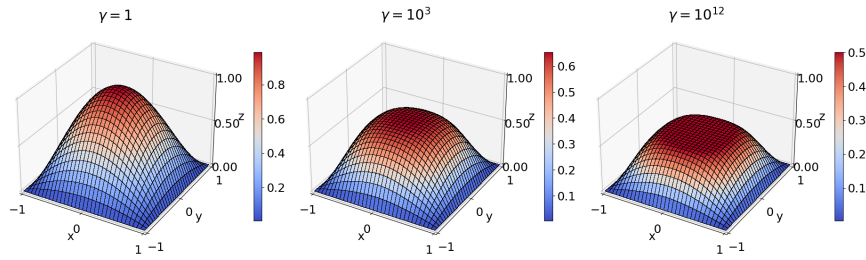


FIGURE 5.3. Results for different choices of regularization parameter γ on state solution $u_{h,\gamma}$ of Problem (P_γ^{MEst}) at refinement level $l = 5$

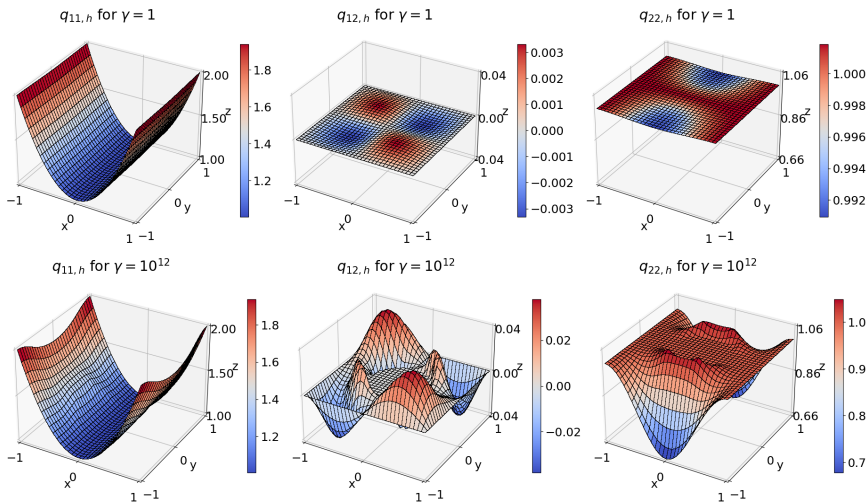


FIGURE 5.4. Results for different choices of regularization parameter γ on control solution $q_{h,\gamma}$ of Problem (P_γ^{MEst}) at refinement level $l = 5$.

We also start our computations with the same initial control q^{init} . We now compute solutions $(q_{h,\gamma}, u_{h,\gamma})$ for (P_γ^{MEst}) at different values of the regularization parameter γ . In Figure 5.3, we have illustrated the impact of increasing γ on the optimal state solution, visibly enforcing the obstacle for higher values of γ . We can also observe that the regularized control, see Figure 5.4, approximates the control solution of obstacle problem (P^{MEst}) for increasing γ . This is supported by our numerical results when comparing solutions of Problem (P_γ^{MEst}) at different regularization values with those of Problem (P^{MEst}) , see Table 5.1 for error computations at different refinement levels.

γ	$\ u_{h_1,\gamma} - u_{h_1}\ _2$	$\ q_{h_1,\gamma} - q_{h_1}\ _2$	$\ u_{h_2,\gamma} - u_{h_2}\ _2$	$\ q_{h_2,\gamma} - q_{h_2}\ _2$
10^0	$3.79579 \cdot 10^{-1}$	$1.8927 \cdot 10^{-1}$	$3.79979 \cdot 10^{-1}$	$1.87395 \cdot 10^{-1}$
10^3	$1.41644 \cdot 10^{-1}$	$6.47868 \cdot 10^{-2}$	$1.42056 \cdot 10^{-1}$	$6.98082 \cdot 10^{-2}$
10^6	$1.59084 \cdot 10^{-2}$	$7.76552 \cdot 10^{-3}$	$1.62702 \cdot 10^{-2}$	$8.16446 \cdot 10^{-3}$
10^9	$1.6923 \cdot 10^{-3}$	$3.57287 \cdot 10^{-3}$	$1.62867 \cdot 10^{-3}$	$1.56167 \cdot 10^{-3}$
10^{12}	$2.0242 \cdot 10^{-4}$	$4.39335 \cdot 10^{-4}$	$1.81648 \cdot 10^{-4}$	$1.19951 \cdot 10^{-3}$

TABLE 5.1. Difference between solution (q_{h_i}, u_{h_i}) of Problem (P^{MEst}) and solution $(q_{h_i,\gamma}, u_{h_i,\gamma})$ of regularized Problem (P_γ^{MEst}) with $i = 1, 2$ for refinement levels $l_1 = 5$ and $l_2 = 7$.

6. EXTENSION TO PHASE-FIELD FRACTURE

Let us introduce a free material optimization problem in the setting of fracture propagation, that is inspired by [27]. The overall goal is to control the behavior of the fracture by optimizing the stiffness tensor with a control in the coefficients and thus achieving a desired crack pattern.

6.1. Problem Statement. The state of the material is given by a pair $\mathbf{u} = (u, \varphi)$, where u denotes a two dimensional displacement field and φ a phase-field, i.e., a smooth indicator function for the fracture, cf., [12, 11], with $\varphi = 0$ in the broken area, and $\varphi = 1$ in the intact area. The symmetric gradient $e(u)$ is defined as

$$e_{ij}(u(x)) := \frac{1}{2} \left(\frac{du_i(x)}{dx_j} + \frac{du_j(x)}{dx_i} \right), \quad i, j = 1, 2,$$

and the strain by $\sigma_{q_{ij}} := q_{ijkl} e_{kl}(u)$, $i, j, k, l = 1, 2$, where q_{ijkl} is the elastic/plane-stress stiffness tensor. In accordance with [27], it is written as the symmetric material matrix

$$(6.1) \quad q = \begin{pmatrix} q_{1111} & q_{1122} & \sqrt{2}q_{1112} \\ & q_{2222} & \sqrt{2}q_{2212} \\ \text{sym} & & 2q_{1212} \end{pmatrix}.$$

As spatial domain Ω , we choose the unit square $(0, 1)^2 \subset \mathbb{R}^2$ with a horizontal notch in the middle of the domain $[0, 1] \times \{0.5\}$. Moreover, the Lipschitz boundary is partitioned into $\partial\Omega := \Gamma_D \dot{\cup} \Gamma_N \dot{\cup} \Gamma_{\text{free}}$, where $\Gamma_D := [0, 1] \times \{0\}$ and $\Gamma_N := [0, 1] \times \{1\}$. On Γ_D we enforce homogeneous Dirichlet boundary conditions for the displacement u . We have homogeneous Neumann boundary conditions for the phase-field and the initial condition $\varphi \equiv 1$ in Ω at $t = 0$. Further, let

$\mathbf{f}|_{\Gamma_N} \in L^2(\Gamma_N)$ be a stationary external orthogonal force. We consider a time-discrete model formulation on the time interval $[0, 1]$ with $M + 1$ equidistant time points, i.e., $0 = t_0 < t_1 < \dots < t_M = 1$. Consequently the state is given by $\mathbf{u} = (\mathbf{u}^i)_{i=1}^M = (u^i, \varphi^i)_{i=1}^M$. However, we will assume both the material matrix q and the external load \mathbf{f} to be constant in time. The fracture problem then reads: For given material matrix $q \in L^2(\Omega, \mathbb{R}_{sym}^{3 \times 3})$, initial values $\mathbf{u}^0 \in V$ and right-hand side \mathbf{f} , find a state $\mathbf{u}^i \in V := H_D^1(\Omega; \mathbb{R}^2) \times H^1(\Omega)$ that solves for all $i = 1, \dots, M$,

$$(\text{PDE}^{\text{Frac}}) \quad \langle A(\mathbf{u}^i, q), \mathbf{v} \rangle + \langle R(\varphi^i; \gamma), v^\varphi \rangle = \langle \mathbf{f}, v^u \rangle_{\Gamma_N}, \quad \forall \mathbf{v} = (v^u, v^\varphi) \in V.$$

The operators $A(\mathbf{u}^i, q)$ and $R(\varphi^i; \gamma)$ are given by

$$\begin{aligned} \langle A(\mathbf{u}^i, q), \mathbf{v} \rangle &:= \left(((1 - \kappa)(\varphi^i)^2 + \kappa) \sigma_q(u^i), e(v^u) \right) \\ &\quad + \varepsilon G_c (\nabla \varphi^i, \nabla v^\varphi) - \frac{G_c}{\varepsilon} (1 - \varphi^i, v^\varphi) + \eta (\varphi^i - \varphi^{i-1}, v^\varphi) \\ &\quad + \left((1 - \kappa) \varphi^i \sigma_q(u^i) : e(u^i), v^\varphi \right), \\ \langle R(\varphi^i; \gamma), v^\varphi \rangle &:= \left(\gamma \max(0, \varphi^i - \varphi^{i-1}), v^\varphi \right), \end{aligned}$$

for any $(v^u, v^\varphi) \in V$, see, [48, 49]. Here, κ denotes a (bulk) regularization parameter that helps extending the displacements to the entire domain Ω , ε is a phase-field regularization parameter, γ is a penalty parameter for the crack irreversibility condition $\varphi^i \leq \varphi^{i-1}$, η denotes a viscosity parameter, and G_c is the critical energy release rate. For further explanation on phase-field fracture, and the physical interpretation of the involved parameters, we refer to [48, 49, 33].

We investigate an optimal control problem with tracking type cost functional J . The objective is to reach a given desired crack pattern $\varphi_d \in V$ as well as a desired material matrix $q_d \in L^2(\Omega, \mathbb{R}_{sym}^{3 \times 3})$. With constraints given by $(\text{PDE}^{\text{Frac}})$, the optimal control problem reads:

$$\begin{aligned} (\text{P}^{\text{Frac}}) \quad \min_{q, \mathbf{u}} J(q, \mathbf{u}) &:= \sum_{i=1}^M \left(\frac{1}{2} \|\varphi^i - \varphi_d\|^2 + \frac{\alpha}{2} \|q - q_d\|_2^2 + \beta B(q) \right), \\ \text{s.t.} \quad \mathbf{u}^i \text{ and } q &\text{ satisfy } (\text{PDE}^{\text{Frac}}) \text{ for all } i = 1, \dots, M, \end{aligned}$$

where $\alpha > 0$ is a Tikhonov cost parameter, and $\beta > 0$ is a barrier parameter. The barrier function is defined by

$$\begin{aligned} -B(q) &:= \int_{\Omega} \log(q_{1:1,1:1} - q_{L1:1,1:1}) + \log(q_{U1:1,1:1} - q_{1:1,1:1}) \\ &\quad + \log \det(q_{1:2,1:2} - q_{L1:2,1:2}) + \log \det(q_{U1:2,1:2} - q_{1:2,1:2}) \\ &\quad + \log \det(q - q_L) + \log \det(q_U - q) \, dx, \end{aligned}$$

where $q_{1:1,1:1}$, $q_{1:2,1:2}$ are the leading principal submatrices of the control matrix q defined in (6.1). Further, $q_L = q_{\min} I \in \mathbb{R}^{3 \times 3}$, $q_{L1:2,1:2} = q_{\min} I \in \mathbb{R}^{2 \times 2}$ and $q_{L1:1,1:1} = q_{\min} \in \mathbb{R}$, respectively for q_U , etc. Note that the integrand in the barrier is finite if and only if $q - q_L$ and $q_U - q$ are positive definite and thus the control fulfills the constraints specified in Q^{ad} , similar to Problem (P^{MEst}) but without the need to check for values q outside of Q^{ad} .

We conduct two numerical test examples, which are both motivated by the single edge notched tension test [40, 41]. The propagating fracture is caused by a constant

orthogonal force $\mathbf{f}_{|\Gamma_N} = (0, \ 2100)^T$. In both examples, we chose the time interval $[0, 1]$, with 501 and 101 equidistant time points in Example 1, and Example 2, respectively. The spatial mesh has 64×64 square elements.

6.2. Example 1: Material Susceptible to Fracture Propagation. In this first example the initial control is defined as

$$q^{\text{init}} = \begin{pmatrix} 2\mu_1 + \lambda_1 & \lambda_1 & 0 \\ \lambda_1 & 2\mu_1 + \lambda_1 & 0 \\ 0 & 0 & 2\mu_1 \end{pmatrix},$$

which represents the standard elasticity tensor for the Lamé parameters $\lambda_1 = \frac{2\nu\mu_1}{1-2\nu}$ and $\mu_1 = \frac{E}{2(1+\nu)}$, cf., [33]. The desired phase-field continues the initial notch to the left, i.e.,

$$\varphi_d(x, y) := \begin{cases} 0, & x \in [0.25, 0.5] \text{ and } y \in [0.5 - 0.0221, 0.5 + 0.0221] \\ 1, & \text{else.} \end{cases}.$$

The desired control q_d is defined as

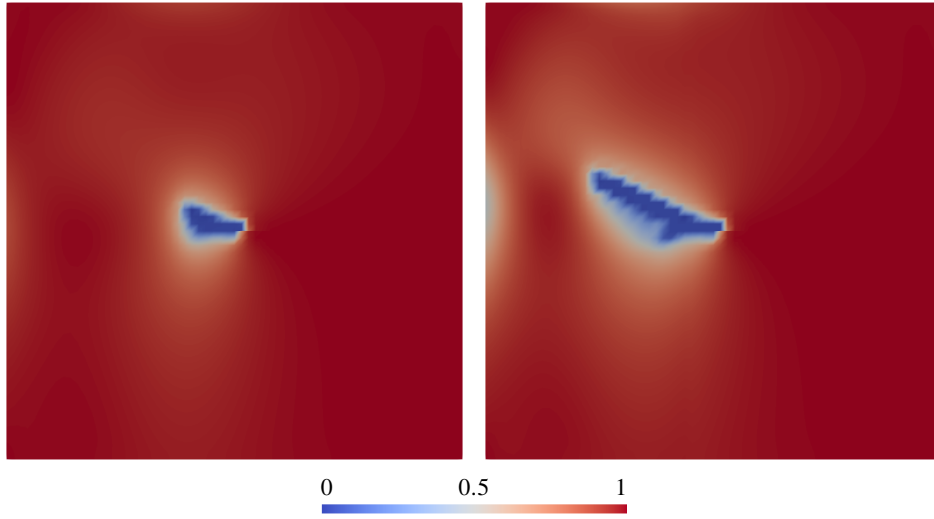
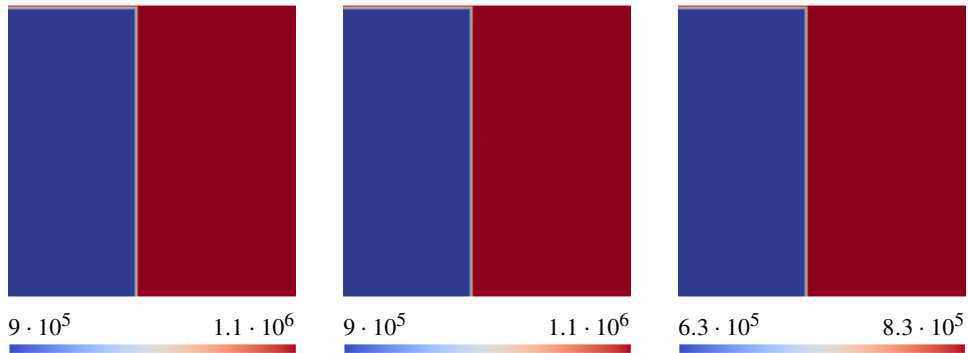
$$q_d = q^{\text{init}} \quad \text{in } [0.45, 1] \times [0, 1],$$

$$q_d = \begin{pmatrix} 2\mu_2 + \lambda_2 & \lambda_2 & 0 \\ \lambda_2 & 2\mu_2 + \lambda_2 & 0 \\ 0 & 0 & 2\mu_2 \end{pmatrix}, \quad \text{in } [0, 0.45] \times [0, 1],$$

which corresponds to the Lamé parameters $\lambda_2 = \lambda_1$ and $\mu_2 = 0.01\mu_1$ in the latter subdomain. The choice of q_d describes a material that is more susceptible to fracture in the left part of the domain. Within the optimization process we seek a control q that is closer to q_d in order to get a different crack pattern, compared to the one that we get from q^{init} . In Table 6.1, we present further numerical parameters that lead to $\text{tr}_\Omega(q^{\text{init}}) := \int_\Omega \text{trace}(q^{\text{init}}) \, dx = 6\mu_1 + 2\lambda_1 = 3.056 \cdot 10^6$. In Figure 6.1, we compare the phase-fields at the final timepoint t_{500} for the initial control q^{init} and the control q^{fin} , where $\text{tr}_\Omega(q^{\text{fin}}) \approx 2.776 \cdot 10^6$, see Figure 6.2 for the corresponding diagonal entries of q^{fin} .

6.3. Example 2: Effects of the Desired Control. In this example, we focus on the effects of adjusting the desired control q^d . On $[0.35, 1] \times [0, 1]$ we set $q_d = q^{\text{init}}$. On $[0, 0.35] \times [0, 1]$ we adjust the Lamé parameters similar to Example 1, but using $\mu_2 = 100\mu_1$. Here we chose a time interval in $[0, 1]$ with 101 equidistant time points. Mesh size, constant orthogonal force $\mathbf{f}_{|\Gamma_N} = (0, \ 2100)^T$, and all other parameters remain the same, see Table 6.1. We want to observe the effects of increasing the Lamé parameter μ_2 on part of the domain to achieve a different crack pattern, as opposed to Example 1 where we observed the effects of decreasing this parameter. In Figure 6.3, we compare the phase fields at final timepoint t_{100} for the initial control q^{init} and the control q^{fin} , where $\text{tr}_\Omega(q^{\text{fin}}) \approx 1.5332 \cdot 10^8$, for the corresponding diagonal entries of q^{fin} we refer to Figure 6.4.

Parameter	Definition	Value
ε	Regularization (crack)	0.0884
κ	Regularization (bulk)	1.0e-10
η	Regularization (viscosity)	1.0e3
γ	Penalty	1.0e5
α	Tikhonov	4.75e-4
G_c	Fracture toughness	1.0
ν	Poisson's	0.2
E	Young's modulus	1.0e6

TABLE 6.1. Parameters for Problem (P^{Frac}).FIGURE 6.1. Crack Pattern of Example 1 after 500 timesteps for initial control (left) and final control (right) on a 64×64 meshFIGURE 6.2. Diagonal entries of final control q^{fin} of Example 1 on a 64×64 mesh

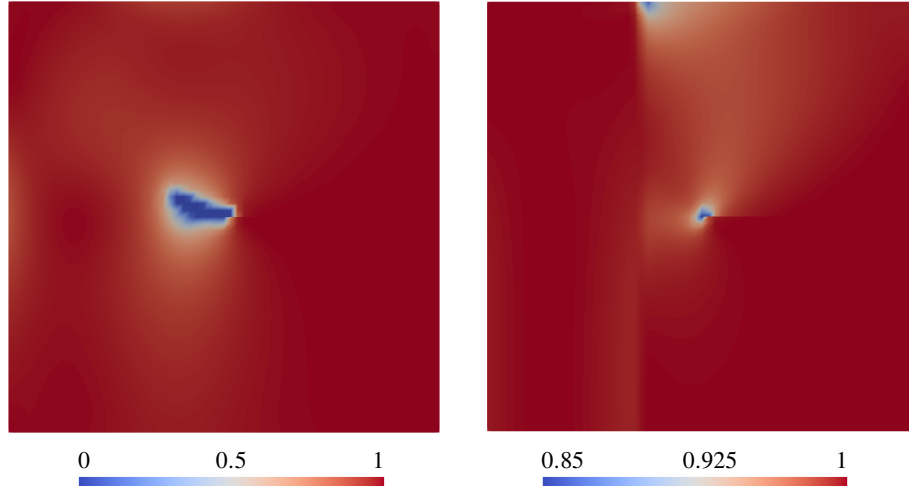


FIGURE 6.3. Crack Pattern of Example 2 after 100 timesteps for initial control (left) and final control (right) on a 64×64 mesh

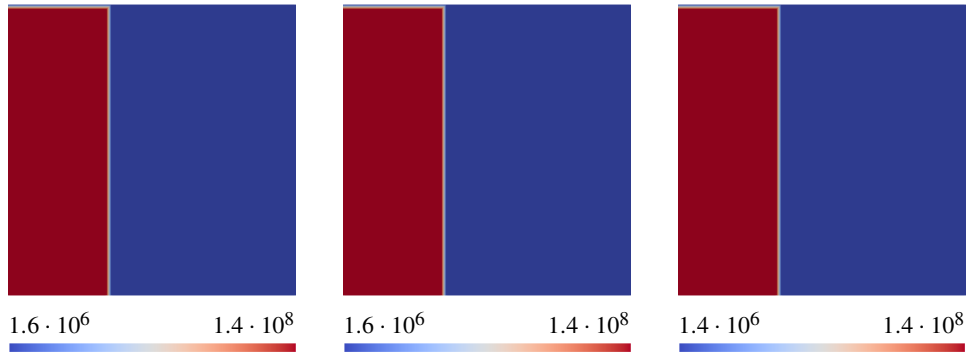


FIGURE 6.4. Diagonal entries of final control q^{fin} of Example 2 on a 64×64 mesh

7. SUMMARY OF FURTHER PROJECT RESULTS AND OUTLOOK

The article summarized some results obtained within the project „Optimizing Fracture Propagation using a Phase-Field Approach” concerning existence and first order optimality conditions for control in the coefficients of a variational inequality. Improved results and detailed proofs for these optimality conditions will be subject of a forthcoming publication. Further, some numerical results for a related coefficient control problem of phase-field fracture are provided. The project analyzed in detail the control of such phase-field fracture problems by the applied forces and the convergence in the regularization limit in [48, 49]. These results were enabled by a fundamental result on higher integrability of solutions to elliptic systems by [24]. The analysis of such phase-field control problems could be extended to second order sufficient conditions [28], and finite element error estimates were obtained in [44] for a linearized fracture control problem. Analysis of local quadratic convergence of the SQP method for regularized fracture with control on a Neumann boundary is subject of a forthcoming publication.

Further results on optimality conditions for control of variational inequalities have been obtained in [47], including state-constraints and control in the right-hand-side, as well as for coefficient control problems in [56]. A posteriori [19] and a priori [30] finite element error analysis for non-smooth control problems of equations with p structure could be carried out within the project. The project was complemented by developments of algorithms for the control of phase-field fracture in [34, 33] and of Lagrange multiplier methods [32] for nonlinear elliptic state-constrained problems.

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REFERENCES

- [1] G. ALLAIRE, *Shape optimization by the homogenization method*, vol. 146 of Applied Mathematical Sciences, Springer-Verlag, New York, 2002.
- [2] A. ALPHONSE, M. HINTERMÜLLER, AND C. N. RAUTENBERG, *Directional differentiability for elliptic quasi-variational inequalities of obstacle type*, Calc. Var. Partial Differential Equations, 58 (2019), p. Article 39.
- [3] M. AMBATI, T. GERASIMOV, AND L. DE LORENZIS, *A review on phase-field models of brittle fracture and a new fast hybrid formulation*, Comput. Mech., 55 (2015), pp. 383–405.
- [4] D. ARNDT, W. BANGERTH, D. DAVYDOV, T. HEISTER, L. HELTAI, M. KRONBICHLER, M. MAIER, J.-P. PELTERET, B. TURCK SIN, AND D. WELLS, *The deal.ii finite element library: Design, features, and insights*, Computers & Mathematics with Applications, (2020).
- [5] D. ARNDT, W. BANGERTH, M. FEDER, M. FEHLING, R. GASSMÖLLER, T. HEISTER, L. HELTAI, M. KRONBICHLER, M. MAIER, P. MUNCH, J.-P. PELTERET, S. STICKO, B. TURCK SIN, AND D. WELLS, *The deal.II library, version 9.4*, Journal of Numerical Mathematics, 30 (2022), pp. 231–246.
- [6] V. BARBU, *Necessary conditions for nonconvex distributed control problems governed by elliptic variational inequalities*, J. Math. Anal. Appl., 80 (1981), pp. 566–597.
- [7] ———, *Optimal control of variational inequalities*, vol. 100 of Research Notes in Mathematics, Pitman (Advanced Publishing Program), Boston, MA, 1984.
- [8] M. BERGOUNIOUX, *Optimal control of an obstacle problem*, Appl. Math. Optim., 36 (1997), pp. 147–172.
- [9] J. F. BONNANS AND A. SHAPIRO, *Perturbation Analysis of Optimization Problems*, Springer Series in Operations Research, Springer, 2000.
- [10] B. BOURDIN AND G. A. FRANCFORT, *Past and present of variational fracture*, SIAM News, 52 (2019).
- [11] B. BOURDIN, G. A. FRANCFORT, AND J.-J. MARIGO, *Numerical experiments in revisited brittle fracture*, J. Mech. Phys. Solids, 48 (2000), pp. 797–826.
- [12] ———, *The variational approach to fracture*, J. Elasticity, 91 (2008), pp. 1–148.
- [13] C. CHRISTOF, *Sensitivity analysis and optimal control of obstacle-type evolution variational inequalities*, SIAM J. Control Optim., 57 (2019), pp. 192–218.
- [14] C. CHRISTOF, J. C. DE LOS REYES, AND C. MEYER, *A nonsmooth trust-region method for locally Lipschitz functions with application to optimization problems constrained by variational inequalities*, SIAM J. Optim., 30 (2020), pp. 2163–2196.
- [15] C. CHRISTOF AND G. WACHSMUTH, *Differential Sensitivity Analysis of Variational Inequalities with Locally Lipschitz Continuous Solution Operators*, Appl. Math. Optim., 81 (2020), pp. 23–62.
- [16] K. DECKELNICK AND M. HINZE, *Identification of matrix parameters in elliptic PDEs*, Control Cybernet., 40 (2011), pp. 957–969.
- [17] K. DECKELNICK AND M. HINZE, *Convergence and error analysis of a numerical method for the identification of matrix parameters in elliptic PDEs*, Inverse Problems, 28 (2012).

- [18] P. DIEHL, R. LIPTON, T. WICK, AND M. TYAGI, *A comparative review of peridynamics and phase-field models for engineering fracture mechanics*, Computational Mechanics, 69 (2022), pp. 1259–1293.
- [19] B. ENDTMAYER, U. LANGER, I. NEITZEL, T. WICK, AND W. WOLLNER, *Multigoal-oriented optimal control problems with nonlinear PDE constraints*, Comput. Math. Appl., 79 (2020), pp. 3001–3026.
- [20] G. FRANCFORT, *Variational fracture: twenty years after*, International Journal of Fracture, (2021), pp. 1–11.
- [21] G. A. FRANCFORT AND J.-J. MARIGO, *Revisiting brittle fracture as an energy minimization problem*, J. Mech. Phys. Solids, 46 (1998), pp. 1319–1342.
- [22] C. GOLL, T. WICK, AND W. WOLLNER, *DOPeLib: Differential equations and optimization environment; A goal oriented software library for solving pdes and optimization problems with pdes*, Archive of Numerical Software, 5 (2017), pp. 1–14.
- [23] K. GRÖGER, *A $W^{1,p}$ -estimate for solutions to mixed boundary value problems for second order elliptic differential equations*, Math. Ann., 283 (1989), pp. 679–687.
- [24] R. HALLER-DINTELMANN, H. MEINLSCHMIDT, AND W. WOLLNER, *Higher regularity for solutions to elliptic systems in divergence form subject to mixed boundary conditions*, Ann. Mat. Pura Appl., 198 (2019), pp. 1227–1241.
- [25] A. HARAUX, *How to differentiate the projection on a convex set in Hilbert space. Some applications to variational inequalities*, J. Math. Soc. Japan, 29 (1977), pp. 615–631.
- [26] F. HARDER AND G. WACHSMUTH, *Comparison of optimality systems for the optimal control of the obstacle problem*, GAMM-Mitt., 40 (2018), pp. 312–338.
- [27] J. HASLINGER, M. KOČVARA, G. LEUGERING, AND M. STINGL, *Multidisciplinary free material optimization*, SIAM J. Appl. Math., 70 (2010), pp. 2709–2728.
- [28] A. HEHL AND I. NEITZEL, *Second order optimality conditions for an optimal control problem governed by a regularized phase-field fracture propagation model*, Optimization, 72 (2022), pp. 1665–1689.
- [29] L. HERTLEIN AND M. ULBRICH, *An inexact bundle algorithm for nonconvex nonsmooth minimization in Hilbert space*, SIAM J. Control Optim., 57 (2019), pp. 3137–3165.
- [30] A. HIRN AND W. WOLLNER, *An optimal control problem for equations with p -structure and its finite element discretization*, in Optimization and Control for Partial Differential Equations, R. Herzog, M. Heinkenschloss, D. Kalise, G. Stadler, and E. Trélat, eds., vol. 29 of Radon Series on Computational and Applied Mathematics, De Gruyter, 2022, ch. 7, pp. 137–166.
- [31] K. ITO AND K. KUNISCH, *Optimal control of elliptic variational inequalities*, Appl. Math. Optim., 41 (2000), pp. 343–364.
- [32] V. KARL, I. NEITZEL, AND D. WACHSMUTH, *A Lagrange multiplier method for semilinear elliptic state constrained optimal control problems*, Comput. Optim. Appl., 77 (2020), pp. 831–869.
- [33] D. KHIMIN, M. STEINBACH, AND T. WICK, *Space-time formulation, discretization, and computational performance studies for phase-field fracture optimal control problems*, Journal of Computational Physics, 470 (2022), p. 111554.
- [34] D. KHIMIN, M. C. STEINBACH, AND T. WICK, *Optimal Control for Phase-Field Fracture: Algorithmic Concepts and Computations*, Springer International Publishing, Cham, 2022, pp. 247–255.
- [35] D. KINDERLEHRER AND G. STAMPACCHIA, *An Introduction to Variational Inequalities and their Applications*, vol. 31 of Classics in applied mathematics, Society for Industrial and Applied Mathematics, Philadelphia, 1. ed., 2000.
- [36] C. KUHN AND R. MÜLLER, *A continuum phase-field model for fracture*, Engineering Fracture Mechanics, 77 (2010), pp. 3625–3634.
- [37] K. KUNISCH AND D. WACHSMUTH, *Path-following for optimal control of stationary variational inequalities*, Comput. Optim. Appl., 51 (2012), pp. 1345–1373.
- [38] ———, *Sufficient optimality conditions and semi-smooth Newton methods for optimal control of stationary variational inequalities*, ESAIM Control Optim. Calc. Var., 18 (2012), pp. 520–547.
- [39] C. MEYER, A. RADEMACHER, AND W. WOLLNER, *Adaptive optimal control of the obstacle problem*, SIAM J. Sci. Comput., 37 (2015), pp. A918–A945.
- [40] C. MIEHE, M. HOFACKER, AND F. WELSCHINGER, *A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits*, Comput. Meth. Appl. Mech. Engrg., 199 (2010), pp. 2765–2778.

- [41] C. MIEHE, F. WELSCHINGER, AND M. HOFACKER, *Thermodynamically consistent phase-field models of fracture: variational principles and multi-field fe implementations*, Internat. J. Numer. Methods Engrg., 83 (2010), pp. 1273–1311.
- [42] F. MIGNOT, *Contrôle dans les inéquations variationnelles elliptiques*, J. Functional Analysis, 22 (1976), pp. 130–185.
- [43] F. MIGNOT AND J.-P. PUEL, *Optimal control in some variational inequalities*, SIAM J. Control Optim., 22 (1984), pp. 466–476.
- [44] M. MOHAMMADI AND W. WOLLNER, *A priori error estimates for a linearized fracture control problem*, Optim. Eng., 22 (2021), pp. 2127–2149.
- [45] F. MURAT AND L. TARTAR, *Calcul des variations et homogénéisation*, in Homogenization methods: theory and applications in physics (Bréau-sans-Nappe, 1983), vol. 57 of Collect. Dir. Études Rech. Élec. France, Eyrolles, Paris, 1985, pp. 319–369.
- [46] ———, *H-convergence*, in Topics in the mathematical modelling of composite materials, vol. 31 of Progr. Nonlinear Differential Equations Appl., Birkhäuser Boston, 1997, pp. 21–43.
- [47] I. NEITZEL AND G. WACHSMUTH, *First-order conditions for the optimal control of the obstacle problem with state constraints*, Pure Appl. Funct. Anal., 7 (2022), pp. 1881–1911.
- [48] I. NEITZEL, T. WICK, AND W. WOLLNER, *An optimal control problem governed by a regularized phase-field fracture propagation model*, SIAM J Control Optim., 55 (2017), pp. 2271–2288.
- [49] I. NEITZEL, T. WICK, AND W. WOLLNER, *An optimal control problem governed by a regularized phase-field fracture propagation model. part II: The regularization limit*, SIAM J. Control Optim., 57 (2019), pp. 1672–1690.
- [50] D. PREISS, *Differentiability of Lipschitz functions on Banach spaces*, J. Funct. Anal., 91 (1990), pp. 312–345.
- [51] A.-T. RAULS AND S. ULBRICH, *Computation of a Bouligand generalized derivative for the solution operator of the obstacle problem*, SIAM J. Control Optim., 57 (2019), pp. 3223–3248.
- [52] J. F. RODRIGUES, *Obstacle Problems in Mathematical Physics*, vol. 134 of Mathematics Studies, North-Holland, 1987.
- [53] A. SCHIELA AND D. WACHSMUTH, *Convergence analysis of smoothing methods for optimal control of stationary variational inequalities*, ESAIM Math. Model. Numer. Anal., 47 (2013), pp. 771–787.
- [54] J. SCHRÖDER, T. WICK, S. REESE, P. WRIGGERS, R. MÜLLER, S. KOLLMANNNSBERGER, M. KÄSTNER, A. SCHWARZ, M. IGLBÜSCHER, N. VIEBAHN, H. R. BAYAT, S. WULFINGHOFF, K. MANG, E. RANK, T. BOG, D. D’ANGELLA, M. ELHADDAD, P. HENNIG, A. DÜSTER, W. GARHUOM, S. HUBRICH, M. WALLOTH, W. WOLLNER, C. KUHN, AND T. HEISTER, *A selection of benchmark problems in solid mechanics and applied mathematics*, Arch. Computat. Methods Eng., 28 (2021), pp. 713–751.
- [55] A. SHAPIRO, *On concepts of directional differentiability*, J. Optim. Theory Appl., 66 (1990), pp. 477–487.
- [56] N. SIMON AND W. WOLLNER, *First order limiting optimality conditions in the coefficient control of an obstacle problem*, in PAMM, vol. 22, 2023.
- [57] S. SPAGNOLO, *Convergence in energy for elliptic operators*, in Numerical solution of partial differential equations, III (Proc. Third Sympos. (SYNSPADE), Univ. Maryland, College Park, Md., 1975), Academic Press, 1976, pp. 469–498.
- [58] L. TARTAR, *Estimations of homogenized coefficients*, in Topics in the mathematical modelling of composite materials, vol. 31 of Progr. Nonlinear Differential Equations Appl., Birkhäuser Boston, Boston, MA, 1997, pp. 9–20.
- [59] G. WACHSMUTH, *Strong stationarity for optimal control of the obstacle problem with control constraints*, SIAM J. Optim., 24 (2014), pp. 1914–1932.
- [60] ———, *Towards M-stationarity for optimal control of the obstacle problem with control constraints*, SIAM J. Control Optim., 54 (2016), pp. 964–986.
- [61] T. WICK, *Multiphysics Phase-Field Fracture: Modeling, Adaptive Discretizations, and Solvers*, De Gruyter, Berlin, Boston, 2020.

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