A REGULARIZATION METHOD FOR THE NUMERICAL SOLUTION OF ELLIPTIC BOUNDARY CONTROL PROBLEMS WITH POINTWISE STATE CONSTRAINTS

F. TRÖLTZSCH* AND I. YOUSEPT*

Abstract. A Lavrentiev type regularization technique for solving elliptic boundary control problems with pointwise state constraints is considered. The main concept behind this regularization is to look for controls in the range of the adjoint control-to-state mapping. After investigating the analysis of the method, a semismooth Newton method based on the optimality conditions is presented. The theoretical results are confirmed by numerical tests. Moreover, they are validated by comparing the regularization technique with standard numerical codes based on the discretize-then-optimize concept.

Key words. Boundary control, state constraints, Lavrentiev type regularization, semismooth Newton method, optimize-then-discretize, nested iteration.

AMS subject classifications. 49J20, 49M05, 65K10.

1. Introduction. In this paper, we suggest a regularization method for solving a class of state-constrained elliptic boundary control problems. We consider the following fairly standard problem:

$$(P) \qquad \text{minimize } J(u,y) := \frac{1}{2}\int_\Omega (y(x) - y_d(x))^2 \, dx + \frac{\alpha}{2}\int_\Gamma u^2(x)\, ds$$

subject to the elliptic boundary value problem

$$(1.1) \qquad \begin{array}{rcll} Ay &=& 0 & \text{in } \Omega \\ \partial_n y &=& u & \text{on } \Gamma \end{array}$$

and to the pointwise state constraints

$$(1.2) \qquad y_a(x) \le y(x) \le y_b(x) \quad \text{for almost all } x \text{ in } \Omega.$$

Here, A is a linear uniformly elliptic differential operator and $\Omega \subset \mathbb{R}^N$, $N \ge 2$, is a bounded domain with sufficiently regular boundary Γ. The functions y_d, y_a, y_b and the cost parameter $\alpha > 0$ are assumed to be given data. We do not require that the state constraints are satisfied for all $x \in \bar{\Omega}$, since this will be meaningful only for two-dimensional domains. If the admissible set of (P) is not empty, then, for any dimension N, the problem (P) admits a unique optimal solution.

If $N = 2$, necessary optimality conditions for this problem follow from Casas [4] or from the Pontryagin principle presented in Casas [5], or Alibert and Raymond [1] for more general problems with semilinear equations (cf. also our remarks on the dimension N below).

When solving this problem numerically, one of the main difficulties is the lack of regularity of the Lagrange multipliers associated with the state constraints. Moreover, there is another, somewhat hidden obstacle in the analysis: To show the existence of these multipliers – i.e. to gain Karush-Kuhn-Tucker type optimality conditions – the constraints (1.2) should be considered in $\mathcal{C}(\bar{\Omega})$. This, however, restricts the

*Institut für Mathematik, Technische Universität Berlin, D-10623 Berlin, Str. des 17. Juni 136, Germany (troeltz@math.tu-berlin.de, yousept@math.tu-berlin.de). The authors acknowledge support through DFG Research Center "Mathematics for Key Technologies" (FZT 86) in Berlin.

theory to two-dimensional domains Ω. In this case, the mapping $u \mapsto y$ defined by (1.1) is continuous from $L^2(\Gamma)$ to $\mathcal{C}(\bar{\Omega})$. Another way would consist of restricting the constraints (1.2) to a compact subset $\Omega' \subset \Omega$.

This obstacle is overcome after regularizing problem (P). Then necessary optimality conditions can be stated for the regularized problem for any dimension $N \geq 2$. To show, however, convergence for vanishing regularization parameter, the restriction to $N = 2$ is more or less needed, again.

It is well known that the numerical treatment of state-constrained problems is a quite difficult issue. On the one hand, the measure type form of Lagrange multipliers complicates the numerical treatment of the problems. On the other hand, in the analysis one is faced with some ill-conditioned equations when dealing with state-constrained problems. This is mostly due to the compactness of the mapping $u \mapsto y$. This is known for distributed optimal control problems and it turns out to be even harder in the case of boundary control.

In the last years, two different regularization concepts were proposed to overcome the difficulties mentioned previously. First, Ito and Kunisch [10] suggested a Moreau-Yosida type regularization approach, which removes the pointwise state inequality constraints by adding a penalty term to the objective functional. Hereafter, the penalized problems are solved in an efficient way. We also refer to [2], [3], and [11].

Later, Meyer et al. [14] came up with a Lavrentiev type regularization to the pointwise state inequality constraints, see also the case of pure state constraints in [15]. In contrast to the first method, it preserves, in some sense, the structure of the state-constrained problem. Let us briefly introduce this regularization technique and compare it with the main issue of our paper. Suppose that the state equation is given by

$$\begin{array}{rcll} Ay & = & u & \text{in } \Omega \\ \partial_n y & = & 0 & \text{on } \Gamma \end{array}$$

with *distributed* control u. Then the Lavrentiev type regularization converts the state constraints (1.2) into the mixed control-state constraints

$$y_a \leq y + \lambda u \leq y_b \quad \text{a.e. in } \Omega \tag{1.3}$$

with a small parameter $\lambda > 0$. This technique is not applicable in the case of boundary control, since the control is defined only on Γ, while (1.3) must be considered on Ω. The domains of u and y do not fit together.

Our main idea to overcome this difficulty is as follows: Let $S : L^2(\Gamma) \to L^2(\Omega)$ denote the control-to-state mapping defined by (1.1). We look for controls in the range of the adjoint operator $S^\star$, i.e., we use the ansatz

$$u = S^\star v$$

with a new control v defined in Ω. Then, the pointwise state constraints (1.2) admit the form $y_a \leq SS^\star v \leq y_b$ and, substituting a new "control function" $w \in L^2(\Omega)$ by $w = SS^\star v$, we obtain the "control constraints"

$$y_a \leq w \leq y_b.$$

However, this is too formal, since $SS^\star$ is compact in $L^2(\Omega)$, and hence the equation $SS^\star v = w$ is ill-posed, if $w \in L^2(\Omega)$ is given. To obtain a well-posed equation, we apply the Lavrentiev type regularization, cf. [12], i.e. we write

$$\lambda v + SS^\star v = w.$$

Finally, we arrive at the constraints

$$y_a \le \lambda v + SS^\star v \le y_b \quad \text{a.e. in } \Omega.$$

There are two reasons for the ansatz $u = S^\star v$. We obtain from the necessary optimality condition (2.3) that the optimal control $\bar{u}$ is in the range of the adjoint control-to-state mapping $G^\star : \mathcal{C}(\bar{\Omega})^\star \to L^2(\Gamma)$ (notice that $p = G^\star(\bar{y} - y_d + \mu_b - \mu_a)$). By restricting the domain of $G^\star$ to $L^2(\Omega)$, we avoid measures and arrive at $S^\star$. Moreover, we obtain the representation $y = SS^\star v$ with a positive semidefinite and self-adjoint operator $SS^\star$, which is useful for computations.

We investigate the analysis of this idea as well as its numerical performance. The method slightly increases the number of unknowns and doubles the number of equations. This is certainly some drawback. However, the numerical results are encouraging. In some cases, the results were even better then those obtained by the discretize-then-optimize concept that was used to compare our method. Our main aim was to find an extension of the Lavrentiev type regularization concept to the case of boundary controls that guarantees the existence of regular Lagrange multipliers. Moreover, it should generate a problem that is equivalent to a control-constrained one. Then, we have access to known results on numerical approximations of control-constrained problems such as error estimates or mesh-independence principles.

To give the reader a better orientation on the possible choices for the dimension N, we mention already here that $N = 2$ is only needed to show the convergence of optimal solutions for vanishing regularization parameter. All other results on the regularized problems hold true for arbitrary dimension. If $N = 2$ is needed, we explicitely state this in the associated theorems.

The paper is organized as follows: After introducing the general assumptions as well as our notation in Section 2, we analyze different aspects of our regularization in Section 3. We discuss the optimality conditions for the regularized version of (P) and based on them, we present a semismooth Newton algorithm in Section 4. Finally, in Section 5, we provide a numerical report including a validation of our theoretical results and a comparison of our technique with the application of the discretize-then-optimize concept.

2. General assumptions and notation. Throughout this paper, we consider a bounded domain $\Omega \subset \mathbb{R}^N$, $N \ge 2$, with a $\mathcal{C}^{0,1}$-boundary Γ. The lower and upper bounds $y_a, y_b \in \mathcal{C}(\bar{\Omega})$ satisfy $y_a(x) < y_b(x)$ for all $x \in \bar{\Omega}$. Furthermore, the desired state y_d is given in $L^2(\Omega)$. If V is a linear normed function space, then we use the notation $\|\cdot\|_V$ for the standard norm used in V. By A, we denote the second-order elliptic partial differential operator defined by

$$Ay(x) = -\sum_{i,j=1}^{N} D_i(a_{ij}(x) D_j y(x)) + c_0(x) y(x),$$

where the coefficient functions $a_{ij} \in C^{0,1}(\bar{\Omega})$ satisfy the ellipticity condition

$$\sum_{i,j=1}^{n} a_{ij}(x)\xi_i\xi_j \ge \theta \|\xi\|^2_{L^2(\Omega)} \quad \forall\ (\xi, x) \in \mathbb{R}^n \times \bar{\Omega}$$

for some constant $\theta > 0$. By $A^\star$, the associated formally adjoint operator is denoted. We assume that $c_0 \in L^\infty(\Omega)$ is non-negative with $\|c_0\|_{L^\infty(\Omega)} \ne 0$. By G, we denote the solution operator $G : L^2(\Gamma) \to H^1(\Omega)$ that assigns to each $u \in L^2(\Gamma)$ the weak solution $y = y(u) \in H^1(\Omega)$ of the elliptic equation

$$\begin{aligned} Ay &= 0 \text{ in } \Omega \\ \partial_n y &= u \quad \text{on } \Gamma, \end{aligned}$$

in which $\partial_n y$ denotes the co-normal derivative of y (often denoted by ∂n_A). For later use, we set $S = i_0 G$, where i_0 is the compact embedding operator from $H^1(\Omega)$ to $L^2(\Omega)$. Now, our problem can be expressed as follows:

$$(P) \qquad \begin{cases} \text{minimize } f(u) := \frac{1}{2}\|Su - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Gamma)} \\ \text{over } u \in L^2(\Gamma) \\ \text{subject to } y_a \le Gu \le y_b \quad \text{a.e. in } \Omega. \end{cases}$$

We still use G instead of S in the constraints, since we need higher regularity of y in Theorem 2.1.

Remark 2.1. Consider the following more general problem

$$(2.1) \qquad \begin{cases} \text{minimize } \frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u - u_d\|^2_{L^2(\Gamma)} \\ \text{over } (u, y) \in L^2(\Omega) \times H^1(\Omega) \\ \text{subject to } Ay = e \quad \text{in } \Omega, \ \partial_n y = u \quad \text{on } \Gamma \\ \qquad\qquad y_a \le y \le y_b \quad \text{a.e. in } \Omega \end{cases}$$

with a fixed function $e \in L^2(\Omega)$ and a fixed shift control $u_d \in L^2(\Gamma)$. By substituting $\mathbf{u} = u - u_d$ and splitting the state into two components $y(e, u) = y_e + Gu$, where y_e is solution of

$$\begin{aligned} Ay &= e \quad \text{in } \Omega \\ \partial_n y &= 0 \quad \text{on } \Gamma, \end{aligned}$$

the problem (2.1) is equivalent to:

$$(2.2) \qquad \begin{cases} \text{minimize } \frac{1}{2}\|S\mathbf{u} - y_\Omega\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|\mathbf{u}\|^2_{L^2(\Gamma)} \\ \text{over } \mathbf{u} \in L^2(\Gamma) \\ \text{subject to } y'_a \le G\mathbf{u} \le y'_b \quad \text{a.e. in } \Omega, \end{cases}$$

with $y_\Omega = y_d - y_e - Su_d$, $y'_a = y_a - Gu_d - y_e$ and $y'_b = y_b - Gu_d - y_e$. Therefore, we are justified to concentrate on the simpler problem (P).

2.1. Standard results. It is well known that the operator $G : L^2(\Gamma) \to H^1(\Omega)$ is continuous. In the case of a two-dimensional domain, $N = 2$, the mapping $G : u \to y$ is even continuous from $L^2(\Gamma)$ into $H^1(\Omega) \cap \mathcal{C}(\bar{\Omega})$, see [5]. One can show that, independently of the dimension $N \ge 2$, the problem (P) admits a unique solution $\bar{u} \in L^2(\Gamma)$ provided that the admissible set $\{u \in L^2(\Gamma) \mid y_a \le G(u) \le y_b \text{ a.e. in } \Omega\}$ is not empty. In the rest of the paper, we assume hence that the admissible set for (P) is not empty and denote the optimal solution to (P) by $\bar{u}$ with the associated state $\bar{y} = G\bar{u}$. In the following, we present the optimality system for (P) in a appropriate sense defined in [5].

Theorem 2.1 (First-order optimality conditions for (P)). *Let $N = 2$ and assume that the following Slater condition is satisfied: There exists a function $u_0 \in L^2(\Gamma)$ (a so-called Slater point) such that*

$$y_a(x) < G(u_0)(x) < y_b(x) \ \forall \ x \in \bar{\Omega}.$$

Then, $\bar{u}$ is optimal for (P) if and only if there exists an adjoint state $p \in W^{1,s}(\Omega)$ for all $1 \leq s < \frac{N}{N-1}$ and Lagrange multipliers $\mu_a, \mu_b \in \mathcal{C}^*(\bar{\Omega})$ such that

$$\begin{array}{rclll rclll} A\bar{y} &=& 0 & \textit{in} & \Omega & A^\star p &=& \bar{y} - y_d + (\mu_b - \mu_a)_{|\Omega} & \textit{in} & \Omega \\ \partial_n \bar{y} &=& \bar{u} & \textit{on} & \Gamma, & \partial_n p &=& (\mu_b - \mu_a)_{|\Gamma} & \textit{on} & \Gamma, \end{array}$$

$$p + \alpha \bar{u} = 0 \quad \textit{on } \Gamma, \tag{2.3}$$

$$< \mu_a, \bar{y} - y_a >_{\mathcal{C}^\star,\mathcal{C}} = < \mu_b, \bar{y} - y_b >_{\mathcal{C}^\star,\mathcal{C}} = 0,$$
$$< \mu_b, w >_{\mathcal{C}^\star,\mathcal{C}} \geq 0, \ < \mu_a, w >_{\mathcal{C}^\star,\mathcal{C}} \geq 0 \quad \forall w \in \mathcal{C}(\bar{\Omega}).$$

Notice that $< \cdot, \cdot >_{\mathcal{C}^\star,\mathcal{C}}$ stands for the duality pairing between $\mathcal{C}^\star(\bar{\Omega})$ and $\mathcal{C}(\bar{\Omega})$.

3. Regularization. As pointed out in the introduction, we look for controls u in the range of the adjoint operator $S^\star$, i.e., we substitute $u = S^\star v$ in (P). This idea leads us to an associated problem with a new control v defined on the domain Ω. In this section, we study this problem with different regularization terms, to motivate the final form of our regularized problem.

We start by investigating the operator $S^\star$. By definition, $S^\star$ is defined from $L^2(\Omega)$ to $L^2(\Gamma)$. It is represented by $S^\star v = w_{|\Gamma}$, where $w = w(v) \in H^1(\Omega)$ is defined as the solution of

$$\left\{ \begin{array}{rcll} A^\star w &=& v & \text{in} \quad \Omega \\ \partial_n w &=& 0 & \text{on} \quad \Gamma. \end{array} \right. \tag{3.1}$$

Hence, for each $v \in L^2(\Omega)$, $w_{|\Gamma}$ possesses at least the regularity $w_{|\Gamma} \in H^{\frac{1}{2}}(\Gamma)$. In convex domains Ω, we obtain even $w_{|\Gamma} \in H^{\frac{3}{2}}(\Gamma)$. This higher regularity raises some difficulties, since it implies that $S^\star : L^2(\Omega) \to L^2(\Gamma)$ is not surjective. However, we have the following result:

LEMMA 3.1. *$S^\star(L^2(\Omega))$ is dense in $L^2(\Gamma)$.*

Proof. Assume the contrary: Then there exists a function $d \in L^2(\Gamma)$ with $d \neq 0$ such that

$$(d, S^\star v)_\Gamma = 0 \quad \forall\, v \in L^2(\Omega).$$

This implies that $(Sd, v)_\Omega = 0$ for all $v \in L^2(\Omega)$ and hence $y(d) = Sd = 0$. Since $y = y(d)$ satisfies

$$\left\{ \begin{array}{rcll} Ay &=& 0 & \text{in} \quad \Omega \\ \partial_n y &=& d & \text{on} \quad \Gamma, \end{array} \right.$$

one finds then $d = 0$, which contradicts our assumption. □

This result shows that $\bar{u}$ can be approximated by functions $S^\star v$. Compared with the regularity of $\bar{u}$, the images of $S^\star$ are too smooth so that $\bar{u}$ cannot in general be represented by $\bar{u} = S^\star v$ with $v \in L^2(\Omega)$. We would need measures v for this representation.

3.1. Auxiliary problem. Substituting $u = S^\star v$ in (P), we obtain the following problem

$$(P_{aux}) \qquad \left\{ \begin{array}{l} \text{minimize } \tilde{f}(v) := f(S^\star v) = \frac{1}{2}\|SS^\star v - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|S^\star v\|^2_{L^2(\Gamma)} \\ \text{over } v \in L^2(\Omega) \\ \text{subject to } y_a \leq GS^\star v \leq y_b \quad \text{a.e. in } \Omega. \end{array} \right.$$

As noticed previously, the operator $S^\star$ is not surjective and consequently the auxiliary problem (P_{aux}) is not necessarily solvable. However, under some assumptions of approximability, we are able to show that (P) and (P_{aux}) have the same infimal value.

DEFINITION 3.1 (Approximability and Slater condition). *We say that $\bar u$ satisfies the approximability condition, if there exists a sequence $\{a_n\}_{n=1}^\infty$ in $L^2(\Omega)$ such that*

$$\lim_{n\to\infty} S^\star a_n = \bar u \quad \text{and} \quad y_a \le GS^\star a_n \le y_b, \tag{3.2}$$

for all n.

If there exists a function $v_0 \in L^\infty(\Omega)$ satisfying the condition

$$y_a + \delta \le GS^\star v_0 \le y_b - \delta \tag{3.3}$$

with some constant $\delta > 0$, then we say that the Slater condition is satisfied.

LEMMA 3.2. *For $N = 2$, the approximability condition is satisfied if the Slater condition (3.3) is fulfilled.*

Proof. Since $S^\star(L^2(\Omega))$ is dense in $L^2(\Gamma)$, there exists a sequence $\{\tilde v_n\}_{n=1}^\infty$ in $L^2(\Omega)$ such that

$$\bar u = \lim_{n\to\infty} S^\star \tilde v_n = \lim_{n\to\infty} u_n \tag{3.4}$$

holds in $L^2(\Gamma)$, where $u_n := S^\star \tilde v_n$. Moreover, by the assumption $N = 2$, G is continuous from $L^2(\Gamma)$ in $H^1(\Omega)\cap \mathcal{C}(\bar\Omega)$. Thus, Gu_n converges uniformly to $G\bar u$. For this reason, we have

$$Gu_n = G\bar u + d_n \quad \forall n, \tag{3.5}$$

where $\{d_n\}_{n=1}^\infty$ is a sequence in $\mathcal{C}(\bar\Omega)$ converging to zero. Define now $a_n = (1 - t_n)\tilde v_n + t_n v_0$, where $\{t_n\}_{n=1}^\infty$ is a sequence of positive numbers tending to zero, given by $t_n = \frac{\|d_n\|_{\mathcal{C}(\bar\Omega)}}{\delta}$. Obviously, due to (3.4), the sequence $\{S^\star a_n\}_{n=1}^\infty$ converges strongly to $\bar u$ in $L^2(\Omega)$. By (3.5) and the *Slater condition* (3.3), we find further for all sufficiently large n:

$$\begin{aligned} GS^\star a_n &= (1-t_n)G\bar u + (1-t_n)d_n + t_n GS^\star v_0 \\ &\le (1-t_n)y_b + (1-t_n)d_n + t_n y_b - t_n\delta \\ &\le y_b + (1-t_n)\|d_n\|_{\mathcal{C}(\bar\Omega)} - t_n\delta \\ &= y_b - t_n\|d_n\|_{\mathcal{C}(\bar\Omega)} \le y_b. \end{aligned}$$

In a similar way, we infer $y_a \le GS^\star a_n$ for all sufficiently large n and hence $\{a_n\}_{n=1}^\infty$ satisfies the property (3.2). □

THEOREM 3.1. *Assume that the optimal solution $\bar u$ satisfies the approximability condition. Then (P) and (P_{aux}) have the same infimal value. Furthermore, there exists an infimal sequence $\{v_n\}_{n=1}^\infty$ for (P_{aux}) such that $\{S^\star v_n\}_{n=1}^\infty$ converges strongly to $\bar u$ in $L^2(\Gamma)$.*

Proof. By the nonnegativity of $\tilde f$, the infimal values of (P_{aux}) and (P), denoted by j_{aux} and j, respectively, exist in $\mathbb{R}_0^+$. Furthermore, since the range of $S^\star$ is dense in $L^2(\Gamma)$, we have obviously $j \le j_{aux}$. On the other hand, by the approximability assumption, there exists a sequence $\{a_n\}_{n=1}^\infty$ in $L^2(\Omega)$ such that $S^\star a_n$ is feasible for (P) for sufficiently large n and $\lim_{n\to\infty} S^\star a_n = \bar u$. Thus, by the continuity of S, we have

$$\lim_{n\to\infty}\Big(\frac12\|SS^\star a_n - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|S^\star a_n\|^2_{L^2(\Gamma)}\Big) = \frac12\|S\bar u - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|\bar u\|^2_{L^2(\Gamma)} = j$$

and consequently it holds that $j_{aux} \leq j$.

Let now $\{v_n\}_{n=1}^{\infty}$ be an infimal sequence for (P_{aux}). Thanks to the Tikhonov regularization parameter $\alpha > 0$, the sequence $\{S^\star v_n\}_{n=1}^{\infty}$ is uniformly bounded in $L^2(\Omega)$. Thus, there exists a subsequence, denoted w.l.o.g. by $\{S^\star v_n\}_{n=1}^{\infty}$, converging weakly to $\tilde{u} \in L^2(\Gamma)$. Due to the compactness of the embedding of $H^1(\Omega)$ in $L^2(\Omega)$, $GS^\star v_n$ converges strongly to $G\tilde{u}$ in $L^2(\Omega)$ as $n \to \infty$ and consequently $\tilde{u}$ is feasible for (P), i.e.

$$y_a \leq G\tilde{u} \leq y_b \text{ a.e. in } \Omega.$$

The optimality of $\tilde{u}$ for (P) follows now from the semicontinuity of f:

$$f(\tilde{u}) \leq \lim_{n\to\infty} \inf f(S^\star v_n) = j_{aux} = j.$$

Therefore, by the uniqueness of the optimal solution, we find $\tilde{u} = \bar{u}$. Finally, due to the weak convergence, the strong convergence of $S^\star v_n$ to $\bar{u}$ can be directly derived from the convergence of $S^\star v_n$ in norm. □

In the preceding proof, we did not show the convergence of $\{v_n\}_{n=1}^{\infty}$. As yet, we are only able to show the strong convergence of $S^\star v_n$ to $\bar{u}$ for the auxiliary problem (P_{aux}). Still, this is not satisfactory due to the possible unsolvability of (P_{aux}). To overcome this difficulty, we next study different kinds of regularization and their specific properties. Finally, we end up with our Lavrentiev-regularized problem. We start with the following problem:

$$(P^\varepsilon) \qquad \begin{cases} \text{minimize } \tilde{g}(v) := \frac{1}{2}\|SS^\star v - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|S^\star v\|^2_{L^2(\Gamma)} + \frac{\varepsilon}{2}\|v\|^2_{L^2(\Omega)} \\ \text{over } v \in L^2(\Omega) \\ \text{subject to } y_a \leq GS^\star v \leq y_b \quad \text{a.e. in } \Omega. \end{cases}$$

Lemma 3.3. *Assume that the admissible set $\tilde{V}_{ad} = \{v \in L^2(\Omega) \mid y_a \leq GS^\star v \leq y_b$ a.e. in $\Omega\}$ is not empty. Then, for every $\varepsilon > 0$, (P^ε) admits a unique solution.*

Proof. The infimal value of (P^ε) exists in $\mathbb{R}_0^+$, since the objective functional $\tilde{g}$ is nonnegative. Let now $\{v_n\}$ be an infimal sequence for (P^ε). Due to the regularization parameter $\frac{\varepsilon}{2}$ in $\tilde{g}$, v_n is uniformly bounded in $L^2(\Omega)$. Consequently, there exists a subsequence of v_n converging weakly to $\tilde{v} \in L^2(\Omega)$. Owing to the continuity of $GS^\star$, the weak limit $\tilde{v}$ belongs obviously to $\tilde{V}_{ad}$. Thus, by the lower semicontinuity of $\tilde{g}$, $\tilde{v}$ is optimal for (P^ε) □

3.2. Lavrentiev type regularization. As mentioned previously, our aim is to propose a Lavrentiev type regularization applied to the boundary control problem. We regularize now (P) in the following way:

$$(P_\lambda) \qquad \begin{cases} \text{minimize } \tilde{g}(v) := \frac{1}{2}\|SS^\star v - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|S^\star v\|^2_{L^2(\Gamma)} + \frac{\varepsilon}{2}\|v\|^2_{L^2(\Omega)} \\ \text{over } v \in L^2(\Omega) \\ \text{subject to } y_a \leq \lambda v + GS^\star v \leq y_b \quad \text{a.e. in } \Omega, \end{cases}$$

with some regularization parameters $\lambda > 0$ and $\varepsilon(\lambda) \geq 0$. We mention here some reasons for regularizing the problem in that way: Without any restriction on the dimension N and without the assumption on approximability and Slater conditions, we always have the solvability of (P_λ) and additionally, we are able to show that the associated Lagrange multipliers exist and belong to $L^2(\Omega)$. However, for the convergence of the regularized solution to the solution of (P) in the case of vanishing regularization parameters, one has to restrict again the theory to the two-dimensional case, $N = 2$. We require this since for $N = 2$, the operator G is continuous from $L^2(\Omega)$ to $\mathcal{C}(\bar{\Omega}) \cap H^1(\Omega)$.

THEOREM 3.2. *Let $\lambda > 0$ and $\varepsilon(\lambda) \geq 0$ be arbitrarily fixed. Then, the regularized problem (P_λ) admits a solution and the solution is unique if $\varepsilon(\lambda) \neq 0$.*

Proof. In the proof, we consider G again as mapping with range in $L^2(\Omega)$, i.e. we subtitute S for G. This does not change the admissible set. First of all, we have to show that the admissible set $V_{ad} := \{v \in L^2(\Omega) \mid y_a \leq \lambda v + SS^\star v \leq y_b \text{ a.e. in } \Omega\}$ is not empty. To this purpose, we consider the operator $\lambda I + SS^\star$, where $I : L^2(\Omega) \to L^2(\Omega)$ denotes the identity operator in $L^2(\Omega)$. Since $SS^\star : L^2(\Omega) \to L^2(\Omega)$ is positive semidefinite and $\lambda > 0$ holds by assumption, the equation $\lambda v + SS^\star v = 0$ admits only the trivial solution $v = 0$. Hence, by the Fredholm alternative, the compactness of $SS^\star$ implies the existence of the inverse operator $(\lambda I + SS^\star)^{-1}$. From this, we infer that V_{ad} is not empty: For instance, we have $(\lambda I + SS^\star)^{-1} y_b \in V_{ad}$.

Next, since the objective functional in (P_λ) is nonnegative, the infimum in (P_λ) exists in $\mathbb{R}_0^+$. Let now $\{v_n\}_{n=1}^\infty$ be an infimal sequence for (P_λ). By the presence of the cost parameter $\alpha > 0$, $S^\star v_n$ is uniformly bounded in $L^2(\Omega)$ and hence we can find a subsequence $\{S^\star v_{n_j}\}_{j=1}^\infty$ of $\{S^\star v_n\}_{n=1}^\infty$ such that $S^\star v_{n_j} \rightharpoonup u'$. Subsequently, invoking again the compactness of S, we infer the strong convergence of $SS^\star v_{n_j}$ to Su'. Moreover, since $v_{n_j} \in V_{ad}$ for all j, the strong convergence of $SS^\star v_{n_j}$ ensures then the uniform boundedness property of v_{n_j}. Thus, we find again a subsequence of v_{n_j} converging weakly to $\bar{v}_\lambda \in L^2(\Omega)$. This weak limit $\bar{v}_\lambda$ is clearly feasible and finally, by the lower semicontinuity of the objective functional in (P_λ), $\bar{v}_\lambda$ is optimal. For $\varepsilon(\lambda) > 0$, $\tilde{g}$ is strictly convex and consequently we obtain the uniqueness of $\bar{v}_\lambda$. ☐

Next, setting $z = \lambda v + SS^\star v$ and hence, $v = (\lambda I + SS^\star)^{-1} z = Rz$, (P_λ) is equivalent to the following control problem:

$$(P_\lambda^z) \qquad \begin{cases} \text{minimize } \mathbf{g}(z) := \tilde{g}(Rz) \\ \text{over } z \in L^2(\Omega) \\ \text{subject to } y_a \leq z \leq y_b \quad \text{a.e. in } \Omega. \end{cases}$$

In this way, we have just transformed (P_λ) into a control problem with a simple box constraint. Subsequently, by standard arguments, cf. [15], the following optimality system can easily be shown.

THEOREM 3.3 (First-order optimality conditions). *Let $\lambda > 0$ be arbitrarily fixed and let $\bar{v}_\lambda$ be an optimal solution to (P_λ). Moreover, we set $\bar{y}_\lambda = GS^\star \bar{v}_\lambda$ and $S^\star \bar{v}_\lambda = w_{|\Gamma}$, with $w = w(\bar{v}_\lambda) \in H^1(\Omega)$ solution of (3.1). Then, there exist Lagrange multipliers $\mu_\lambda^a, \mu_\lambda^b \in L^2(\Omega)$ and adjoint states $p, q \in H^1(\Omega)$ such that the following optimality system is satisfied:*

$$\begin{array}{rclll} A\bar{y}_\lambda &=& 0 & \text{in} & \Omega \\ \partial_n \bar{y}_\lambda &=& w & \text{on} & \Gamma, \end{array} \qquad \begin{array}{rclll} A^\star w &=& \bar{v}_\lambda & \text{in} & \Omega \\ \partial_n w &=& 0 & \text{on} & \Gamma, \end{array} \tag{3.6}$$

$$\begin{array}{rclll} A^\star p &=& \bar{y}_\lambda - y_d + \mu_\lambda^b - \mu_\lambda^a & \text{in} & \Omega \\ \partial_n p &=& 0 & \text{on} & \Gamma, \end{array} \qquad \begin{array}{rclll} A^\star q &=& 0 & \text{in} & \Omega \\ \partial_n q &=& \alpha w + p & \text{on} & \Gamma, \end{array} \tag{3.7}$$

$$\varepsilon(\lambda)\bar{v}_\lambda + q + \lambda(\mu_\lambda^b - \mu_\lambda^a) = 0, \tag{3.8}$$

$$y_a \leq \lambda \bar{v}_\lambda + \bar{y}_\lambda \leq y_b \quad \text{a.e. in } \Omega, \tag{3.9}$$

$$(3.10)\qquad \begin{gathered}\mu_\lambda^a \geq 0, \mu_\lambda^b \geq 0,\\ (\mu_\lambda^a, y_a - \lambda\bar{v}_\lambda - \bar{y}_\lambda)_{L^2(\Omega)} = (\mu_\lambda^b, \lambda\bar{v}_\lambda + \bar{y}_\lambda - y_b)_{L^2(\Omega)} = 0.\end{gathered}$$

3.3. Pass to the limit $\lambda \to 0$. We study now the convergence of the solution to the regularized problem in the case of vanishing Lavrentiev parameter λ.

ASSUMPTION 3.1. *The regularization parameter $\varepsilon = \varepsilon(\lambda)$ satisfies*

$$(3.11)\qquad \varepsilon = \sigma_0 \lambda^{1+\sigma_1}$$

with some constants $\sigma_0 > 0$ and $0 \leq \sigma_1 < 1$. Moreover, there exists a function $v_0 \in L^\infty(\Omega)$ such that

$$(3.12)\qquad y_a + \delta \leq G(\bar{u} + S^\star v_0) \leq y_b - \delta$$

is satisfied with some constant $\delta > 0$.

Let $\{\lambda_n\}_{n=1}^\infty$ be a sequence of positive real numbers converging to zero and by $\{v_n\}_{n=1}^\infty$, we denote the sequence of optimal solutions to (P_{λ_n}). The presence of the Tikhonov parameter $\alpha > 0$ in (P_{λ_n}) ensures the boundedness of the sequence $\{S^\star v_n\}_{n=1}^\infty$ in $L^2(\Gamma)$. For this reason, we can find a subsequence of $\{S^\star v_n\}_{n=1}^\infty$, denoted w.l.o.g. again by $\{S^\star v_n\}_{n=1}^\infty$, converging weakly to some $\tilde{u} \in L^2(\Gamma)$. Our goal now is to show that $\tilde{u}$ minimizes the original unregularized problem. For this purpose, we should show first the feasibility of $\tilde{u}$ for (P), i.e., $y_a \leq G\tilde{u} \leq y_b$ a.e. in Ω.

LEMMA 3.4. *Let Assumption 3.1, (3.11), be satisfied. Then the weak limit $\tilde{u}$ of the sequence $\{S^\star v_n\}_{n=1}^\infty$ defined above is feasible for (P).*

Proof. We know that it holds

$$y_a \leq \lambda_n v_n + GS^\star v_n \leq y_b \quad \forall n.$$

Therefore, it suffices to show that $\lambda_n v_n$ converges to zero. Clearly, by the presence of the regularization parameter $\varepsilon(\lambda) > 0$ in the objective functional $\tilde{g}$, one has:

$$\frac{\varepsilon(\lambda_n)}{2}\|v_n\|^2_{L^2(\Omega)} \leq c \quad \forall n$$

with some constant $c > 0$ and hence

$$\frac{\varepsilon(\lambda_n)}{2\lambda_n^2}\|\lambda_n v_n\|^2_{L^2(\Omega)} \leq c \quad \forall n.$$

From Assumption 3.1, we infer then

$$(3.13)\qquad \|\lambda_n v_n\|^2_{L^2(\Omega)} \leq \frac{2c\lambda_n^2}{\varepsilon(\lambda_n)} \leq \lambda_n^{1-\sigma_1}\frac{2c}{\sigma_0}.$$

This implies $\lambda_n v_n \to 0$ in $L^2(\Omega)$ as $n \to \infty$ and hence the Lemma is shown. ◻

THEOREM 3.4. *Let $N = 2$. Then, under Assumption 3.1, the sequence $\{S^\star v_n\}$ converges strongly in $L^2(\Gamma)$ to the optimal solution of the unregularized problem (P).*

Proof. Since $\mathcal{C}(\bar{\Omega})$ is dense in $L^2(\Omega)$ and due to Lemma 3.1, we can find a sequence $\{z_k\}_{k=1}^\infty$ in $\mathcal{C}(\bar{\Omega})$ such that

$$(3.14)\qquad \|\bar{u} - S^\star z_k\|_{L^2(\Gamma)} \leq \frac{1}{k} \quad \forall\, k \in \mathbb{N}.$$

Moreover, continuity and linearity of G from $L^2(\Gamma)$ to $H^1(\Omega)\cap\mathcal{C}(\bar\Omega)$ ensure the existence of a real positive number c_0 such that

$$\|G(\bar u - S^\star z_k)\|_{\mathcal{C}(\bar\Omega)} \le c_0\|\bar u - S^\star z_k\|_{L^2(\Gamma)} \le c_0\frac{1}{k} \quad \forall\, k\in\mathbb{N}. \tag{3.15}$$

We define now an auxiliary sequence $\{v_k^0\}_{k=1}^\infty$ in $L^\infty(\Omega)$ by

$$v_k^0 = z_k + \frac{2c_0}{k\delta}v_0 = z_k + \frac{c_1}{k}v_0, \tag{3.16}$$

where v_0 satisfies (3.12) and $c_1 = \frac{2c_0}{\delta}$. In a view of (3.14), the definition above implies the strong convergence of $S^\star v_k^0$ in $L^2(\Gamma)$ to $\bar u$, i.e.

$$\lim_{k\to\infty}\|S^\star v_k^0 - \bar u\|_{L^2(\Gamma)} = 0. \tag{3.17}$$

First, we show that, for every $k\in\mathbb{N}$ with $k\ge c_1$, one can find an index number $n_k\in\mathbb{N}$ such that v_k^0 is feasible for (P_{λ_n}) for all $n\ge n_k$. Let now $k\in\mathbb{N}$ with $k\ge c_1$ be arbitrarily fixed. Then, by our assumptions, it holds that

$$\begin{aligned}
&\lambda_n v_k^0 + GS^\star v_k^0 = \lambda_n v_k^0 + G(S^\star z_k - \bar u) + (1-\tfrac{c_1}{k})G\bar u + \tfrac{c_1}{k}(GS^\star v_0 + G\bar u)\\
&\le \lambda_n\|v_k^0\|_{L^\infty(\Omega)} + c_0\|S^\star z_k - \bar u\|_{L^2(\Gamma)} + (1-\tfrac{c_1}{k})y_b + \tfrac{c_1}{k}(y_b-\delta)\\
&\le y_b + (\lambda_n\|v_k^0\|_{L^\infty(\Omega)} + \tfrac{c_0}{k} - 2\tfrac{c_0}{k})\\
&= y_b + (\lambda_n\|v_k^0\|_{L^\infty(\Omega)} - \tfrac{c_0}{k}).
\end{aligned} \tag{3.18}$$

Since λ_n converges to zero, we can find then an index $n_k\in\mathbb{N}$ such that $\lambda_n\|v_k^0\|_{L^\infty(\Omega)}\le \frac{c_0}{k}$ for all $n\ge n_k$. Inserting this in (3.18), we obtain

$$\lambda_n v_k^0 + GS^\star v_k^0 \le y_b \quad \forall\, n\ge n_k.$$

In the same way, one derives $y_a \le \lambda_n v_k^0 + GS^\star v_k^0$ for all $n\ge n_k$. This implies the feasibility of v_k^0 for all (P_{λ_n}) with $n\ge n_k$.

Since v_n is optimal to (P_{λ_n}) for each n, we infer further that

$$f(S^\star v_n) \le f(S^\star v_n) + \frac{\varepsilon_n}{2}\|v_n\|^2_{L^2(\Omega)} \le f(S^\star v_k^0) + \frac{\varepsilon_n}{2}\|v_k^0\|^2_{L^2(\Omega)}\ \forall\, n\ge n_k.$$

Hence, due to the lower semicontinuity of f, one finds by passing to the limit $n\to\infty$

$$f(\tilde u) \le \lim_{n\to\infty}\inf f(S^\star v_n) \le \lim_{n\to\infty}\sup f(S^\star v_n) \le f(S^\star v_k^0),$$

where $\tilde u$ is the weak limit introduced in Lemma 3.4. Finally, letting k pass to infinity, we infer from (3.17) that

$$f(\tilde u) \le \lim_{k\to\infty} f(S^\star v_k^0) = f(\bar u).$$

Hence, we have shown the optimality of $\tilde u$ to (P) and again, due to the uniqueness of $\bar u$, we have $\tilde u = \bar u$. Notice that the latter equality $\lim_{n\to\infty} f(S^\star v_n) = f(\bar u)$ implies the convergence of $\{S^\star v_n\}$ in norm and hence, together with the weak convergence, the strong convergence of $\{S^\star v_n\}$ to $\tilde u$ is verified. ◻

4. Semismooth Newton algorithm. Based on the experience in [11, 8, 9], the semismooth Newton method is quite efficient when dealing with state-constrained optimal control problems. Mainly due to its superlinear convergence and mesh-independence properties, the method is highly efficient in many applications. This was analyzed and verified numerically, quite recently, also for a similar Lavrentiev regularization technique applied to distributed optimal control problem, [9]. Our goal in this section is to present a semismooth Newton algorithm based on the first-order optimality conditions (3.6)-(3.10) for the regularized problem (P_λ). The analysis for the mesh-independence principle is not included here. This is a subject of our ongoing research. Following [6, 8], we define now the Newton generalized differentiability.

DEFINITION 4.1. *Let X, Y be Banach spaces and U be an open set in X. A mapping $F: U \to Y$ is said to be semismooth (or Newton differentiable) in U if there exists a (possibly set-valued) mapping $\partial F : U \rightrightarrows \mathscr{L}(X,Y)$ such that*

$$\sup_{V \in \partial F(x+s)} \|F(x+s) - F(x) - Vs\|_Y = o(\|s\|_X) \quad \text{as } \|s\|_X \to 0 \tag{4.1}$$

is satisfied for all $x \in U$. We call ∂F the Newton differential*, and its elements V are referred to as* Newton maps.

In the following, we derive a semismooth Newton algorithm based on the concept above. Let us start by reformulating the complementarity system (3.10) in the optimality conditions by the following max-formulation.

LEMMA 4.1. *The complementarity conditions (3.10) are equivalent to:*

$$\mu_\lambda^a = \max(0, \mu_\lambda^a - \mu_\lambda^b + \gamma(y_a - \lambda \bar{v}_\lambda - \bar{y}_\lambda)), \tag{4.2}$$

$$\mu_\lambda^b = \max(0, \mu_\lambda^b - \mu_\lambda^a + \gamma(\lambda \bar{v}_\lambda + \bar{y}_\lambda - y_b)), \tag{4.3}$$

for arbitrarily fixed $\gamma > 0$.

We sketch the proof for the convenience of the reader. First, the complementarity conditions (3.10) imply obviously (4.2)-(4.3). Furthermore, (4.2)-(4.3) imply the nonnegativity of μ_λ^a and μ_λ^b. Let now $\mathcal{A}$ be a set in Ω such that $\mu_\lambda^a = \mu_\lambda^a - \mu_\lambda^b + \gamma(y_a - \lambda \bar{v}_\lambda - \bar{y}_\lambda)$ on $\mathcal{A}$. Thus $\mu_\lambda^b = \gamma(y_a - \lambda \bar{v}_\lambda - \bar{y}_\lambda)$ on $\mathcal{A}$. Furthermore, (4.3) implies

$$\mu_\lambda^b = \max(0, -\mu_\lambda^a + \gamma(y_a - y_b)) = 0 \quad \text{on } \mathcal{A}.$$

Therefore, $y_a - \lambda \bar{v}_\lambda - \bar{y}_\lambda = 0$ on $\mathcal{A}$. For this reason, we have

$$(\mu_\lambda^a, y_a - \lambda \bar{v}_\lambda - \bar{y}_\lambda)_{L^2(\Omega)} = 0.$$

In the same way, we infer

$$(\mu_\lambda^b, \lambda \bar{v}_\lambda + \bar{y}_\lambda - y_b)_{L^2(\Omega)} = 0$$

and hence (4.2)-(4.3) imply the complementarity system (3.10).

In [8], the investigation of the Newton differentiability of the maximum-operation has been analyzed. As demonstrated, a class of corresponding Newton maps for the maximum operator $\mathbb{M}(z) = \max(0, z)$ are given by

$$\partial \mathbb{M}_\xi(z)(x) = \begin{cases} 1 \text{ if } z(x) > 0, \\ 0 \text{ if } z(x) < 0, \\ \xi \text{ if } z(x) = 0, \end{cases} \tag{4.4}$$

with arbitrarily fixed $\xi \in \mathbb{R}$, provided that $\mathbb{M}$ is defined from $L^{q_2}(\Omega)$ to $L^{q_1}(\Omega)$ with $1 \leq q_1 < q_2 \leq \infty$.

Setting now a special choice $\gamma := \varepsilon(\lambda)/\lambda^2$ in (4.2)-(4.3), short computations show that due to the equation (3.8) in the optimality system, i.e.,

$$\varepsilon(\lambda)\bar{v}_\lambda + q + \lambda(\mu_\lambda^b - \mu_\lambda^a) = 0,$$

the complementarity system is equivalent to

$$\mu_\lambda^a = \max(0, \frac{1}{\lambda}q + \frac{\varepsilon(\lambda)}{\lambda^2}(y_a - \bar{y}_\lambda)), \tag{4.5}$$

$$\mu_\lambda^b = \max(0, -\frac{1}{\lambda}q + \frac{\varepsilon(\lambda)}{\lambda^2}(\bar{y}_\lambda - y_b)). \tag{4.6}$$

The maximum operators above are defined from $L^{q_2}(\Omega)$ to $L^{q_1}(\Omega)$ with $1 \leq q_1 < q_2$ and thus the application of semismooth Newton method is justified. Our algorithm is based on the particular choice $\xi = 0$ for the Newton map. Then, the semismooth Newton algorithm is equivalent to an active-set-strategy. The complete algorithm is defined by the following steps, cf. also [8, 9] for the details.

Algorithm 4.1.

(i) Initialization: Choose initial data $q^0, y^0 \in L^2(\Omega)$ *and set* $l = 0$.

(ii) Set the active and inactive sets:

$$\begin{aligned}
\mathcal{A}_a^l &= \{x \in \Omega \ : \ \frac{1}{\lambda}q^l(x) + \frac{\varepsilon(\lambda)}{\lambda^2}(y_a(x) - y^l(x)) > 0 \ a.e. \ in \ \Omega\},\\
\mathcal{A}_b^l &= \{x \in \Omega \ : \ -\frac{1}{\lambda}q^l(x) + \frac{\varepsilon(\lambda)}{\lambda^2}(y^l(x) - y_b(x)) > 0 \ a.e. \ in \ \Omega\},\\
\mathcal{I}^l &= \Omega \backslash (\mathcal{A}_a^l \cup \mathcal{A}_b^l).
\end{aligned}$$

(iii) Find the solution $(y^{l+1}, q^{l+1}, p^{l+1}, w^{l+1}, v^{l+1}, \mu_a^{l+1}, \mu_b^{l+1})$ *of*

$$\begin{array}{rclll rclll}
Ay^{l+1} &=& 0 & in & \Omega, & A^\star w^{l+1} &=& v^{l+1} & in & \Omega,\\
\partial_n y^{l+1} &=& w^{l+1} & on & \Gamma, & \partial_n w^{l+1} &=& 0 & on & \Gamma,
\end{array}$$

$$\begin{array}{rclll}
A^\star p^{l+1} &=& y^{l+1} - y_d + \mu_b^{l+1} - \mu_a^{l+1} & in & \Omega,\\
\partial_n p^{l+1} &=& 0 & on & \Gamma,\\
\\
A^\star q^{l+1} &=& 0 & in & \Omega,\\
\partial_n q^{l+1} &=& \alpha w^{l+1} + p^{l+1} & on & \Gamma,
\end{array}$$

$$\varepsilon(\lambda)v^{l+1} + q^{l+1} + \lambda(\mu_b^{l+1} - \mu_a^{l+1}) = 0,$$

$$\begin{array}{rclll}
\mu_a^{l+1} &=& \frac{1}{\lambda}q^{l+1} + \frac{\varepsilon(\lambda)}{\lambda^2}(y_a - y^{l+1}) & on \ \ \mathcal{A}_a^l, & \mu_a^{l+1} = 0 \ on \ \mathcal{I}^l \cup \mathcal{A}_b^l,\\
\mu_b^{l+1} &=& -\frac{1}{\lambda}q^{l+1} + \frac{\varepsilon(\lambda)}{\lambda^2}(y^{l+1} - y_b) & on \ \ \mathcal{A}_b^l, & \mu_b^{l+1} = 0 \ on \ \mathcal{I}^l \cup \mathcal{A}_a^l.
\end{array}$$

(iv) Stop or set $l = l + 1$ *and go to (ii).*

Unless otherwise specified, we initialize Algorithm 4.1 with $y^0 = q^0 = 0$ and terminate it using the stopping criterion: $\mathcal{A}_a^n = \mathcal{A}_a^{n-1}$ and $\mathcal{A}_b^n = \mathcal{A}_b^{n-1}$.

5. Numerical Experiments. Our numerical report is splitted into two parts. First, we confirm the numerical reliability of our regularization approach to solve some classes of state-constrained optimal boundary control problems. In particular, we aim at investigating the influence of the regularization parameter on the algorithm. To this purpose, a test example with analytically known solution to the problem (2.1) will be considered. As pointed out in Remark 2.1, our theory is applicable also to this more general problem (2.1). By means of this example, the numerical approximation of our method as well as its convergence behavior will be analyzed. We also study briefly a nested iteration technique, based on a multigrid concept, to gain a higher efficiency of the algorithm.

Second, we compare our technique based on the "optimize-then-discretize" concept with the standard numerical optimization code QUADPROG of the MATLAB optimization toolbox applied to the discretized problem ("discretize-then-optimize"). We mainly aim at showing that our method exhibits a reasonable performance. We do not intend to compare the concepts "optimize-then-discretize" and "discretize-then-optimize", since this would require various test runs with common available nonlinear optimization codes. A detailed study of the method "discretize-then-optimize" was carried out by Maurer and Mittelmann [13].

Our experience showed that the semismooth Newton method applied to the Lavrentiev type regularization was as efficient as QUADPROG and partially even more advantageous. We point out that all the numerical computations in this paper were carried out on a PC with a 250-GHz AMD processor and a 16-gigabyte memory.

5.1. Discretization. As noticed early, the regularization technique that we propose here is based on the optimize-then-discretize strategy. In the following, we explain the discretization of Algorithm 4.1 and call later the algorithm under this discretization "OTD".

Throughout the experiment, we use for simplicity the unit square domain $\Omega = (0,1) \times (0,1)$ and set $A = -\Delta + I$. We discretize Ω by a regular Friedrichs-Keller triangulation with mesh size h and the mesh on Γ is induced by that on Ω. The partial differential equations (PDEs) are approximated by the finite element method. The state space $H^1(\Omega) \cap \mathcal{C}(\bar{\Omega})$ is discretized by the span of the standard finite element basis $\{\phi_h^1(x), \ldots, \phi_h^{N_h}(x)\}$ consisting of the piecewise linear and continuous hat functions on $\bar{\Omega}$. Analogously, we define the discrete control space with the standard finite element basis $\{\psi_h^1(x), \ldots, \psi_h^{M_h}(x)\}$, composed of the piecewise linear and continuous hat functions defined on the boundary Γ. Hence, the state equation is approximated by the system of linear equations

$$A_h y_h = B_h u_h + M_h e_h,$$

where the matrices $A_h, M_h \in \mathbb{R}^{N_h \times N_h}$ and $B_h \in \mathbb{R}^{N_h \times M_h}$ are given by

$$\begin{aligned}(A_h)_{ij} &= (\nabla \phi_h^i, \nabla \phi_h^j)_{L^2(\Omega)} + (\phi_h^i, \phi_h^j)_{L^2(\Omega)},\\ (B_h)_{i,j} &= (\phi_h^i, \psi_h^j)_{L^2(\Gamma)},\\ (M_h)_{ij} &= (\phi_h^i, \phi_h^j)_{L^2(\Omega)}.\end{aligned}$$

Here, the vectors $y_h \in \mathbb{R}^{N_h}$, $u_h \in \mathbb{R}^{M_h}$ and $e_h \in \mathbb{R}^{N_h}$ serve for the discrete approximations of the state, the control and the fixed function e, respectively, with mesh size h. For instance, y_{h_i} is the numerical approximation of the value $y(x_i)$ in the node point x_i that is associated with the ansatz function ϕ_h^i. The remaining PDEs in the optimality system associated with (P_λ) are analogously discretized. The active sets are discretized by the approximated values of corresponding functions at the nodes. For instance, the discretization of $\mathcal{A}_a$ is given by

$$\{i: \frac{1}{\lambda}q_{h_i} + \frac{\varepsilon(\lambda)}{\lambda^2}(y_{a,h_i} - y_{h_i}) > 0\},$$

where the vectors $q_h \in \mathbb{R}^{M_h}$ and $y_{a,h} \in \mathbb{R}^{N_h}$ serve for the discrete approximations of q and y_a, respectively, with mesh size h. Algorithm 4.1 is implemented in this way.

5.2. Test example 1. To construct the example, we first define the optimal state y_{opt}, the adjoint state p_{opt}, the upper bound ψ and the fixed function e by

$$\begin{aligned} y_{opt}(x) &= \frac{2}{\pi}\sin(\pi x_1)\sin(\pi x_2), \\ p_{opt}(x) &= -0.5, \\ \psi(x) &= \max(\frac{1}{\pi}, y_{opt}(x)), \\ e(x) &= -\Delta y_{opt}(x) + y_{opt}(x). \end{aligned}$$

Notice that, in our test examples, we only consider an upper bound constraint

$$y_{opt}(x) \le \psi(x) \quad \forall x \in \bar{\Omega}.$$

Clearly, our theory applies to this case as well. Short computations show that

$$\mu_{opt}(x) := \begin{cases} 1.7 & \text{if} \quad y(x) > \frac{1}{\pi} \\ 0 & \text{if} \quad y(x) \le \frac{1}{\pi} \end{cases}$$

fulfills the complementarity slackness condition for (P). Setting for the desired state

$$y_d = y_{opt} - p_{opt} + \mu_{opt},$$

μ_{opt} can serve for the Lagrange multiplier associated with (P). Next, by computing the normal derivative of y_{opt}, one obtains the optimal boundary control u_{opt}, which is identical on all edges of Ω. For example, on the lower boundary of Ω, $u_{opt} = -2\sin(\pi x_1)$. Finally, for the cost parameter α and the desired control u_d, we set:

$$\begin{aligned} \alpha &= 10^{-2}, \\ u_d &= u_{opt} + \tfrac{1}{\alpha}p_{opt\,\Gamma}. \end{aligned}$$

For the choice of the parameter $\varepsilon = \varepsilon(\lambda)$, we select throughout the numerical test $\varepsilon(\lambda) = \lambda^{1+\frac{1}{2}}$. This satisfies clearly Assumption 3.1.

Our aim now consists of investigating the numerical approximations based on Algorithm 4.1 in the case of vanishing Lavrentiev parameter λ. In Table 5.1, we report on the numerical results when solving the problem utilizing Algorithm 4.1. We found out in our test runs ($h = 1/128$) that the problem is becoming harder to be solved for decreasing λ. Observing the second and third columns of Table 5.1, we notice that the distance to the optimal solution is quite satisfactory and getting smaller with respect to decreasing Lavrentiev parameter λ. This confirms the result of Theorem 3.4. At the same time, it indicates the applicability of our technique when dealing with state-constrained optimal boundary control problems.

TABLE 5.1
Convergence behavior of Algorithm 4.1 with respect to decreasing Lavrentiev parameter.

λ	$\|u_h - u_{opt}\|_{L^2}$	$\|y_h - y_{opt}\|_{L^2}$	$\|\mu_h - \mu_{opt}\|_{L^2}$	$\|p_h - p_{opt}\|_{L^2}$
$10^{-2.0}$	3.1880078e-01	3.9198985e-01	6.2201011e-01	3.5549336e-03
$10^{-3.0}$	3.2990915e-02	2.0899831e-02	2.4068944e-01	1.1464553e-03
$10^{-4.0}$	4.4104922e-03	4.5454556e-03	1.2453488e-01	7.7483476e-04
$10^{-5.0}$	2.5020193e-03	2.6584714e-03	6.3426567e-02	3.5686997e-04
$10^{-6.0}$	1.8128938e-03	1.0053254e-03	4.2474621e-02	2.6608656e-04
$10^{-7.0}$	1.1850217e-03	3.5760613e-04	4.0462811e-02	4.1388376e-04
$10^{-8.0}$	8.1408314e-04	1.3624889e-04	9.2715530e-02	1.0450310e-03
$10^{-9.0}$	7.3457286e-04	6.5919685e-05	2.6964435e-01	3.0716652e-03
$10^{-10.0}$	7.2968216e-04	4.5600222e-05	7.6555488e-01	8.5845442e-03

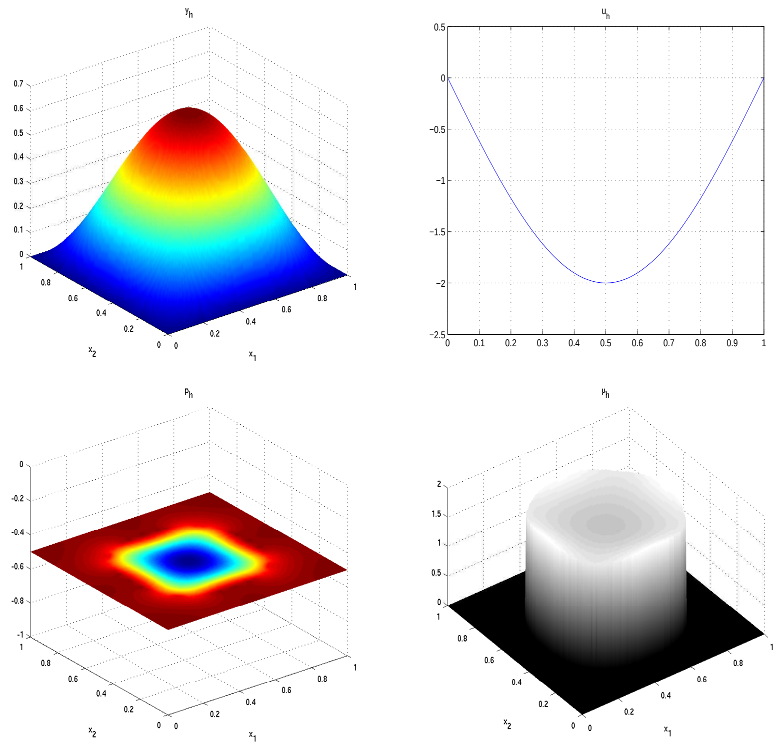

FIG. 5.1. *Computed solution based on Algorithm 4.1 for $h = 1/128$ and $\lambda = 10^{-7}$: Optimal state (upper left), optimal control (upper right), adjoint state (lower left) and Lagrange multiplier (lower right).*

If the selection of the parameter λ is too small, the approximation to the Lagrange multiplier turns out to be rather poor. In the fourth column of Table 5.1, we observe that the distance to the Lagrange multiplier is increasing with respect to decreasing $\lambda \leq 10^{-7}$, see Figure 5.2. This effect occurred most likely due to the noticeably-increasing ill-conditioning, which is monitored in the experiment for decreasing $\lambda < 10^{-8}$.

Therefore, we suggest to choose a moderate Lavrentiev parameter, $\lambda \approx 10^{-7}$. For this selection, we obtained the best approximation of the desired Lagrange multiplier, see Figure 5.1.

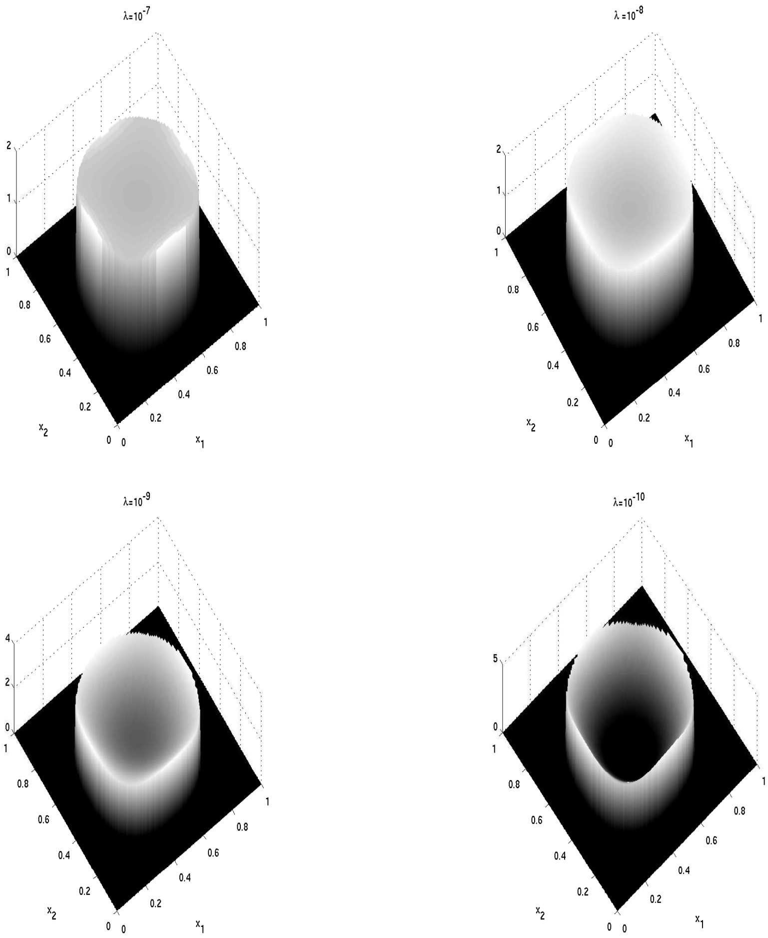

FIG. 5.2. *Spurious oscillation of the Lagrange multipliers with respect to decreasing* λ.

5.3. Comparison with a commercial optimization code. As noted earlier, it is one of our goals to compare our regularization technique based on "optimize-then-discretize" (OTD) with a commercial code applied to the discretized problem ("discretize-then-optimize", DTO). To this aim, we selected the code *QUADPROG* from the MATLAB optimization toolbox, since this is often applied by users of MATLAB.

We start by defining briefly the discretized version of (P):

$$(P_h) \qquad \begin{cases} \text{minimize } \frac{1}{2}(y_h - y_{d_h})^T M_h (y_h - y_{d_h}) + \frac{\alpha}{2}(u_h - u_{d_h})^T \tilde{M}_h (u_h - u_{d_h}) \\ \text{subject to } A_h y_h = M_h e_h + B_h u_h \\ \qquad\qquad\quad y_h \leq \psi_h \\ \qquad\qquad\quad (u_h, y_h) \in \mathbb{R}^{M_h} \times \mathbb{R}^{N_h}, \end{cases}$$

where the mass matrix $\tilde{M}_h$ is given by $\tilde{M}_{h_{ij}} = (\psi_h^i, \psi_h^j)_{L^2(\Gamma)}$ and the vectors $\psi_h, y_{d_h} \in \mathbb{R}^{N_h}$ and $u_{d_h} \in \mathbb{R}^{M_h}$ stand for the discretization of the upper bound function ψ, the desired state y_d and the desired control u_d, respectively. *QUADPROG* was used to solve this linear quadratic problem (P_h).

Table 5.3 shows the results when solving the previous test example. Considering the first and second columns of Table 5.3, the numerical approximations of DTO to the optimal state and optimal control with respect to decreasing mesh size are quite satisfactory just as those of OTD. We point out here that, in contrast to the previous

Table 5.2
The L^2-error to the optimal values

N	$\|u_h - u_{opt}\|_{L^2}$	$\|y_h - y_{opt}\|_{L^2}$
8	2.453490834802477e-01	4.004580211912924e-03
16	7.119225785142243e-02	1.533151564674966e-03
32	1.901332987811985e-02	4.525371992082597e-04
64	4.927627144442628e-03	1.156125655672012e-04

numerical test for OTD, the computation based on DTO for the test example with mesh size $h = 1/128$ failed due to exceeding the memory of the PC.

Next, we aim at comparing the efficiency of our methods OTD with that of *QUADPROG* based on the discretize-then-optimize concept. For this purpose, we test again OTD at $\lambda = 10^{-7}$ as well as DTO with various mesh sizes and report on their required CPU-time for each grid. Observing Table 5.3, we detect that OTD was more efficient. On the finest grid of the numerical tests ($h = 1/64$), DTO required about 6.46e+03 seconds to converge, whereas OTD was at least 50 times faster. This demonstrates the computational efficiency of our regularization strategy.

Table 5.3
CPU times for various mesh sizes.

h	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{32}$	$\frac{1}{64}$
DTO	4.00e-02	1.18e+00	1.23e+02	6.46e+03
OTD $\lambda = 10^{-7}$	2.00e-01	1.85e+00	1.33e+01	9.89e+01

5.4. Test example 2. We consider now an example without given analytical solution.

Example 5.1. We choose:

$$\begin{aligned} y_d &= (x_1 - 0.5)^2 + (x_2 - 0.5)^2 - 3, \\ u_d &= 0, \\ e &= 0, \\ \alpha &= 10^{-2}, \end{aligned}$$

and the state constraint is given by

$$y(x) \le -2.723 \quad \forall x \in \bar{\Omega}.$$

Figure 5.3 displays the computed solution for $\lambda = 10^{-9}$. Again, the optimal control is identical on all edges of Ω and hence is only plotted on the lower boundary.

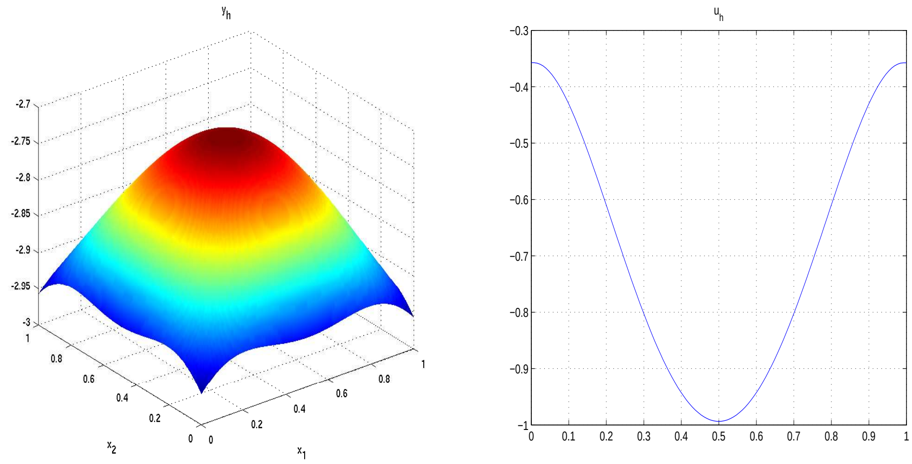

FIG. 5.3. *Computed solution based on Algorithm 4.1 for* $h = 1/128$ *and* $\lambda = 10^{-9}$

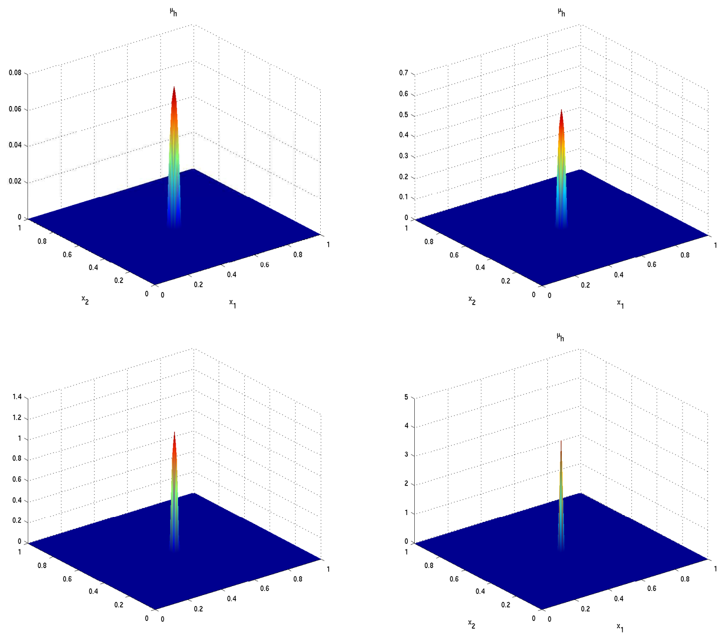

FIG. 5.4. *Computed Lagrange multipliers associated with the upper bound:* $\lambda = 10^{-4}, \lambda = 10^{-6}, \lambda = 10^{-7}$ *and* $\lambda = 10^{-9}$ *(from left to right).*

In Table 5.4, we provide the required iteration numbers when solving the problem using our algorithm with fixed initial data $p_0 = y_0 = 0$. Just as before, we detect that the problem is harder to be solved if the choice of λ is too small. Based on our numerical observation, this effect occurred mostly due to the following two reasons: the linear equations solved by the algorithm are ill-conditioned. This behavior is monitored particularly if the selection of the Lavrentiev-parameter is too small. Furthermore, the measure structure of the Lagrange multipliers associated with the

TABLE 5.4
Number of iterations for several Lavrentiev-parameter choices with fixed mesh size $h = 1/128$.

λ	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}
# It.	7	9	10	10	16	29	34

upper bound complicates considerably the numerical computation. As $\lambda \to 0$, the computed Lagrange multiplier approaches a Dirac measure concentrated in a single point, cf. Figure 5.4.

5.5. Nested iteration. In this last part of the paper, we briefly introduce an interpolation technique with the objective to gain a faster method. Our experience in handling the regularized distributed control problem, cf. [9], indicates that a simple nested iteration scheme, based on the coarse-to-fine grid strategy, may improve the efficiency of the algorithm. In fact, this method is also reliable for boundary control problems and can significantly accelerate the convergence. First, let us shortly explain the nested iteration method: We set a sequence of grids Ω_k with mesh size $h_k = 2h_{k-1}$ and start by solving the problem over the coarsest grid Ω_0. Subsequently, we interpolate the result to the next finer grid Ω_1 by the nine prolongation method, see [7], and utilize it as initial data for the algorithm with finer mesh size h_1. We repeat this process until the desired mesh size is reached. In table 5.5, we present a comparison of the results for the first test example with $\lambda = 10^{-5}$ based on Algorithm 4.1 (OTD) and those based on the nested iteration strategy.

In the second row of Table 5.5, we report on the iteration numbers as well as the CPU-time required by OTD with fixed initial data $y_0 = q_0 = 0$. The row with title *Interpolation* displays the performance of the algorithm combined with the nested iteration scheme (NIS) including its required CPU-time for each grid. Clearly, we find a significant speed-up of the algorithm under this coarse to fine grid sweep: By comparing the accumulated CPU-time of NIS with that of OTD at $h = 1/128$ with fixed initial data, we infer that NIS is more than three times faster than OTD with fixed initial data.

Certainly, under this nested iteration scheme, a similar improvement of the performance might have obtained for DTO based on *QUADPROG*. We did not investigate this alternative.

Our second noticeable observation is the mesh-independence behavior of OTD. Regardless of the mesh size of the discretization, the iteration numbers of OTD with fixed initial data remain constant equal to six. This might correspond to the mesh independence principle for a similar regularization technique applied to distributed optimal control problems [9]. Notice that after regularization, our problem is equivalent to a control-constrained one (cf. our remarks before Theorem 3.3).

TABLE 5.5
Mesh independence behavior of OTD and speed-up under a coarse-to-fine mesh sweep.

h	$\frac{1}{32}$	$\frac{1}{64}$	$\frac{1}{128}$
Fixed mesh (OTD)	6	6	6
CPU-time	6.420e+00	4.600e+01	4.208e+02
Interpolation (NIS)	6	1	1
CPU-time	6.420e+00	1.221e+01	1.278e +02

REFERENCES

[1] J.-J. Alibert and J.-P. Raymond. Boundary control of semilinear elliptic equations with discontinuous leading coefficients and unbounded controls. *Numer. Funct. Anal. and Optimization*, 3&4:235–250, 1997.

[2] M. Bergounioux, K. Ito, and K. Kunisch. Primal-dual strategy for constrained optimal control problems. *SIAM J. Control and Optimization*, 37:1176–1194, 1999.

[3] M. Bergounioux and K. Kunisch. Primal-dual active set strategy for state-constrained optimal control problems. *Computational Optimization and Applications*, 22:193–224, 2002.

[4] E. Casas. Control of an elliptic problem with pointwise state constraints. *SIAM J. Control and Optimization*, 4:1309–1322, 1986.

[5] E. Casas. Boundary control of semilinear elliptic equations with pointwise state constraints. *SIAM J. Control and Optimization*, 31:993–1006, 1993.

[6] X. Chen, Z. Nashed, and L. Qi. Smoothing methods and semismooth methods for nondifferentiable operator equations. *SIAM J. Numer. Anal.*, 38(4):1200–1216 (electronic), 2000.

[7] W. Hackbusch. *Multigrid methods and applications*, volume 4 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 1985.

[8] M. Hintermüller, K. Ito, and K. Kunisch. The primal-dual active set strategy as a semismooth Newton method. *SIAM J. Optim.*, 13:865–888, 2003.

[9] M. Hintermüller, F. Tröltzsch, and I. Yousept. Mesh-independence of semismooth Newton methods for Lavrentiev-regularized state constrained nonlinear optimal control problems. 2006.

[10] K. Ito and K. Kunisch. Augmented Lagrangian methods for nonsmooth, convex optimization in Hilbert spaces. *Nonlinear Analysis TMA*, 41:591–616, 2000.

[11] K. Ito and K. Kunisch. Semi-smooth Newton methods for state-constrained optimal control problems. *Systems and Control Letters*, 50:221–228, 2003.

[12] Lavrentiev, M. M. *Some Improperly Posed Problems of Mathematical Physics.* Springer, New York, 1967.

[13] H. Maurer and H. D. Mittelmann. Optimization techniques for solving elliptic control problems with control and state constraints. I: Boundary control. *J. of Computational and Applied Mathematics*, 16:29–55, 2000.

[14] C. Meyer, A. Rösch, and F. Tröltzsch. Optimal control of PDEs with regularized pointwise state constraints. *Computational Optimization and Applications*, 33:209–228, 2006.

[15] C. Meyer and F. Tröltzsch. On an elliptic optimal control problem with pointwise mixed control-state constraints. In A. Seeger, editor, *Recent Advances in Optimization. Proceedings of the 12th French-German-Spanish Conference on Optimization held in Avignon, September 20-24, 2004*, Lectures Notes in Economics and Mathematical Systems, Vol. 563, pages 187–204. Springer-Verlag, 2006.