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**Arnd Rösch and Daniel Wachsmuth**

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DFG-Research Center Matheon, Mathematics for key technologies  
Technische Universität Berlin, Sekr. MA 3-1  
Straße des 17. Juni 136 D-10623 Berlin, Germany

# SEMI-SMOOTH NEWTON METHOD FOR AN OPTIMAL CONTROL PROBLEM WITH CONTROL AND MIXED CONTROL-STATE CONSTRAINTS

ARND RÖSCH<sup>1</sup>, DANIEL WACHSMUTH<sup>2</sup>

**Abstract.** A class of optimal control problems for a semilinear parabolic partial differential equation with control and mixed control-state constraints is considered. For this problem, a projection formula is derived that is equivalent to the necessary optimality conditions. As main result, the superlinear convergence of a semi-smooth Newton method is shown. Moreover we show the numerical treatment and several numerical experiments.

**Key words.** Nonlinear programming, optimal control, semilinear elliptic equation, mixed control-state constraint, optimality conditions, semi-smooth Newton method, primal-dual active set strategy.

**AMS subject classifications.** 49K20, 49N60, 35J60

**1. Introduction.** In this paper, we consider the optimal control problem to minimize the function  $J$  given by

$$J(y, u) = \frac{1}{2} \|y(T) - y_d\|_{L^2(\Omega)}^2 + \frac{\nu}{2} \|u\|_{L^2(\Sigma)}^2 \quad (1.1)$$

subject to the initial boundary value problem

$$\begin{aligned} y_t - \Delta y &= 0 && \text{in } Q, \\ \partial_\nu y &= u && \text{on } \Sigma, \\ y(0) &= y_0 && \text{on } \Omega \end{aligned} \quad (1.2)$$

and to the mixed control-state constraints

$$0 \leq u(x, t) \leq c(x, t) + \gamma(x, t)y(x, t) \quad \text{a.e. in } \Sigma. \quad (1.3)$$

In this setting  $\Omega$  is a bounded domain of  $\mathbb{R}^N$ ,  $N = 2, 3$ , with boundary  $\Gamma$  and outward unit normal  $\nu$ . Moreover  $\nu$  is a fixed positive number and we define  $Q = (0, T) \times \Omega$ ,  $\Sigma = (0, T) \times \Gamma$ . Precise assumptions on and definitions of the quantities introduced above are formulated at the end of this section.

Our main issue is the discussion of the semi-smooth Newton method for this problem. Convergence of a semi-smooth Newton method in a general setting was shown in a paper of Ulbrich [17], see also Kummer [7, 8]. Mesh-independent convergence of this algorithm was shown by Hintermüller and Ulbrich [6].

In the control constrained case, the semi-smooth Newton method is under certain assumptions equivalent to the primal-dual active set strategy, see Hintermüller, Ito and Kunisch [5]. Similarly, we will formulate an active set algorithm for this type of problems.

However, the problem under consideration contains two different types of inequalities: a control constraint and a mixed control-state constraint. Therefore, it seems to be difficult

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<sup>1</sup> Universität Duisburg-Essen, Fachbereich Mathematik, Forsthausweg 2, D-47057 Duisburg, Germany

<sup>2</sup>Institut für Mathematik, Technische Universität Berlin, Str. des 17. Juni 136, D-10623 Berlin, Germany, wachsmut@math.tu-berlin.de.

to apply the general theory. We will overcome this problem by a reformulation of the optimality condition. Such a reformulation was introduced in [13] by the authors to show optimal regularity of the solution of a semilinear elliptic optimal control problem.

In our theory we will benefit from the specific structure of the constraints of problem (1.1)-(1.3). Here, the existence of Lagrange multipliers in function spaces (instead of measure spaces) is guaranteed. We refer to Arada, Raymond [1], Bergounioux, Tröltzsch [3], and Tröltzsch [14] for the parabolic case, and to Rösch, Tröltzsch [11, 12] for the elliptic case. A second essential advantage, which we will exploit, is that the active sets to the different constraints are disjoint.

The paper is structured as follows: In Section 2 we establish the optimality system and a suitable reformulation. The formulation of the semi-smooth setting and the presentation of the complete algorithm is contained in Section 3. Section 4 is devoted to the convergence theory. The paper ends with numerical experiments in Section 5.

**Assumptions.** The set  $\Omega \subset \mathbb{R}^N$ ,  $N = 2, 3$  is a bounded domain of the class  $C^{1,1}$ . The functions  $\gamma, c \in C(\bar{\Sigma})$  are nonnegative. Moreover, we require for the function  $c$

$$\inf_{x \in \Sigma} c(x) = c_m > 0.$$

The data of the optimization problem satisfy  $y_0, y_d \in C(\bar{\Omega})$ .

**2. The optimality system.** At first we discuss the properties of the state equation. Let us consider the following linear parabolic problem with some data  $f, g, y_0$

$$\begin{aligned} y_t - \Delta y &= f && \text{in } Q, \\ \partial_\nu y &= g && \text{on } \Sigma, \\ y(0) &= y_0 && \text{on } \Omega. \end{aligned} \tag{2.1}$$

Existence and uniqueness of solutions in the space

$$W(0, T) := \{y \in L^2(0, T; H^1(\Omega)) : y_t \in L^2(0, T; H^1(\Omega)')\}$$

are classical results, see e.g. Lions [9]. Let us denote the mapping from  $(f, g, y_0)$  to  $(y, y|_\Sigma, y(T))$  by  $\Lambda$ , i.e.  $\Lambda(f, g, y_0) = (y, y|_\Sigma, y(T))$ , where  $y$  is the corresponding solution of (2.1). It is well known that the equation (2.1) admits for  $L^2$ -data a unique solution in  $W(0, T)$ . By trace theorems, it holds  $y|_\Sigma \in L^2(0, T; L^2(\Gamma)) = L^2(\Sigma)$  and  $y(T) \in L^2(\Omega)$ . Hence, the objective  $J$  is well defined.

In the sequel, we will need estimates of  $\Lambda$  as mapping between different  $L^p$ -spaces.

**THEOREM 2.1.** *For any  $(f, g, y_0) \in L^2(Q) \times L^2(\Sigma) \times L^2(\Omega)$ , there exists a unique solution  $y \in W(0, T)$  of (2.1) with*

$$\|y\|_{W(0, T)} \leq c(\|f\|_{L^2(Q)} + \|g\|_{L^2(\Sigma)} + \|y_0\|_{L^2(\Omega)}). \tag{2.2}$$

*That is, the mapping  $\Lambda$  is linear and bounded, hence continuous, from  $L^2(Q) \times L^2(\Sigma) \times L^2(\Omega)$  to  $L^2(Q) \times L^2(\Sigma) \times L^2(\Omega)$ .*

*Moreover, there is a constant  $\delta > 0$ , such that the mapping  $\Lambda$  is continuous from  $L^r(Q) \times L^r(\Sigma) \times L^r(\Omega)$  to  $L^{r+\delta}(Q) \times L^{r+\delta}(\Sigma) \times L^{r+\delta}(\Omega)$  for all  $r \geq 2$ .*

*For  $r > N/2 + 1$ ,  $s > N + 1$ , it holds that  $\Lambda$  is continuous from  $L^r(Q) \times L^s(\Sigma) \times L^\infty(\Omega)$  to  $L^\infty(Q) \times L^\infty(\Sigma) \times L^\infty(\Omega)$ . It is moreover continuous from  $L^r(Q) \times L^s(\Sigma) \times C(\bar{\Omega})$  to  $C(\bar{Q}) \times C(\Sigma) \times C(\bar{\Omega})$ .*

*Proof.* The  $L^2$ -regularity result can be found in [9]. The smoothing property is proven in [15]. The  $L^\infty$ -regularity result can be found for instance in [10].  $\square$

With the help of  $\Lambda$ , we can express the solution  $y$  of (1.2) as  $(y, y|_\Sigma, y(T)) = \Lambda(0, u, y_0)$ . The previous theorem states regularity of  $y$  in  $L^p$ -spaces. Of course, one can find more detailed regularity results for  $y$  for instance in  $W^{1,p}$ -spaces.

Now, we can prove also an existence result for the optimal control problem under consideration.

LEMMA 2.2. *There exists a uniquely determined optimal control  $\bar{u} \in L^2(\Sigma)$ .*

*Proof.* Since  $u = 0$  is feasible, the set of admissible controls is nonempty. Moreover this set is convex and closed. The objective is strictly convex and radially unbounded. Consequently, we have the existence of a unique optimal solution  $\bar{u} \in L^2(\Sigma)$ .  $\square$

In all what follows, we denote the optimal control by  $\bar{u}$ . Moreover, we use the notation  $\bar{y}$  for the corresponding optimal state (as solution of (1.2)). By  $\bar{p}$  we will denote the solution of the adjoint equation

$$\begin{aligned} -p_t - \Delta p &= 0 && \text{in } Q, \\ \partial_\nu p &= -\gamma\mu_2 && \text{on } \Sigma, \\ p(T) &= y(T) - y_d && \text{on } \Omega \end{aligned} \quad (2.3)$$

Existence and regularity of solutions of that equation can be derived from Theorem 2.1. Here, we cannot apply directly the operator  $\Lambda$ , since (2.3) is backward in time. Let us define the operator  $\tau$ , which describes the time transform  $t \mapsto T - t$ , for abstract functions  $v \in L^2(0, T; X)$  by  $(\tau v)(t) := v(T - t)$ . Using the solution operator  $\Lambda$ , we can write  $(p, p|_\Sigma, p(0)) = (\tau q, \tau q|_\Sigma, q(T))$  with  $(q, q|_\Sigma, q(T)) = \Lambda(0, \tau(-\gamma\mu_2), y(T) - y_d)$ . Let us denote the solution operator of (2.3) by  $\Lambda^*$ , i.e.  $(p, p|_\Sigma, p(0)) = \Lambda^*(0, -\gamma\mu_2, y(T) - y_d)$ . By Theorem 2.1, we get similar regularity results for  $\Lambda^*$  as for  $\Lambda$ .

Now, let us state the necessary – and by convexity sufficient – first-order optimality conditions. For the proof we refer to [2] and [3].

THEOREM 2.3. *There exists a uniquely determined adjoint state  $\bar{p} \in W(0, T)$  and Lagrange multipliers  $\bar{\mu}_1, \bar{\mu}_2 \in L^2(\Sigma)$  such that the following necessary and sufficient first-order optimality conditions are satisfied together with (1.2), (1.3), and (2.3):*

$$\nu\bar{u} + \bar{p} + \bar{\mu}_2 - \bar{\mu}_1 = 0, \quad (2.4)$$

$$\bar{\mu}_i \geq 0 \text{ for } i = 1, 2, \quad (2.5)$$

$$(\bar{u} - \gamma\bar{y} - c)\bar{\mu}_2 = 0, \quad (2.6)$$

$$\bar{u}\bar{\mu}_1 = 0. \quad (2.7)$$

The formulation of the optimality system in Theorem 2.3 has to be modified for the semi-smooth setting. One has to reformulate that system as a non-smooth equation. For instance, one can write an equation for  $\mu_2$  like

$$\mu_2 = \max(0, \mu_2 - C(u - c - \gamma y)) \quad (2.8)$$

with some  $C > 0$ . However, due to the appearance of  $\mu_2$  itself in the argument of the max-function, this equation is not semi-smooth with respect to  $\mu_2 \in L^p(\Sigma)$ . Fortunately, one can find an equivalent reformulation in terms of semi-smooth equations. Similar to [13, Section 4] one can show the following result

THEOREM 2.4. *The formulas*

$$\bar{\mu}_2 = \max(0, -(\bar{p} + \nu(\gamma\bar{y} + c))), \quad (2.9)$$

$$\bar{u} = \max(0, -\frac{1}{\nu}(\bar{p} + \bar{\mu}_2)) \quad (2.10)$$

are equivalent to (1.3) and (2.4)–(2.7).

In the proof it is essential that the active sets  $\{\sigma \in \Sigma : \bar{u}(\sigma) = 0\}$  and  $\{\sigma \in \Sigma : \bar{u}(\sigma) = c(\sigma) + \gamma(\sigma)y(\sigma)\}$  have no common points. This implies  $\bar{\mu}_1\bar{\mu}_2 = 0$  a.e. on  $\Sigma$ . Then both multipliers can be treated separately, and equation (2.8) can be transformed to (2.9). Below, we will prove that this equation is indeed semi-smooth.

These projection formulas are the base to formulate a semi-smooth Newton method to solve the original optimal control problem (1.1)–(1.3). As a by-product, they allow to prove higher regularity of optimal solutions.

THEOREM 2.5. *The solution of the optimal control problem satisfies  $\bar{u}, \bar{\mu}_1, \bar{\mu}_2 \in L^\infty(\Sigma)$ . The regularity of  $\bar{y}, \bar{p}$  is determined by Theorem 2.1.*

*Proof.* The proof uses a bootstrapping procedure. By Theorem 2.3, we know  $\bar{u}, \bar{\mu}_2 \in L^2(\Sigma)$ . Then by Theorem 2.1 there is a  $\delta > 0$  such that  $\bar{y}|_\Sigma, \bar{p}|_\Sigma \in L^{2+\delta}(\Sigma)$  holds. Applying the projection formulas (2.9)–(2.10) we obtain  $\bar{u}, \bar{\mu}_2 \in L^{2+\delta}(\Sigma)$  as well. Again using Theorem 2.1 we find  $\bar{y}|_\Sigma, \bar{p}|_\Sigma \in L^{2+2\delta}(\Sigma)$ . After finitely many steps we arrive at  $\bar{u}, \bar{\mu}_2, \bar{y}|_\Sigma, \bar{p}|_\Sigma \in L^{2+k\delta}(\Sigma)$  with  $2 + k\delta > N + 1$ . Finally, the  $L^\infty$ -part of Theorem 2.1 gives  $\bar{y}|_\Sigma, \bar{p}|_\Sigma \in L^\infty(\Sigma)$ , which implies by the projection representation of  $\bar{u}$  and  $\bar{\mu}_2$  the regularity  $\bar{u}, \bar{\mu}_2 \in L^\infty(\Sigma)$ . And the claim  $\bar{\mu}_1 \in L^\infty(\Sigma)$  follows from (2.4).  $\square$

**3. Semi-smooth Newton method.** In order to apply Newton's method, we write the optimality system as an semi-smooth equation  $F(y, p, u, \mu_2) = 0$ . Let us define the space, where we will look for solutions  $y$  and  $p$ , by

$$Y := W(0, T) \cap C(\bar{Q}), \quad \|v\|_Y := \|v\|_{W(0, T)} + \|v\|_{C(\bar{Q})}.$$

Further let us fix two exponents  $r$  and  $s$  by

$$N + 1 < r < s < \infty.$$

In the sequel, we are looking for controls  $u \in L^r(\Sigma)$  and multipliers  $\mu_2 \in L^s(\Sigma)$ . The multiplier  $\mu_1$  can be reconstructed afterwards by (2.4).

Defining the function  $F : Y \times Y \times L^r(\Sigma) \times L^s(\Sigma) \rightarrow Y \times Y \times L^r(\Sigma) \times L^s(\Sigma)$  by

$$F(y, p, u, \mu_2) = \begin{pmatrix} y - \Lambda(0, u, y_0) \\ p - \Lambda^*(0, -\gamma\mu_2, y(T) - y_d) \\ u - \max(0, -\frac{1}{\nu}(p|_\Sigma + \mu_2)) \\ \mu_2 - \max(0, -(p|_\Sigma + \nu(\gamma y|_\Sigma + c))) \end{pmatrix} \quad (3.1)$$

we can write the optimality system as the equation  $F(\bar{y}, \bar{p}, \bar{u}, \bar{\mu}_2) = 0$ . For the sake of brevity we will omit henceforth the trace operator in the third and fourth component of  $F$ . Due to the appearance of the max-function the function  $F$  cannot be Fréchet differentiable in general. Hence, we resort to a weaker form of differentiability. Here, we use the concept of semi-smoothness as developed in [17]. See also the work of Kummer [7, 8].

DEFINITION 3.1. *Let  $G : X \rightarrow Y$  be a mapping between to Banach spaces  $X$  and  $Y$ .*

Further, let be given a set-valued function  $\partial G : X \rightsquigarrow L(X, Y)$ . Then  $G$  is  $\partial G$ -semi-smooth at  $x \in X$ , if  $G$  is continuous in a neighborhood of  $x$  and it holds

$$\sup_{M \in \partial G(x+s)} \|f(x+s) - f(x) - Ms\|_Y = o(\|s\|_X) \quad \text{as } \|s\|_X \rightarrow 0.$$

Now let us define the set-valued mapping  $\partial F$

$$\partial F(\tilde{y}, \tilde{p}, \tilde{u}, \tilde{\mu}_2)(y, p, u, \mu_2) = \left( \begin{array}{l} y - \Lambda(0, u, 0) \\ p - \Lambda^*(0, -\gamma\mu_2, y(T)) \\ u - D(-\frac{1}{\nu}(\tilde{p} + \tilde{\mu}_2))(-\frac{1}{\nu}(p + \mu_2)) \\ \mu_2 - D(-(\tilde{p} + \nu(\gamma\tilde{y} + c)))(-(p + \nu\gamma y)) \end{array} \right) \quad (3.2)$$

with the set-valued function  $D : L^2(\Sigma) \rightsquigarrow L^\infty(\Sigma)$  given by

$$D(w) = \left\{ v \in L^\infty(\Sigma) : v(x, t) \in \left\{ \begin{array}{ll} \{0\} & \text{if } w(x, t) < 0 \\ [0, 1] & \text{if } w(x, t) = 0 \text{ a.e. on } \Sigma \\ \{1\} & \text{if } w(x, t) > 0 \end{array} \right. \right\}.$$

Let us use in the sequel for abbreviation the space  $X$ , defined by

$$X := Y \times Y \times L^r(\Sigma) \times L^s(\Sigma)$$

and equipped with the norm

$$\|x\|_X = \|(y, p, u, \mu)\|_X := \|y\|_Y + \|p\|_Y + \|u\|_{L^r(\Sigma)} + \|\mu\|_{L^s(\Sigma)}.$$

**COROLLARY 3.2.** *The function  $F : X \rightarrow X$  given by (3.1) is  $\partial F$ -semi-smooth.*

*Proof.* The operators  $\Lambda$  and  $\Lambda^*$  are linear with respect to each variable, hence we have by Theorem 2.1 the semi-smoothness as in the statement of the corollary. It remains to investigate the components  $F_3$  and  $F_4$ , which contain the max-function. It is known that the function  $\max(0, z)$  is  $D(z)$ -semi-smooth from  $L^p \rightarrow L^q$  for  $p > q$ , see e.g. [17]. The trace operator is linear and continuous from  $Y$  to  $L^\infty(\Sigma)$ . Hence, the function  $m_1(p, \mu_2) := \max(0, -\frac{1}{\nu}(p + \mu_2))$  is a semi-smooth mapping from  $Y \times L^s(\Sigma)$  to  $L^r(\Sigma)$ . Analogously, the function  $m_2(y, p) := \max(0, -(p + \nu(\gamma y + c)))$  is semi-smooth from  $Y \times Y \rightarrow L^s(\Sigma)$ .  $\square$

Now, we can apply Newton's method in its semi-smooth variant. For a detailed analysis, we refer to [17]. Let  $x_n = (y_n, p_n, u_n, \mu_n)$  be an iterate in  $X = Y \times Y \times L^r(\Sigma) \times L^s(\Sigma)$ . Then the next iterate  $x_{n+1} = (y_{n+1}, p_{n+1}, u_{n+1}, \mu_{n+1})$  will be determined as the solution of

$$M_n(x_{n+1} - x_n) = -F(x_n). \quad (3.3)$$

Here, the operator  $M_n$  have to be chosen from the subdifferential  $\partial F(x_n)$ . To prove convergence of that method, one has to investigate the solvability of that equation. Furthermore, a uniform bound on  $\|M_n^{-1}\|_{\mathcal{L}(X, X)}$  is needed.

**3.1. Analysis of the subproblems.** Before we start with the investigation of the Newton step (3.3), let us abbreviate the arguments of the subdifferential  $D$  in (3.2) by  $g_n := -\frac{1}{\nu}(p_n + \mu_n)$  and  $h_n := -(p_n + \nu(\gamma y_n + c))$ . At first, we have to chose an element

$M$  of  $\partial F$ . This means, we have to chose in the third and fourth component of (3.2) elements  $d_n^u \in D(g_n)$  and  $d_n^\mu \in D(h_n)$ , respectively. Now, it turns out that the solution of equation (3.3) is equivalent to the solution of the following set of equations for given  $(y_n, p_n, u_n, \mu_n)$ :

$$\begin{aligned} y_{n+1} - y_n - \Lambda(0, u_{n+1} - u_n, 0) &= -y_n + \Lambda(0, u_n, y_0) \\ p_{n+1} - p_n - \Lambda^*(-\gamma(\mu_{n+1} - \mu_n), y_{n+1}(T) - y_n(T)) &= -p_n + \Lambda^*(-\gamma\mu_n, y_n(T) - y_d) \\ u_{n+1} - u_n - d_n^u(g_{n+1} - g_n) &= -u_n + \max(0, g_n) \\ \mu_{n+1} - \mu_n - d_n^\mu(h_{n+1} - h_n) &= -\mu_n + \max(0, h_n). \end{aligned} \quad (3.4)$$

Here, the functions  $d_n^u$  and  $d_n^\mu$  satisfy a.e. on  $\Sigma$

$$d_n^u(x, t) \in \begin{cases} \{0\} & \text{if } -\frac{1}{\nu}(p_n(x, t) + \mu_n(x, t)) < 0, \\ [0, 1] & \text{if } -\frac{1}{\nu}(p_n(x, t) + \mu_n(x, t)) = 0, \\ \{1\} & \text{if } -\frac{1}{\nu}(p_n(x, t) + \mu_n(x, t)) > 0, \end{cases} \quad (3.5)$$

and

$$d_n^\mu(x, t) \in \begin{cases} \{0\} & \text{if } -(p_n(x, t) + \nu(\gamma(x, t)y_n(x, t) + c(x, t))) < 0, \\ [0, 1] & \text{if } -(p_n(x, t) + \nu(\gamma(x, t)y_n(x, t) + c(x, t))) = 0, \\ \{1\} & \text{if } -(p_n(x, t) + \nu(\gamma(x, t)y_n(x, t) + c(x, t))) > 0. \end{cases} \quad (3.6)$$

Since  $\Lambda$  and  $\Lambda^*$  are linear in all arguments, the first and the second equation in (3.4) are equivalent to

$$y_{n+1} = \Lambda(0, u_{n+1}, y_0) \quad \text{and} \quad p_{n+1} = \Lambda^*(0, -\gamma\mu_{n+1}, y_{n+1}(T) - y_d), \quad (3.7)$$

which are the full state and adjoint equations. The third and fourth equation of (3.4) have to be studied pointwise. We distinguish whether  $-\frac{1}{\nu}(p_n(x, t) + \mu_n(x, t))$  is greater, equal, or less than zero. We obtain

$$u_{n+1}(x, t) = \begin{cases} 0 & \text{if } g_n(x, t) = -\frac{1}{\nu}(p_n(x, t) + \mu_n(x, t)) < 0 \\ d_n^u(x, t)g_{n+1}(x, t) & \text{if } g_n(x, t) = -\frac{1}{\nu}(p_n(x, t) + \mu_n(x, t)) = 0 \\ g_{n+1}(x, t) & \text{if } g_n(x, t) = -\frac{1}{\nu}(p_n(x, t) + \mu_n(x, t)) > 0 \end{cases}$$

for the third equation, which can be written as

$$\nu u_{n+1} + d_n^u(p_{n+1} + \mu_{n+1}) = 0.$$

For the fourth equation, we get analogously

$$\mu_{n+1} + d_n^\mu(p_{n+1} + \nu(\gamma y_{n+1} + c)) = 0. \quad (3.8)$$

This equation allows us to eliminate  $\mu_{n+1}$  from the adjoint equation in (3.7). Altogether we then have to solve the following coupled system:

$$\begin{aligned} y_t - \Delta y &= 0 & \text{in } Q, & & -p_t - \Delta p &= 0 & \text{in } Q, \\ \partial_\nu y &= u & \text{on } \Sigma, & & \partial_\nu p &= \gamma d_n^\mu(p + \nu(\gamma y + c)) & \text{on } \Sigma, \\ y(0) &= y_0 & \text{on } \Omega, & & p(T) &= y(T) - y_d & \text{on } \Omega, \end{aligned} \quad (3.9)$$

$$\nu u + d_n^u(1 - d_n^\mu)p - \nu d_n^u d_n^\mu(\gamma y + c) = 0 \quad \text{on } \Sigma. \quad (3.10)$$

Now, we try to reduce the complexity of that system. On the sets, where  $g_n$  and  $h_n$  are zero, we are free to choose the values of  $d_n^u$  and  $d_n^\mu$  from  $[0, 1]$ , respectively. It turns out that it is advantageous to take only values from  $\{0, 1\}$ . Let us define the following sets

$$\mathcal{A}^u = \{(x, t) \in \Sigma : d_n^u(x, t) = 0\}, \quad \mathcal{A}^\mu = \{(x, t) \in \Sigma : d_n^\mu(x, t) = 0\}.$$

The first one,  $\mathcal{A}^u$ , will be the set of active control constraints. The set  $\mathcal{A}^\mu$  corresponds to the active multiplier constraint  $\mu = 0$ , and thus is connected in some sense to inactive control-state constraints. In view of the definition of  $d_n^u$  and  $d_n^\mu$  in (3.5) and (3.6), respectively, we have the following inclusions

$$\mathcal{A}^u \subset \left\{ (x, t) \in \Sigma : -\frac{1}{\nu}(p_n(x, t) + \mu_n(x, t)) \leq 0 \right\} \quad (3.11)$$

and

$$(\Sigma \setminus \mathcal{A}^\mu) \subset \{(x, t) \in \Sigma : -(p_n(x, t) + \nu(\gamma(x, t)y_n(x, t) + c(x, t))) \geq 0\}. \quad (3.12)$$

Equation (3.10) can be rewritten as

$$\begin{aligned} u &= 0 && \text{on } \mathcal{A}^u, \\ \nu u + p &= 0 && \text{on } (\Sigma \setminus \mathcal{A}^u) \cap \mathcal{A}^\mu, \\ u &= \gamma y + c && \text{on } \Sigma \setminus (\mathcal{A}^u \cup \mathcal{A}^\mu). \end{aligned} \quad (3.13)$$

Let us have a look on the boundary conditions of (3.9) and substitute the control  $u$  by the quantities obtained just now:

$$\begin{aligned} \partial_\nu y &= 0, & \partial_\nu p &= 0 && \text{on } \mathcal{A}^u \cap \mathcal{A}^\mu, \\ \partial_\nu y &= 0, & \partial_\nu p - \gamma p &= \gamma\nu(\gamma y + c) && \text{on } \mathcal{A}^u \cap (\Sigma \setminus \mathcal{A}^\mu), \\ \partial_\nu y &= u, & \partial_\nu p &= 0 && \text{on } (\Sigma \setminus \mathcal{A}^u) \cap \mathcal{A}^\mu, \\ \partial_\nu y - \gamma y &= c, & \partial_\nu p - \gamma p &= \gamma\nu(\gamma y + c) && \text{on } \Sigma \setminus (\mathcal{A}^u \cup \mathcal{A}^\mu). \end{aligned} \quad (3.14)$$

With this reformulation we obtain a system for the unknown control  $u|_{(\Sigma \setminus \mathcal{A}^u) \cap \mathcal{A}^\mu}$ , the state  $y$ , and the adjoint state  $p$ . The unknowns have to fulfill the parabolic equations with boundary conditions (3.14) and the second equation of (3.13). The remaining parts of  $u$  and  $\mu$  can be computed afterwards according to (3.8) and (3.13).

We will now answer the question of existence of solutions of that system. Here, it would be nice to find an optimal control problem such that our system is in fact its first order necessary optimality condition. Unfortunately, this is not the case in general. If we look at the boundary conditions (3.14) we see that on  $\mathcal{A}^u \cap (\Sigma \setminus \mathcal{A}^\mu)$  the coefficients in the boundary condition are not the same for  $y$  and for  $p$ :  $\partial_\nu y = ..$  vs.  $\partial_\nu p - \gamma p = ...$ . Hence, the equation for  $p$  is not the adjoint equation to the equation in  $y$ . To avoid this case, let us assume

$$\mathcal{A}^u \cap (\Sigma \setminus \mathcal{A}^\mu) = \emptyset. \quad (3.15)$$

As mentioned above, the set  $\mathcal{A}^u$  corresponds to active control constraints, whereas  $\Sigma \setminus \mathcal{A}^\mu$  is associated with active mixed control-state constraints. Thus, in (3.15) we assume that these active sets do not have common points. We will see that this is a reasonable assumption, since it is fulfilled for the solution of the original problem and in a neighborhood



thereof. Under that assumption, it is easy to verify that the system (3.9)–(3.10) forms the first-order necessary optimality condition of the following optimal control problem:

$$\min \frac{1}{2} \|y(T) - y_d\|_{L^2(\Omega)}^2 + \frac{\nu}{2} \|u\|_{L^2((\Sigma \setminus \mathcal{A}^u) \cap \mathcal{A}^\mu)}^2 + \frac{\nu}{2} \|\gamma y + c\|_{L^2(\Sigma \setminus (\mathcal{A}^u \cup \mathcal{A}^\mu))}^2 \quad (3.16)$$

subject to

$$\begin{aligned} y_t - \Delta y &= 0 && \text{in } Q, \\ \partial_\nu y &= 0 && \text{on } \mathcal{A}^u \cap \mathcal{A}^\mu, \\ \partial_\nu y &= u && \text{on } (\Sigma \setminus \mathcal{A}^u) \cap \mathcal{A}^\mu, \\ \partial_\nu y - \gamma y &= c, && \text{on } \Sigma \setminus (\mathcal{A}^u \cup \mathcal{A}^\mu). \\ y(0) &= y_0 && \text{on } \Omega. \end{aligned} \quad (3.17)$$

This problem is a convex optimization problem. Hence, it admits a unique solution  $(u|_{(\Sigma \setminus \mathcal{A}^u) \cap \mathcal{A}^\mu}, y)$ . Using relation (3.13) it is possible to extend the control to whole  $\Sigma$ . It remains to show that the norm of the solution is bounded independently of the choice of the sets  $\mathcal{A}^u$  and  $\mathcal{A}^\mu$ .

**THEOREM 3.3.** *The system (3.16)–(3.17) is solvable for all sets  $\mathcal{A}^u, \mathcal{A}^\mu \subset \Sigma$  with  $\mathcal{A}^u \cap (\Sigma \setminus \mathcal{A}^\mu) = \emptyset$ . The set of solutions  $(u, y)$  for all the possible choices of  $\mathcal{A}^u, \mathcal{A}^\mu$  is bounded, i.e. it holds*

$$\|u\|_{L^r(\Sigma)} + \|y\|_Y \leq C$$

for all solutions of (3.16)–(3.17) with a constant  $C > 0$  independently of  $\mathcal{A}^u, \mathcal{A}^\mu$ .

*Proof.* Let us abbreviate the domain of the control functions by  $\mathcal{U} := (\Sigma \setminus \mathcal{A}^u) \cap \mathcal{A}^\mu$ .

At first, we have to mention that the parabolic equation (3.17) is uniquely solvable. The coefficient in the boundary condition is negative but bounded from below by  $-\|\gamma\|_{L^\infty(\Sigma)}$  independently of  $\mathcal{A}^u, \mathcal{A}^\mu$ . Unlike to elliptic equations, this fact does not influence the existence of solutions. Furthermore, we have similar smoothing and regularity properties as in Theorem 2.1, see [10, Prop. 3.3]. Moreover, as argued in [10], the norms of the associated solution operator depend only on the lower bound of the coefficient. We have for instance for given  $u \in L^2(\mathcal{U})$  the existence of a solution  $y$  of (3.17) that satisfies

$$\|y\|_{W(0,T)} + \|y\|_{L^2(\Sigma)} + \|y(T)\|_{L^2(\Omega)} \leq c_1 (\|u\|_{L^2(\mathcal{U})} + \|c\|_{L^\infty(\Sigma)} + \|y_0\|_{L^2(\Omega)}), \quad (3.18)$$

and for  $u \in L^r(\mathcal{U})$ ,  $r > N + 1$ , this solution  $y$  is in  $L^\infty$  and satisfies the estimate

$$\|y\|_{L^\infty(\Sigma)} + \|y(T)\|_{L^\infty(\Omega)} \leq c_2 (\|u\|_{L^r(\mathcal{U})} + \|c\|_{L^\infty(\Sigma)} + \|y_0\|_{L^r(\Omega)}). \quad (3.19)$$

In both inequalities, the constants  $c_1, c_2$  depend on  $\|\gamma\|_{L^\infty(\Sigma)}$  but not on  $\mathcal{A}^u, \mathcal{A}^\mu$ . A similar estimate holds also for the bootstrapping result as in Theorem 2.1. There is a  $\delta > 0$  and a constant  $c_{3,q} = c_{3,q}(q)$  such that for all  $q \geq 2$  it holds

$$\|y\|_{L^{q+\delta}(\Sigma)} + \|y(T)\|_{L^{q+\delta}(\Omega)} \leq c_{3,q} (\|u\|_{L^q(\mathcal{U})} + \|c\|_{L^\infty(\Sigma)} + \|y_0\|_{L^\infty(\Omega)}). \quad (3.20)$$

Since the proof uses only interpolation arguments as in [15], it follows that  $c_{3,q}$  depends on  $q, \|\gamma\|_{L^\infty(\Sigma)}$  but not on  $\mathcal{A}^u, \mathcal{A}^\mu$ .

By convexity, the problem under consideration admits a unique solution  $(u, y)$ . It remains to prove an uniform upper bound of the  $L^r$ -norm of  $u$  and of the  $L^\infty$ -norm of  $y$ , which is independent of the choice of  $\mathcal{A}^u$  and  $\mathcal{A}^\mu$ .

To this end, we test (3.13)<sub>2</sub> by  $u$ . We use the well-known method of transposition, see e.g. [16, Satz 3.18], and obtain

$$\begin{aligned} 0 &= \nu \|u\|_{L^2(\mathcal{U})}^2 + (p|_{\mathcal{U}}, u) = \nu \|u\|_{L^2(\mathcal{U})}^2 + (y(T) - y_d, y(T)) \\ &= \nu \|u\|_{L^2(\mathcal{U})}^2 + \|y(T)\|_{L^2(\Omega)}^2 - (y(T), y_d), \end{aligned}$$

which directly leads to the estimate

$$\|u\|_{L^2(\mathcal{U})} \leq \frac{1}{\sqrt{2\nu}} \|y_d\|_{L^2(\Omega)} =: M_1.$$

Using the estimate (3.18) and the relation (3.13)<sub>3</sub> we find

$$\begin{aligned} \|y\|_{W(0,T)} + \|y\|_{L^2(\Sigma)} + \|y(T)\|_{L^2(\Omega)} &\leq c_1 (M_1 + \|c\|_{L^\infty(\Sigma)} + \|y_0\|_{L^\infty(\Omega)}), \\ \|u\|_{L^2(\Sigma)} &\leq M_1 + \|\gamma\|_{L^\infty(\Sigma)} \|y\|_{L^2(\Sigma)} + \|c\|_{L^2(\Sigma)}. \end{aligned}$$

Altogether, we have the existence of an upper bound  $M_2$  independently of the actual choice of  $\mathcal{A}^u, \mathcal{A}^\mu$ ,

$$\|u\|_{L^2(\Sigma)} + \|y\|_{W(0,T)} + \|y\|_{L^2(\Sigma)} + \|y(T)\|_{L^2(\Omega)} \leq M_2. \quad (3.21)$$

Now, we will apply the same bootstrapping procedure as in Theorem 2.5. We will need estimates for the adjoint state  $p$ , which is the solution of the following equation

$$\begin{aligned} -p_t - \Delta p &= 0 && \text{in } Q, \\ \partial_\nu p &= 0 && \text{on } \mathcal{A}^u \cap \mathcal{A}^\mu, \\ \partial_\nu p &= 0 && \text{on } (\Sigma \setminus \mathcal{A}^u) \cap \mathcal{A}^\mu, \\ \partial_\nu p - \gamma p &= \gamma \nu (\gamma y + c) && \text{on } \Sigma \setminus (\mathcal{A}^u \cup \mathcal{A}^\mu), \\ p(T) &= y(T) - y_d && \text{on } \Omega. \end{aligned} \quad (3.22)$$

It turns out, that the estimates (3.18)–(3.20) are also applicable to (3.22). The system is uniquely solvable and satisfies the following estimates depending on the regularity of the data: if  $y \in L^s(\Sigma)$  for  $s > N + 1$  then it holds

$$\|p\|_{L^\infty(\Sigma)} \leq c_2 \left( \nu \|\gamma\|_{L^\infty(\Sigma)}^2 \|y\|_{L^s(\Sigma)} + \nu \|\gamma\|_{L^\infty(\Sigma)} \|c\|_{L^\infty(\Sigma)} + \|y(T) - y_d\|_{L^\infty(\Omega)} \right), \quad (3.23)$$

and there is a constant  $\delta > 0$  such that for all  $q \geq 2$  it holds

$$\|p\|_{L^{q+\delta}(\Sigma)} \leq c_{3,q} \left( \nu \|\gamma\|_{L^\infty(\Sigma)}^2 \|y\|_{L^q(\Sigma)} + \nu \|\gamma\|_{L^\infty(\Sigma)} \|c\|_{L^\infty(\Sigma)} + \|y(T) - y_d\|_{L^q(\Omega)} \right). \quad (3.24)$$

Now, the claim follows by a simple bootstrapping procedure using the smoothing properties of (3.19)–(3.20) and (3.23)–(3.24). Since all constants in these estimates and the bound (3.21) are independent of the choice of  $\mathcal{A}^u$  and  $\mathcal{A}^\mu$ , the final bound of  $\|u\|_{L^r(\Sigma)} + \|y\|_Y$  is also independent of that sets.  $\square$

Let us summarize the results obtained so far concerning the solvability of the system (3.9)–(3.10) arising in a step of the semi-smooth Newton method.

**THEOREM 3.4.** *Under the assumption  $d_n^u(x, t), d_n^\mu(x, t) \in \{0, 1\}$  a.e. on  $\Sigma$  and the assumption (3.15), the system (3.9)–(3.10) admits a unique solution  $(y, u, p, \mu)$ . Moreover, there is a constant  $C > 0$  independent of  $d_n^u, d_n^\mu$  such that*

$$\|y\|_Y + \|p\|_Y + \|u\|_{L^r(\Sigma)} + \|\mu\|_{L^s(\Sigma)} \leq C.$$

*Proof.* The bound for  $y, u, p$  was derived in the proof of the previous Theorem 3.3. The claim for  $\mu$  follows then by the representation (3.8).  $\square$

**3.2. Convergence result.** We are now in the position to prove the convergence of the semi-smooth variant of Newton's method. In the previous section, we investigated the properties of the equation that has to be solved in each step. Under the separation assumption (3.15), we proved solvability and uniform boundedness of solutions of the subproblem (3.16). It remains to ensure that the active sets associated to the iterates fulfill this assumption.

Let us recall for convenience the definition of the sets  $\mathcal{A}_n^u$  and  $\mathcal{A}_n^\mu$ . Let  $(y_n, p_n, u_n, \mu_n)$  be some iterate, then it holds

$$\mathcal{A}_n^u \subset \left\{ (x, t) \in \Sigma : -\frac{1}{\nu}(p_n(x, t) + \mu_n(x, t)) \leq 0 \right\} =: \tilde{\mathcal{A}}_n^u$$

$$(\Sigma \setminus \mathcal{A}_n^\mu) \subset \left\{ (x, t) \in \Sigma : -(p_n(x, t) + \nu(\gamma(x, t)y_n(x, t) + c(x, t))) \geq 0 \right\} =: \tilde{\mathcal{I}}_n^\mu$$

cf. (3.5) and (3.6). Now, let us prove that under certain assumptions the intersection  $\tilde{\mathcal{A}}_n^u \cap \tilde{\mathcal{I}}_n^\mu$  is empty, which implies condition (3.15) for  $\mathcal{A}_n^u$  and  $\mathcal{A}_n^\mu$ , i.e.  $\mathcal{A}_n^u \cap (\Sigma \setminus \mathcal{A}_n^\mu) = \emptyset$ .

**LEMMA 3.5.** *Let  $(y_n, p_n, u_n) \in Y \times Y \times L^r(\Sigma)$  be given with  $\gamma(x, t)y_n(x, t) + c(x, t) > 0$  a.e. on  $\Sigma$ . And let  $\mu_n$  satisfy*

$$\mu_n + \chi_{\Sigma \setminus \mathcal{A}_{n-1}^\mu}(p_n + \nu(\gamma y_n + c)) = 0 \quad (3.25)$$

for a given set  $\mathcal{A}_{n-1}^\mu$ , cf. (3.8).

Then, the corresponding sets  $\tilde{\mathcal{A}}_n^u$  and  $\tilde{\mathcal{I}}_n^\mu$  fulfill  $\tilde{\mathcal{A}}_n^u \cap \tilde{\mathcal{I}}_n^\mu = \emptyset$ .

*Proof.* If  $\tilde{\mathcal{I}}_n^\mu = \emptyset$ , holds nothing has to be proven. Otherwise, let us take  $(x, t) \in \tilde{\mathcal{I}}_n^\mu$ , which implies the inequality  $-(p_n(x, t) + \nu(\gamma(x, t)y_n(x, t) + c(x, t))) \geq 0$  by construction of  $\tilde{\mathcal{I}}_n^\mu$ .

If on one hand  $(x, t)$  belongs to  $\Sigma \setminus \mathcal{A}_{n-1}^\mu$  then we have using (3.25)

$$\begin{aligned} -(p_n(x, t) + \mu_n(x, t)) &= -p_n(x, t) + (p_n(x, t) + \nu(\gamma(x, t)y_n(x, t) + c(x, t))) \\ &= \nu(\gamma(x, t)y_n(x, t) + c(x, t)) > 0. \end{aligned}$$

On the other hand,  $(x, t) \notin \Sigma \setminus \mathcal{A}_{n-1}^\mu$  implies  $\mu_n(x, t) = 0$ , which gives together with the definition of  $\tilde{\mathcal{I}}_n^\mu$  gives

$$-(p_n(x, t) + \mu_n(x, t)) = -p_n(x, t) \geq \nu(\gamma(x, t)y_n(x, t) + c(x, t)) > 0.$$

It follows  $(x, t) \notin \tilde{\mathcal{A}}_n^u$ , and the claim is proven.  $\square$

Please note, that we did not use any information about the set  $\mathcal{A}_{n-1}^\mu$ . Moreover, the proof remains true, if one substitutes (3.25) by  $\mu_n = \max(0, -(p_n + \nu(\gamma_n y + c)))$ .

Now, we are ready to prove the convergence of the method. A crucial point is that the separation of the active sets can be maintained to apply the uniform bound in Theorem 3.4. Let  $\bar{x} = (\bar{y}, \bar{p}, \bar{u}, \bar{\mu}_2)$  be the solution of the optimal control problem (1.1)–(1.3).

**THEOREM 3.6.** *Let us choose in each step  $d_n^u(x, t), d_n^\mu(x, t) \in \{0, 1\}$  a.e. on  $\Sigma$ . Then there is a constant  $\rho > 0$  such that for all  $x_0 = (y_0, p_0, u_0, \mu_0)$  with  $\|\bar{x} - x_0\|_X < \rho$*

and  $\mathcal{A}_0^u \cap (\Sigma \setminus \mathcal{A}_0^\mu) = \emptyset$  the semi-smooth Newton's method either terminates with the solution  $x_k = \bar{x}$  or converges  $q$ -superlinearly to  $\bar{x}$  in  $X = Y \times Y \times L^r(\Sigma) \times L^s(\Sigma)$ .

*Proof.* At first, there is a constant  $\rho_0 > 0$  such that for all  $u$  with  $\|\bar{u} - u\|_{L^r(\Sigma)} < \rho_0$  the corresponding solution  $y$  of the state equation (2.1) fulfills  $\gamma y + c > 0$ . This is a direct consequence of Theorem 2.1 and the assumption on  $c$ .

If all iterates  $u_n$  of the method stay in that neighborhood of  $\bar{u}$ ,  $\gamma y_n + c > 0$  would hold for all  $n$ . This would imply by the previous Lemma 3.5 that the sets  $\mathcal{A}_n^u, \mathcal{A}_n^\mu$  would fulfill  $\mathcal{A}_n^u \cap (\Sigma \setminus \mathcal{A}_n^\mu) = \emptyset$  for all  $n$ .

However, the general convergence result of [17, Theorem 6.5] is not directly applicable, since the uniform bound in Theorem 3.4 holds only in a neighborhood of the solution. Fortunately, one can use the argumentation in the proof of [17, Theorem 6.5] to conclude the existence of a constant  $\rho$  with  $0 < \rho < \rho_0$ , such that the iterates of the algorithm stay in that neighborhood and converge  $q$ -superlinearly (or the solution is found in finitely many steps).  $\square$

**4. Numerical results.** Let us now present some numerical experiments. We show results for an optimal control problem with known solution. We consider the following problem, which is a slight modification of the problem analysed in the present article:

$$\min \frac{1}{2} \|y(T) - y_T\|_{L^2(\Omega)}^2 + \frac{1}{2} \|y|_{\Sigma} - y_{\Sigma}\|_{L^2(\Sigma_o)}^2 + \frac{\nu}{2} \|u - u_d\|_{L^2(\Sigma_c)}^2$$

subject to the parabolic equation

$$\begin{aligned} y_t - \Delta y &= 0 && \text{in } Q, \\ \partial_\nu y &= u && \text{on } \Sigma_c, \\ \partial_\nu y &= 0 && \text{on } \Sigma \setminus \Sigma_c, \\ y(0) &= y_0 && \text{on } \Omega \end{aligned}$$

and to the mixed control-state constraints

$$u_a(x, t) \leq u(x, t) \leq c(x, t) + \gamma(x, t)y(x, t) \quad \text{a.e. in } \Sigma_c.$$

Here, the domain  $\Omega$  is the unit square  $(0, 1)^2$ , the final time is  $T = 1$ , the control acts on

$$\Sigma_c = \Sigma_o = \{(x_1, x_2, t) \in \Sigma : x_1 = 1\}.$$

Given are the following quantities in the cost functional

$$\begin{aligned} y_0(x_1, x_2) &= \cos(\pi x_1), \\ y_T(x_1, x_2) &= e^{-\pi^2 T} \cos(\pi x_1) - \cos(2\pi x_1), \\ y_G(x_2, t) &= -\mu_2 - e^{-\pi^2 t}, \\ u_d(x_2, t) &= \frac{1}{\nu} (e^{-4\pi^2(T-t)} + \chi_{[0.5, 1]}(t) - \chi_{[0, 0.4]}(t)), \end{aligned}$$

and for the control and mixed control-state constraints

$$\begin{aligned} u_a(x_2, t) &= -\chi_{[0.4, 1]}(t), \\ c(x_2, t) &= (1 + \chi_{[0, 0.5]}(t))e^{-\pi^2 t}, \\ \gamma(x_2, t) &= 1. \end{aligned}$$

Then our test problem admits the the solution

$$\begin{aligned} y(x_1, x_2, t) &= e^{-\pi^2 t} \cos(\pi x_1), \\ p(x_1, x_2, t) &= e^{-4\pi^2(T-t)} \cos(2\pi x_1), \\ u(x_2, t) &= 0, \\ \mu_2(x_2, t) &= \chi_{[0.5,1]}(t). \end{aligned}$$

The projection representation (2.9)–(2.10) transforms to

$$\begin{aligned} \bar{\mu}_2 &= \max(0, -(\bar{p} + \nu(\gamma\bar{y} + c - u_d))), \\ \bar{u} &= \max(u_a, u_d - \frac{1}{\nu}(\bar{p} + \bar{\mu}_2)). \end{aligned}$$

For the computations the problem was discretized by finite differences on an equidistant grid with  $n_{x_1} \times n_{x_2} = 200 \times 200$  grid points. The time axis was divided in  $n_t = 2000$  subintervals.

We started the method with a randomly chosen control  $u_0$  and multiplier  $\mu_2 \equiv 0$ . The starting values for state and adjoint were then computed as the corresponding solutions of (1.2) and (2.3), respectively. The regularization parameter for the control was set to  $\nu = 0.1$ .

In Table 4.1, we report about the convergence history. In the second and fourth columns, the differences  $\|u_n - \bar{u}\|_{L^3(\Sigma)}$  and  $\|\mu_n - \bar{\mu}\|_{L^4(\Sigma)}$  can be found. The convergence we tried two measure with  $q_u := \frac{\|u_n - \bar{u}\|_{L^3(\Sigma)}}{\|u_{n+1} - \bar{u}\|_{L^3(\Sigma)}}$  and  $q_\mu := \frac{\|\mu_n - \bar{\mu}\|_{L^4(\Sigma)}}{\|\mu_{n+1} - \bar{\mu}\|_{L^4(\Sigma)}}$ . The iterates show a superlinearly convergence as proven in Theorem 3.6.

$n$	$\ u_n - \bar{u}\ _{L^3(\Sigma)}$	$q_u$	$\ \mu_n - \bar{\mu}\ _{L^4(\Sigma)}$	$q_\mu$
0	$5.80 \cdot 10^{-3}$		$1.77 \cdot 10^{-5}$	
1	$4.28 \cdot 10^{-5}$	0.01	$2.36 \cdot 10^{-5}$	1.33
2	$5.65 \cdot 10^{-5}$	1.32	$5.62 \cdot 10^{-6}$	0.24
3	$1.09 \cdot 10^{-5}$	0.19	$7.35 \cdot 10^{-7}$	0.13
4	$1.36 \cdot 10^{-6}$	0.12	$8.13 \cdot 10^{-8}$	0.11
5	$4.55 \cdot 10^{-8}$	0.03	$2.20 \cdot 10^{-8}$	0.27

TABLE 4.1  
Iteration history of the numerical example

**5. Conclusions.** In this section we will comment briefly on the specifics of the considered problem and on possible extensions.

**5.1. Other state equations.** In the analysis of the subproblems arising in semi-smooth Newton's method we relied heavily on the fact that the solvability of the state equation is not affected by changes in the coefficients. The situation changes in general for other equations. To see this, let us briefly look at the linear elliptic case: Similar to (3.17) we have to investigate the solvability of the following equation:

$$\begin{aligned} -\Delta y &= 0 && \text{in } \Omega, \\ \partial_\nu y &= 0 && \text{on } \mathcal{A}^u \cap \mathcal{A}^\mu, \\ \partial_\nu y &= u && \text{on } (\Gamma \setminus \mathcal{A}^u) \cap \mathcal{A}^\mu, \\ \partial_\nu y - \gamma y &= c, && \text{on } \Gamma \setminus (\mathcal{A}^u \cup \mathcal{A}^\mu). \end{aligned}$$

Because of the term  $-\gamma y$  in the last line one has to avoid explicitly the eigenvalue case.

If the state equation is no longer a linear one, then the situation becomes much more difficult. At first, the necessary optimality conditions are not longer also sufficient, since the problem is not convex anymore in general. To compensate this, one has to assume the satisfaction of a second-order sufficient optimality condition at the optimal point. The theory of such a method would require a combination of the methods of this paper with the proving technique of the convergence of the SQP method, see Griesse, Metla, and Rösch [4]. However, one can view on such problems also from another side: The presented results are used for solving the quadratic subproblems of the SQP-methods. Then, both results can be directly applied.

**5.2. Other constraints.** The presented theory used specific properties of the inequality constraints: First, we were able to prove a reformulation of the optimality system which fits to the theory of semi-smooth Newton methods. Consequently this technique cannot be applied to pointwise state constraints. Moreover, the derivation of the corresponding projection formulas for a finite number of mixed constraints and control constraints requires additional assumptions, see Rösch and Tröltzsch [12].

Second, we were able to show that the active sets for the control and the mixed constraint are separated in the optimal point. Moreover these sets stay separated in a small  $L^r$ -neighborhood of the optimal control, see Lemma 3.5. Consequently, the discussion of more general constraints requires a careful analysis of the active sets. In particular, working with only one  $L^r$ -space for the control cannot guarantee the desired results. We will investigate this general situation in a forthcoming paper.

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