On a Lagrange–Newton method for a nonlinear parabolic boundary control problem *

H. Goldberg and F. Tröltzsch†
Technical University of Chemnitz–Zwickau
Faculty of Mathematics

July 17, 1997

Abstract

An optimal control problem governed by the heat equation with nonlinear boundary conditions is considered. The objective functional consists of a quadratic terminal part and a quadratic regularization term. On transforming the associated optimality system to a generalized equation, an SQP method for solving the optimal control problem is related to the Newton method for the generalized equation. In this way, the convergence of the SQP method is shown by proving the strong regularity of the optimality system. After explaining the numerical implementation of the theoretical results some high precision test examples are presented.

AMS subject classification: 49M40, 49M05

Keywords: optimal control, semilinear parabolic equation, multigrid method, SQP method

1 Introduction

Lagrange-Newton-SQP methods in infinite-dimensional spaces have received much attention during the past years. For general investigations in Banach spaces and their application to the optimal control of ordinary differential equations we refer, for instance, to Alt [1], [2], Alt and Malanowski [4], to the mesh independence principle in Alt [3], and to the numerical application in Machielsen [23]. The control of weakly singular integral equations was considered by Alt, Sontag and Tröltzsch [5].

*Supported by Deutsche Forschungsgemeinschaft (DFG), under grant "Tr 302/1–3"
†D–09107 Chemnitz, Germany

Paralleling this development, the case of nonlinear partial differential equations was investigated. Numerical aspects of SQP and related methods are considered for problems without control constraints by Kupfer and Sachs [21], Heinkenschloss [14], and with additional control constraints by Heinkenschloss and Sachs [15], who report on different techniques for an effective numerical implementation. Moreover, we refer to the convergence analysis done by Ito and Kunisch [17], [18] in a Hilbert space setting and to associated numerical test examples.

First rigorous proofs of convergence in the presence of constraints on the control were given for semilinear partial differential equations by Tröltzsch [29] for a 1-D nonlinear parabolic boundary control problem with the integral equation method and by Heinkenschloss and Tröltzsch [16] for a system of phase-field equations in the framework of weak solutions. A semigroup approach for a particular parabolic model in N-dimensional domains is contained for a simplified model in [28].

Our paper concentrates on two main points. In contrast to [16], [28], and [29], where the convergence analysis is based on a quite strong second order sufficient optimality condition, we follow Dontchev, Hager, Poore and Yang [10] and include here first order sufficient conditions to tighten the inevitable gap between second order necessary and sufficient conditions. This is worked out for a simplified model including terminal observations to make the analysis more transparent. The convergence analysis for general semilinear parabolic problems is very extensive and will be presented in the forthcoming paper [30].

Moreover, we report on our computational experience for the 1-D heat equation including pointwise constraints on the control. The SQP method was implemented as close as possible to its infinite-dimensional version and shows the expected fast convergence. We should underline that we did not concentrate on the numerical efficiency of the single SQP steps. In fact, modifications of the technique can be more effective, and we refer the reader to the papers [14], [15], [21], mentioned above. A computational verification of our (infinite-dimensional) analysis is the main aim of the numerical part (cf. the remarks at the beginning of section 7).

We consider the optimal boundary control problem to *minimize*

$$\varphi(y,u) = \frac{1}{2}\|y(T,\cdot) - y_T\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|u\|^2_{L^2(\Sigma)} \tag{1.1}$$

subject to

$$\begin{array}{rcll} y_t(t,x) & = & \Delta_x y(t,x) & \text{in} \quad Q \\ y(0,x) & = & y_0(x) & \text{in} \quad \Omega \\ \partial_n y(t,x) & = & b(y(t,x)) + u(t,x) & \text{on} \quad \Sigma \end{array} \tag{1.2}$$

and

$$u_a \le u(t,x) \le u_b \qquad \text{a.e. on } \Sigma. \tag{1.3}$$

Although the problem can be discussed under much weaker conditions and in more generality, we study for convenience this simplified version of a control problem and rely on the following strong assumptions: $\Omega \in I\!R^n$ is a bounded domain with boundary Γ of class $C^{2,\alpha}$, $Q = (0,T) \times \Omega$, $\Sigma = (0,T) \times \Gamma$, $T > 0$, $\lambda > 0$, $u_a \le u_b$ are fixed real numbers, and y_0, $y_T \in C(\overline{\Omega})$ are given functions. By ∂_n the (outward) normal derivative on Γ is denoted. We assume that $b = b(y)$ belongs to $C^{2,1}(I\!R)$ and is monotone non–increasing. The *control* function $u = u(t,x)$ is looked upon in $L^\infty(\Sigma)$, while the *state* $y = y(t,x)$ is defined as weak solution of (1.2) in $Y = W(0,T) \cap C(\overline{Q})$, where $W(0,T) = \{y \in L^2(0,T;H^1(\Omega)) | \, y_t \in L^2(0,T;H^1(\Omega)')\}$ (cf. Lions and Magenes [22]). A weak solution y of (1.2) is defined by $y(0,x) = y_0$ and

$$(y_t(t),v)_{(H^1)',H^1} + \int\limits_\Omega \nabla y(t) \nabla v \, dx = \int\limits_\Gamma (b(y(t,\cdot)) + u(t,\cdot)) v \, dS \qquad \text{a.e. } t \in (0,T) \quad (1.4)$$

for all $v \in H^1(\Omega)$ (dS: surface measure on Γ). Note that $W(0,T) \subset C([0,T],L^2(\Omega))$, continuously. We endow Y with the norm

$$\|y\|_Y = \|y\|_{W(0,T)} + \|y\|_{C(\overline{Q})}.$$

2 The parabolic initial–boundary value problem

In this section we provide some important properties of (1.2) and a linearized version of it without proof. First, we consider the linear system

$$\begin{aligned} y_t &= \Delta_x y && \text{in } Q && (2.1)\\ y(0) &= y_0 && \text{in } \Omega && (2.2)\\ \partial_n y + \beta y &= g && \text{in } \Sigma. && (2.3) \end{aligned}$$

Lemma 2.1 *Let $p > n+1$ and $\beta \in L^\infty(\Sigma)$, $\beta \ge 0$. If $g \in L^p(\Sigma)$ and $y_0 = 0$, then the unique weak solution y of (2.1)–(2.3) belongs to Y. The linear mapping $G : g \mapsto y$ is continuous from $L^p(\Sigma)$ to Y. If $g = 0$ and $y_0 \in C(\overline{\Omega})$, then $y \in Y$, too. The linear mapping $G_0 : y_0 \mapsto y$ is continuous from $C(\overline{\Omega})$ to Y.*

The Lemma follows from Theorem 3.1 and Proposition 3.1 in Raymond and Zidani [24]. Next, we consider the nonlinear system (1.2).

Lemma 2.2 *Let $p > n+1$. Then (1.2) admits for each $u \in L^p(\Sigma)$ a unique weak solution $y \in Y$. The mapping $u \mapsto y = y(u)$ is of class C^2 from $L^p(\Sigma)$ to Y. There is a constant c_L such that*

$$\|y(u_1) - y(u_2)\|_Y \le c_L \, \|u_1 - u_2\|_{L^p(\Sigma)}$$

holds for all u_1, u_2 satisfying the constraints (1.3).

This result can be derived from [24].

In what follows, we define the "boundary operator " G, and the "initial operator" G_0 according to Lemma 2.1 for $\beta = 0$. Moreover, we introduce a Nemytskiĭ operator $B : C(\overline{Q}) \to L^p(\Sigma)$ by

$$B(y)(t,x) = b(y(t,x)), \qquad\qquad (t,x) \in \Sigma.$$

In this way, the nonlinear parabolic system (1.2) can be re–formulated as equation in $C(\overline{Q})$ by

$$y = G_0 y_0 + G(B(y) + u). \tag{2.4}$$

B is of class C^2, as the trace mapping $y \mapsto \gamma y$ is linear and continuous from $C(\overline{Q})$ to $C(\overline{\Sigma})$ and $y \mapsto b(y)$ is C^2 from $C(\overline{\Sigma})$ to $C(\overline{\Sigma}) \hookrightarrow L^p(\Sigma)$.

3 First and second order optimality conditions

We assume once and for all that a fixed *reference control* $\bar{u} \in U_{ad} = \{u \in L^\infty(\Sigma) | u_a \le u \le u_b\}$ is given, which satisfies together with its associated state $\bar{y} = y(\bar{u}) \in Y$ and an adjoint state $\bar{p} \in Y$ the standard *first order optimality system* consisting of (1.2), the control constraint $\bar{u} \in U_{ad}$, the *adjoint equation*

$$\begin{array}{rcll} -\bar{p}_t(t,x) & = & \Delta_x \bar{p}(t,x) & \text{in } Q \\ \bar{p}(T,x) & = & \bar{y}(T,x) - y_T(x) & \text{in } \Omega \\ \partial_n \bar{p}(t,x) & = & b'(\bar{y}(t,x))\bar{p}(t,x) & \text{on } \Sigma \end{array} \tag{3.1}$$

and the *variational inequality*

$$\int_\Sigma (\lambda \bar{u} + \bar{p})(u - \bar{u})\, dS\, dt \ge 0 \qquad\qquad \forall u \in U_{ad}. \tag{3.2}$$

Existence and uniqueness for (3.1) can be discussed by means of Lemma 2.1 and the transformation of time $t' = T - t$. In particular, this yields $\bar{p} \in C(\overline{Q})$. A well known argument shows that (3.2) is equivalent to

$$\bar{u}(t,x) = P_{[u_a,u_b]}\{-\lambda^{-1}\bar{p}(t,x)\} \qquad \text{a.e. } (t,x) \in \Sigma, \tag{3.3}$$

where $P_{[u_a,u_b]} : I\!R \to [u_a, u_b]$ denotes projection onto $[u_a, u_b]$. The continuity of $\bar{p}$ and (3.3) show that $\bar{u}$ is continuous.

For convenience we introduce the *Lagrange function* $\mathcal{L} : Y \times L^\infty(\Sigma) \times Y \to I\!R$ by

$$\mathcal{L}(y,u,p) = \varphi(y,u) - \int_Q (y_t p + \nabla y \nabla p)\, dx\, dt + \int_\Sigma (b(y) + u) p\, dS\, dt. \tag{3.4}$$

In (3.4) the integral over $y_t\, p$ stands for the value of the functional $y_t \in L^2(0,T;H^1(\Omega)')$ at $p \in L^2(0,T;H^1(\Omega))$. $\mathcal{L}$ is of class C^2 w.r. to (y,u). By $\mathcal{L}'$, $\mathcal{L}''$ we denote the first and second order Fréchet derivative of $\mathcal{L}$ w.r. to (y,u) in $Y \times L^\infty(\Sigma)$. We write $\mathcal{L}''(y,u,p)[v]^2$ for $\mathcal{L}''(y,u,p)[v,v]$ to shorten long expressions. It should be mentioned that (3.1)–(3.2) can be formulated also by

$$\mathcal{L}'(\bar{y},\bar{u},\bar{p})(y,u-\bar{u}) \geq 0 \qquad \forall y \in W(0,T) \quad \text{with} \quad y(0)=0 \quad \text{and } \forall u \in U_{ad}. \tag{3.5}$$

To establish a second order sufficient optimality condition being arbitrarily close to the corresponding necessary ones, we consider also first order sufficient conditions: Following [10] we define for fixed (arbitrarily small) $\sigma > 0$

$$I_\sigma = \{(t,x) \in \Sigma \mid \qquad |\lambda \bar{u}(t,x) + \bar{p}(t,x)| \geq \sigma\}. \tag{3.6}$$

Note that (3.2) (or (3.3)) implies $\bar{u}(t,x) \in \{u_a, u_b\}$ a.e. on I_σ. In fact, we have $\bar{u}(t,x) = u_a$, where $\lambda\bar{u}(t,x) + \bar{p}(t,x)$ is positive and $\bar{u}(t,x) = u_b$, if the expression is negative.

We suppose that the triplet $(\bar{y},\bar{u},\bar{p})$ satisfies the *second order sufficient optimality condition* (SSC): There are $\delta > 0$, $\sigma > 0$ such that

(SSC)

$$\mathcal{L}''(\bar{y},\bar{u},\bar{p})[(y,u),(y,u)] \geq \delta \|u\|^2_{L^2(\Sigma)} \tag{3.7}$$

holds for all $(y,u) \in W(0,T) \times L^2(\Sigma)$ such that $u = 0$ on I_σ and

$$\begin{aligned} y_t &= \Delta_x y \\ y(0) &= 0 \\ \partial_n y &= b'(\bar{y})y + u. \end{aligned} \tag{3.8}$$

We assume in our analysis below that $mes\, I_\sigma < mes \Sigma$, i.e. that (3.7) is not trivially satisfied. In the opposite case, first order sufficiency holds a.e. on Σ. Then the theory of the next chapters simplifies in an obvious way.

One can show that $(\bar{y},\bar{u})$ is locally optimal for the control problem in the sense of $Y \times L^\infty(\Sigma)$, if $(\bar{y},\bar{u},\bar{p})$ satisfies the first order optimality system together with (SSC). We refer to the elliptic case discussed in Casas, Tröltzsch and Unger [7]. The extension to the parabolic case is straightforward.

4 The Generalized Newton method

Completely analogous to (2.4) we can formulate the adjoint equation (3.1) as

$$p = G_T(y(T) - y_T) + DB'(y)p, \tag{4.1}$$

where the "final operator" $G_T : C(\overline{\Omega}) \to Y$ gives the solution of (3.1) with homogeneous boundary condition $\partial_n p = 0$ and $D : L^\infty(\Sigma) \to Y$ is the corresponding "boundary operator". Moreover, we introduce the set–valued mapping $N : L^\infty(\Sigma) \to 2^{L^\infty(\Sigma)}$ by

$$N(u) = \{v \in L^\infty(\Sigma) | \int_\Sigma v(z-u)\, dS\, dt \le 0 \quad \forall z \in U_{ad}\}.$$

N is the *normal cone* of U_{ad} at u. Then (3.2) reads $0 \in \lambda\bar{u} + \bar{p} + N(\bar{u})$. Let $W := C(\overline{Q})^2 \times L^\infty(\Sigma)$, f_1, $f_2 : W \to C(\bar{Q})$, $f_3 : W \to L^\infty(\Sigma)$ be defined by

$$\begin{aligned} f_1(y,p,u) &= -y + G_0 y_0 + G(B(y)+u) \\ f_2(y,p,u) &= -p + G_T(y(T) - y_T) + DB'(y)p \\ f_3(y,p,u) &= \lambda u + p \end{aligned} \tag{4.1'}$$

and introduce set–valued mappings by $F_1(y,p,u) = F_2(y,p,u) = \{0\}$, $F_3(y,p,u) = N(u)$. Writing $f = (f_1, f_2, f_3)$, $F = (F_1, F_2, F_3)$, $w = (y,p,u)$, the optimality system (1.2), (3.1)–(3.2) admits finally the form

$$0 \in f(w) + F(w), \tag{4.2}$$

where $f : W \to W$ is of class $C^{1,1}$ (note that $b'' \in C^{0,1}(I\!R)$) and $F : W \to 2^W$ has closed graph ($u_n \to u$, $v_n \to v$ in $L^\infty(\Sigma)$ and $v_n \in N(u_n)$ implies $v \in N(u)$).

The *generalized Newton method* for solving (4.2) can be described as follows: Let w_n be the last (current) iterate. Then the new iterate w_{n+1} is obtained from the *linearized generalized equation*

$$0 \in f(w_n) + f'(w_n)(w - w_n) + F(w). \tag{4.3}$$

To show the convergence of the method, we shall make use of a generalization of the well known Newton-Kantorovich theorem. It relies mainly on the assumption of *strong regularity* of the generalized equation. This notion goes back to Robinson [25]: The generalized equation (4.2) is said to be *strongly regular* at $\bar{w} \in W$, if there are positive constants $r(\bar{w})$ and $c_L(\bar{w})$ such that the perturbed linearized equation

$$e \in f(\bar{w}) + f'(\bar{w})(w - \bar{w}) + F(w) \tag{4.4}$$

has a unique solution $w = w(\bar{w}, e)$ for all $e \in B_{r(\bar{w})}(0)$, and the mapping $e \mapsto w(\bar{w}, e)$ is Lipschitz continuous on $B_{r(\bar{w})}(0)$ with modulus $c_L(\bar{w})$.

Here and in the sequel $B_r(w)$ denotes the closed ball of W around w with radius r, where W is endowed with its natural norm $\|\cdot\|_W$.

Theorem 4.1 *Let $\bar{w}$ be a solution of (4.2) such that this generalized equation is strongly regular at $\bar{w}$. Assume further that $F : W \to 2^W$ has closed graph, $f : W \to W$ is of class C^1, and that for all $M > 0$ there is a constant $l_M > 0$ with*

$$\|f'(w_1) - f'(w_2)\|_{W \to W} \le l_M \|w_1 - w_2\|_W \tag{4.5}$$

for all w_1, w_2 in $B_M(0)$. Then there is a $\rho_N > 0$ such that for any starting point $w_1 \in B_{\rho_N}(\bar{w})$ the generalized Newton method generates a unique sequence $\{w_k\}$ convergent to $\bar{w}$. Moreover,

$$\|w_{k+1} - \bar{w}\|_W \le c_N \|w_k - \bar{w}\|_W^2 \tag{4.6}$$

holds with some positive constant c_N for all $k \ge 1$.

(4.6) expresses the quadratic convergence of the Newton method. For the proof we refer to a recent paper by Alt [3], Theorem 2.6, and to the references therein. A generalization of this theorem can be found in Dontchev [8], [9], where the so-called Aubin continuity of the inverse mapping associated to the linearized generalized equation is introduced and assumed instead of strong stability.

Let $e = (e_y, e_p, e_u) \in C(\bar{Q})^2 \times L^\infty(\Sigma)$ be the perturbation standing in (4.4). Transforming (4.4) back into three separate equations of the type (4.1') we get the linearized system

$$\begin{aligned} 0 &= -y - e_y + G_o y_o + G(B(\bar{y}) + B'(\bar{y})(y - \bar{y}) + u), \\ 0 &= -p - e_p + G_T(y(T) - y_T) + D\left(B'(\bar{y})p + B''(\bar{y})\bar{p}(y - \bar{y})\right) \\ \lambda u + p - e_u &\in N(u). \end{aligned}$$

In this form, it is difficult to interprete y, p as solutions of perturbed partial differential equations. After introducing $\tilde{y} = y + e_y$, $\tilde{p} = p + e_p$ we see that (4.4) is equivalent to

$$\begin{aligned} \tilde{y} &= G_0 y_0 + G(B(\bar{y}) + B'(\bar{y})(\tilde{y} - \bar{y}) - B'(\bar{y})e_y) \\ \tilde{p} &= G_T(\tilde{y}(T) - y_T - e_y(T)) \\ &+ D(B'(\bar{y})\tilde{p} + B''(\bar{y})\bar{p}(\tilde{y} - \bar{y}) - B'(\bar{y})e_p - B''(\bar{y})\bar{p}e_y) \\ (\lambda u &+ \tilde{p} - e_p - e_u, v - u)_{L_2(\Sigma)} \ge 0 \quad \forall v \in U_{ad}. \end{aligned} \tag{4.7}$$

This is the abstract form of an optimality system of a *perturbed linear quadratic control problem* $(QP)_z$ depending on a new perturbation z. In fact, it corresponds to

$$\textbf{(}\boldsymbol{QP}\textbf{)}_z \qquad \varphi'(\bar{y}, \bar{u})(y - \bar{y}, u - \bar{u}) + \frac{1}{2}\mathcal{L}''(\bar{y}, \bar{u}, \bar{p})[(y - \bar{y}, u - \bar{u})]^2 + d_z(y - \bar{y}, u - \bar{u}) = \min!$$

subject to

$$\begin{aligned} y_t &= \Delta y \\ y(0) &= y_0 \\ \partial_n y &= b(\bar{y}) + b'(\bar{y})(y - \bar{y}) + u + z_y, \quad u \in U_{ad}, \end{aligned} \tag{4.8}$$

where we have introduced $y := \tilde{y}$, $z := (z_T, z_y, z_p, z_u)$, $z_T = e_y(T)$, $z_y := -B'(\bar{y})e_y$, $z_p := -B'(\bar{y})e_p - B''(\bar{y})\bar{p}e_y$, $z_u := -(e_p + e_u)$ regarding the restrictions of z_y, z_p, z_u to Σ. The linear perturbation functional d_z is defined by

$$d_z(y,u) := \int\limits_{\Omega} z_T(x)y(T,x)\,dx + \int\limits_{\Sigma} z_p(t,x)y(t,x)\,dS\,dt + \int\limits_{\Sigma} z_u(t,x)u(t,x)\,dS\,dt. \qquad (4.9)$$

To check the assumptions of Theorem 4.1 we shall investigate the stability of (QP_z) with respect to z in the next section. It is obvious that stability with respect to z implies stability of (4.4) with respect to $e = (e_y, e_p, e_u)$, as $\|z\|_{C(\bar{\Omega})\times(L^\infty(\Sigma))^3} \le c\,\|e\|_{C(\bar{\Omega})\times(L^\infty(\Sigma))^2}$.

5 Stability of (QP_z)

The linear–quadratic programming problem (QP_z) cannot assumed to be convex, since $\mathcal{L}''$ is coercive on a subspace only. Regarding (QP_z) for all controls $u \in U_{ad}$ may therefore lead to different local minima. This is the reason for regarding (QP_z) in a local setting, i.e. in a neighborhood of $\bar{u}$.

Let us start with (QP_z) restricted to $\overline{U_{ad}} = \{u \in U_{ad} |\, u = \bar{u} \quad \text{on } I_\sigma\}$ and call this problem $(\overline{QP_z})$.

Theorem 5.1 *Problem $(\overline{QP_z})$ admits for all perturbations $z \in C(\bar{\Omega}) \times (L^\infty(\Sigma))^3$ a unique solution $(y_z, u_z) \in Y \times \overline{U_{ad}}$.*

Proof: In $(\overline{QP_z})$ we set $u = u_1 + u_2$, where $u_1 = \chi_{I_\sigma}\bar{u}$ and $u_2 = \chi_{\Sigma\setminus I_\sigma}u$. Let y_i, $i = 1, 2$, denote associated states satisfying $y_1(0) = y_0$, $y_2(0) = 0$, and the heat equation in (4.8) subject to

$$\begin{aligned} \partial_n y_1 &= b(\bar{y}) + b'(\bar{y})(y_1 - \bar{y}) + z_y + u_1 \\ \partial_n y_2 &= b'(\bar{y})y_2 + u_2. \end{aligned} \qquad (5.1)$$

Then $y = y_1 + y_2$ is the state associated to $u \in \overline{U_{ad}}$. Moreover, (y_1, u_1) is a fixed element and (y_2, u_2) belongs to the subspace, where $\mathcal{L}''(\bar{y}, \bar{u}, \bar{p})$ is coercive. Now we get by standard arguments the existence of a globally optimal control $u_{2,z}$ in $U_{ad} \cap \{u |\, u = 0 \text{ on } I_\sigma\}$ with state $y_{2,z}$. Obviously $u_z = u_1 + u_{2,z}$, $y_z = y_1 + y_{2,z}$ forms an optimal pair for $(\overline{QP_z})$. □

This solution (y_z, u_z) fulfils the optimality system consisting of (4.8), the adjoint equation

$$\begin{aligned} -p_t &= \Delta p \\ p(T) &= y_z(T) - y_T + z_T \\ \partial_n p &= b'(\bar{y})p + b''(\bar{y})\bar{p}(y_z - \bar{y}) + z_p \end{aligned} \qquad (5.2)$$

and

$$\int\limits_{\Sigma} (\lambda u_z + p + z_u)(u - u_z)\,dS\,dt \ge 0 \quad \forall u \in \overline{U_{ad}} \qquad (5.3)$$

with the adjoint state $p = p_z \in Y$.

In the next theorem, we use the norms

$$\begin{aligned} \|(y,p,u)\|_2 &= \|y\|_{W(0,T)} + \|p\|_{W(0,T)} + \|u\|_{L^2(\Sigma)} \\ \|z\|_q &= \|z_T\|_{L^q(\Omega)} + \|z_y\|_{L^q(\Sigma)} + \|z_u\|_{L^q(\Sigma)} + \|z_p\|_{L^q(\Sigma)}, \ (2 \le q \le \infty). \end{aligned}$$

Theorem 5.2 *Let (y_i, u_i) , $i = 1,2$, be the unique solutions of $(\overline{QP_{z_i}})$ and p_i be the associated adjoint states. Then the Lipschitz estimate*

$$\|(y_1,p_1,u_1) - (y_2,p_2,u_2)\|_2 \le l\|z_1 - z_2\|_2 \tag{5.4}$$

holds with some $l > 0$, which does not depend on z_1, z_2.

Proof: We first mention the system for $y_1 - y_2$: It holds $(y_1 - y_2)(0) = 0$, and $(y_1 - y_2)$ solves the heat equation together with the boundary condition

$$\partial_n(y_1 - y_2) = b'(\bar y)(y_1 - y_2) + (u_1 - u_2) + z_y^1 - z_y^2. \tag{5.5}$$

The objective functionals of (QP_{z_i}) are

$$\begin{aligned} \tilde\varphi_i &= (\bar y(T) - y_T + z_T^i, y(T) - \bar y(T))_{L^2(\Omega)} + (\lambda \bar u + z_u^i, u - \bar u)_{L^2(\Sigma)} \\ &+ (z_p^i, y - \bar y)_{L^2(\Sigma)} \\ &+ \frac{1}{2}\|y(T) - \bar y(T)\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|u - \bar u\|^2_{L^2(\Sigma)} + \frac{1}{2}\int_\Sigma b''(\bar y)\bar p(y - \bar y)^2\, dS\, dt. \end{aligned} \tag{5.6}$$

The Lagrange functions $\tilde{\mathcal{L}}^i$ associated to $(\overline{QP_{z_i}})$ are

$$\begin{aligned} \tilde{\mathcal{L}}^i(y,u,p_i) &= \tilde\varphi_i(y,u) - (y_t, p_i) - (\nabla y, \nabla p_i)_{L^2(Q)} \\ &+ (b(\bar y) + b'(\bar y)(y - \bar y) + u + z_y^i, p_i)_{L^2(\Sigma)}. \end{aligned}$$

We used (y_t, p) to denote the value of the functional y_t applied to p. Since $u = \bar u$ on I_σ, the problems $(\overline{QP_{z_i}})$ are convex. Therefore, the necessary and sufficient optimality condition for (y_i, u_i) is

$$(\tilde{\mathcal{L}}^i)'(y_i, u_i, p_i)(v - v_i) \ge 0 \tag{5.7}$$

for all $v = (y,u) \in Y \times U_{ad}$, where $v_i := (y_i, u_i)$, $i = 1,2$. Now we insert $v = v_2$ in the inequality for $i = 1$, $v = v_1$ in the corresponding one for $i = 2$ and add the two inequalities. After several computations we arrive at

$$-\mathcal{L}''(\bar y, \bar u, \bar p)[v_1 - v_2]^2 + < d_{z_1} - d_{z_2}, v_2 - v_1 > + (z_y^1 - z_y^2, p_2 - p_1)_{L^2(\Sigma)} \ge 0. \tag{5.8}$$

The difference $v_1 - v_2$ does not belong to the subspace, where (SSC) applies. Therefore we split $v_1 - v_2 = v + \hat v$, where $v = (y, u_1 - u_2)$, $\hat v = (\hat y, 0)$, y, $\hat y$ solve the heat equation in (4.8) with homogeneous initial condition and

$$\begin{aligned} \partial_n y &= b'(\bar y)y + u_1 - u_2 \\ \partial_n \hat y &= b'(\bar y)\hat y + z_y^1 - z_y^2. \end{aligned} \tag{5.9}$$

Note, that $u_1 - u_2 = 0$ on I_σ. Thus (SSC) applies to v and $\mathcal{L}''(\bar{y}, \bar{u}, \bar{p})[v]^2 \geq \delta \|u_1 - u_2\|^2_{L^2(\Sigma)}$ is obtained. Moreover, known results on parabolic regularity yield

$$\|\hat{y}\|_{W(0,T)} \leq c\|z_y^1 - z_y^2\|_{L^2(\Sigma)}. \tag{5.10}$$

Inserting the preceding two estimates in (5.8) we deduce after some formal manipulations and estimates (in particular for $\|p_2 - p_1\|_{W(0,T)}$) that

$$\begin{aligned} \delta\|u_1 - u_2\|^2_{L^2(\Sigma)} &\leq c(\|z_1 - z_2\|_2^2 + \|z_1 - z_2\|_2\|v_1 - v_2\|_2) \\ &\leq \tilde{c}(\|z_1 - z_2\|_2^2 + \|z_1 - z_2\|_2\|u_1 - u_2\|_2) \end{aligned} \tag{5.11}$$

with some constants c, $\tilde{c} > 0$. The last estimate follows from $\|y_1 - y_2\|_{W(0,T)} \leq c(\|z_y^1 - z_y^2\|_{L^2(\Sigma)} + \|u_1 - u_2\|_{L^2(\Sigma)})$. We have used $\|v_1 - v_2\|_2 = \|y_1 - y_2\|_{W(0,T)} + \|u_1 - u_2\|_{L^2(\Sigma)}$. Now there are two possibilities in (5.11). The first is $\|u_1 - u_2\|_{L^2(\Sigma)} \leq \|z_1 - z_2\|_2$. The second is $\|z_1 - z_2\|_2 < \|u_1 - u_2\|_{L^2(\Sigma)}$. Then (5.11) implies $\|u_1 - u_2\|_{L^2(\Sigma)} \leq \tilde{c}\delta^{-1}\|z_1 - z_2\|_2$. (5.4) follows first for $\|u_1 - u_2\|$ with $l = \max(1, \tilde{c}\delta^{-1})$. The remaining estimates of $y_1 - y_2$, $p_1 - p_2$ follow from estimates for the associated parabolic initial–boundary value problems.

□

Theorem 5.3 *There is a constant $l' > 0$, such that the statement of Theorem 5.2 holds true in the form*

$$\|(y_1, p_1, u_1) - (y_2, p_2, u_2)\|_{C(\bar{Q})^2 \times L^\infty(\Sigma)} \leq l'\|z_1 - z_2\|_\infty. \tag{5.12}$$

This result can be shown by a bootstrapping argument relying on parabolic regularity. We refer to Tröltzsch [27].

Corollary 5.1 *It holds*

$$\|u_1 - u_2\|_{L^\infty(\Sigma)} \leq l'\|z_1 - z_2\|_\infty. \tag{5.13}$$

Corollary 5.2 *The unique solution (y_z, u_z) of $(\overline{QP_z})$ satisfies (5.3) for all $u \in U_{ad}$, i.e.*

$$\int_\Sigma (\lambda u_z + p_z + z_u)(u - u_z)\, dS\, dt \geq 0 \quad \forall u \in U_{ad}, \tag{5.14}$$

if $\|z\|_\infty \leq \bar{\rho}$, and $\bar{\rho}$ is sufficiently small.

Proof: It follows from Corollary 5.1 that $u_z \to \bar{u}$ in $L^\infty(\Sigma)$, if $\bar{\rho} \to 0$. This implies in turn $p_z \to \bar{p}$ in $C(\bar{Q})$. Therefore, on I_σ the signs of $\lambda u_z + p_z + z_u$ and $\lambda\bar{u} + \bar{p}$ coincide almost everywhere for $\bar{\rho}$ sufficiently small. In (5.3) we have $u = u_z = \bar{u}$ on I_σ, hence

$$\int_{\Sigma \setminus I_\sigma} (\lambda u_z + p_z + z_u)(u - u_z)\, dS\, dt \geq 0 \quad \forall u \in U_{ad}. \tag{5.15}$$

On I_σ, $(\lambda u_z + p_z + z_u)(t,x)(u - u_z(t,x)) \geq 0 \quad \forall u \in [u_a, u_b]$, as $u_z = \bar{u}$, $\bar{u}$ solves (3.2) and the signs of $\lambda u_z + p_z + z_u$ and $\lambda \bar{u} + \bar{p}$ coincide. Obviously this yields together with (5.15) the inequality (5.14). □

Up to now, we have shown Lipschitz stability of $(\overline{QP_z})$. In view of the equivalence between the solutions of $(\overline{QP_z})$ and those of the optimality system (4.7) and of the remark closing section 4, this implies Lipschitz stability of the solutions of the linearized generalized equation (4.4) with respect to e. This shows the strong regularity of (4.2) at $\bar{w} = (\bar{y}, \bar{p}, \bar{u})$. All this, however, holds so far only true for $\overline{U_{ad}}$. Moreover, we have to re-define $N(u)$ in this sense, too, to make this result true. Unfortunately, we cannot entirely avoid certain restrictions, but we are able to weaken them essentially. In the next statement, we use

$$U_{ad}^\varepsilon = \{u \in U_{ad} |\, \|u - \bar{u}\|_{L_\infty(\Sigma)} \leq \varepsilon\}.$$

Theorem 5.4 *There are positive numbers ε and $\bar{\rho}'$, which do not depend on the perturbation z, such that for each z with $\|z\|_\infty \leq \bar{\rho}'$ the unique stationary control for (QP_z) in U_{ad}^ε is u_z.*

Proof: Suppose that a perturbation z with $\|z\|_\infty \leq \rho$ is given. If $\rho \leq \bar{\rho}$, then Corollary 5.2 shows that $u_z \in \overline{U_{ad}}$ is stationary for (QP_z). According to the construction we have $u_z = \bar{u}$ on I_σ. Let $\varepsilon > 0$ be given. Then $u_z \in U_{ad}^\varepsilon$, if ρ is sufficiently small, say $\rho \leq \rho_1(\varepsilon) \leq \bar{\rho}$. This follows from Corollary 5.1. Assume now that $\hat{u} \in U_{ad}^\varepsilon$ is another stationary control of (QP_z) with associated state $\hat{y}$ and adjoint state $\hat{p}$. We first estimate $\hat{y} - y_z$, $\hat{p} - p_z$: The difference $\hat{y} - y_z$ solves the heat equation with homogeneous initial condition and boundary condition

$$\partial_n(\hat{y} - y_z) - b'(\bar{y})(\hat{y} - y_z) = \hat{u} - u_z,$$

hence

$$\|\hat{y} - y_z\|_{C(\bar{Q})} \leq \|\hat{y} - y_z\|_Y \leq c_y \, \|\hat{u} - u_z\|_{L_\infty(\Sigma)} \tag{5.16}$$

holds with some $c_y > 0$. Similarly, $\hat{p} - p_z$ satisfies the backward heat equation with

$$\begin{aligned} (\hat{p} - p_z)(T) &= \hat{y}(T) - y_z(T) \\ \partial_n(\hat{p} - p_z) - b'(\bar{y})(\hat{p} - p_z) &= b''(\bar{y})\, \bar{p}\, (\hat{y} - y_z). \end{aligned}$$

Lemma 2.1 yields

$$\|\hat{p} - p_z\|_{C(\bar{Q})} \leq c_p \|\hat{y} - y_z\|_{C(\bar{Q})}. \tag{5.17}$$

Moreover, $\|\hat{u} - u_z\|_{L^\infty(\Sigma)} \leq 2\varepsilon$, since u_z, $\hat{u} \in U_{ad}^\varepsilon$. Therefore, the estimates (5.16), (5.17) imply

$$\|\hat{p} - p_z\|_{C(\bar{Q})} \leq c_p \cdot c_y \cdot 2\varepsilon. \tag{5.18}$$

We have

$$\int_\Sigma (\lambda \hat{u} + \hat{p} + z_u)(u - \hat{u}) \, dS dt \geq 0 \quad \forall u \in U_{ad} \tag{5.19}$$

($\hat{u}$ is stationary for (QP_z)). After splitting

$$\lambda\hat{u} + \hat{p} + z_u = \lambda\bar{u} + \bar{p} + z_u + \lambda(\hat{u} - u_z) + \lambda(u_z - \bar{u}) + (\hat{p} - p_z) + (p_z - \bar{p})$$

we deduce from (5.18) and the fact that $\bar{u}$, $\bar{p}$ are the unique solution and adjoint state to $(\overline{QP_z})$ for $z = 0$

$$\begin{aligned} |\lambda\hat{u} + \hat{p} + z_u - (\lambda\bar{u} + \bar{p})| &\leq \|z\|_\infty + 2\varepsilon\lambda + \lambda l'\|z\|_\infty + 2c_p c_y \varepsilon + l'\|z\|_\infty \\ &\leq (1 + (\lambda+1)l')\rho + 2\varepsilon(\lambda + c_p c_y) \leq \sigma/2, \end{aligned}$$

if $\rho \leq \rho_2 = \sigma(4(1 + (\lambda+1)l'))^{-1}$, $\varepsilon \leq \sigma(8(\lambda + c_p c_y))^{-1}$. We define ε in this way and choose $\rho \leq \bar{\rho}' = min(\rho_1(\varepsilon), \rho_2)$. On I_σ we have $|\bar{p} + \lambda\bar{u}| \geq \sigma$, hence the signs of $\bar{p} + \lambda\bar{u}$ and $\lambda\hat{u} + \hat{p} + z_u$ coincide for this choice of ρ and ε. Consequently, $\hat{u} = \bar{u}$ ($= u_a$ or u_b) on I_σ, i.e. $\hat{u} \in \overline{U_{ad}}$. $(\overline{QP_z})$ admits a unique solution, this is u_z. On the other hand, $\hat{u}$ is stationary, hence by convexity optimal for the same problem, too. This shows $\hat{u} = u_z$. □

Let $(\boldsymbol{QP}_z^\varepsilon)$ denote the linear-quadratic control problem obtained from (QP_z) on replacing the admissible set U_{ad} by U_{ad}^ε. The next statement shows that this does not change the solution set for sufficiently small ε:

Lemma 5.1 *If $\varepsilon > 0$ is sufficiently small, then the unique solution of (QP_z^ε) is u_z.*

Proof: The variational inequality (5.14) is satisfied in particular for all $u \in U_{ad}^\varepsilon$. Therefore, u_z is stationary for (QP_z^ε). Note that Theorem 5.4 cannot be directly applied, as (QP_z) is based on U_{ad}, while (QP_z^ε) is connected with U_{ad}^ε. Let $u_\varepsilon \in U_{ad}^\varepsilon$ be another stationary control, and let y_ε, p_ε be the associated state and adjoint state. For $\varepsilon \to 0$ we have $u_\varepsilon \to \bar{u}$ in $L_\infty(\Sigma)$ by the definition of U_{ad}^ε, hence $y_\varepsilon \to \bar{y}$, $p_\varepsilon \to \bar{p}$ in $C(\bar{Q})$. Following the proof of Corollary 5.2 we find $u_\varepsilon = \bar{u} = u_z$ on I_σ, hence $u_\varepsilon - u_z = 0$ on I_σ, if ε is sufficiently small. Now we repeat the transformations in the proof of Theorem 5.2 for the choice $(y_1, p_1, u_1) := (y_z, p_z, u_z)$, $(y_2, p_2, u_2) := (y_\varepsilon, p_\varepsilon, u_\varepsilon)$ to find

$$-\mathcal{L}''(\bar{y}, \bar{u}, \bar{p})[y_z - y_\varepsilon, u_z - u_\varepsilon]^2 \geq 0$$

instead of (5.8) (note that u_ε and u_z are stationary for the same perturbation). Obviously, (SSC) applies to $v_z - v_\varepsilon$, thus the last inequality implies $v_z = v_\varepsilon$, hence $u_z - u_\varepsilon$. Therefore, u_z is the unique stationary solution for (QP_z^ε). It can be shown by standard arguments that (QP_z^ε) is solvable (U_{ad}^ε is weakly compact in $L_p(\Sigma)$, the functional lower semicontinuous w.r. to u, the mapping $u \mapsto y(u)$ compact from $L_p(\Sigma)$ to Y). This solution is necessarily u_z, since no other control satisfies the optimality system. □

Let us finally introduce

$$N^\varepsilon(u) = \{v \in L^\infty(\Sigma) | \int_\Sigma v(z - u)\, dS\, dt \leq 0 \quad \forall z \in U_{ad}^\varepsilon\}.$$

It is easy to check that $N^\varepsilon(\bar{u}) = N(\bar{u})$ for all $\varepsilon > 0$.

(Let $v \in N^\varepsilon(\bar{u})$ be given. Define $\Sigma_a = \{(t,x) | \, \bar{u}(t,x) = u_a\}$, $\Sigma_b = \{(t,x) | \, \bar{u}(t,x) = u_b\}$, $\Sigma_0 = \Sigma \setminus (\Sigma_a \cup \Sigma_b)$. On Σ_b the constraint $z \in U_{ad}^\varepsilon$ means $z(t,x) \in [u_b - \varepsilon, u_b]$, hence $z - \bar{u}$ can admit all values in $[-\varepsilon, 0]$ on Σ_b. This yields $v \geq 0$ a.e. on Σ_b. In the same way we find $v \leq 0$ a.e. on Σ_a. On Σ_0 we have $u_a < \bar{u}(t,x) < u_b$, hence $z - \bar{u}$ can have all signs, and we obtain in turn $v = 0$ a.e. on Σ_0. Thus $N^\varepsilon(\bar{u}) = \{v \in L^\infty(\Sigma) | \, v \geq 0 \quad \text{a.e. on} \, \Sigma_b, \, v \leq 0 \quad \text{a.e. on} \, \Sigma_a, \, v = 0 \quad \text{on} \, \Sigma_0\}$. The discussion for all $v \in N(\bar{u})$ leads to the same representation for $N(\bar{u})$.)

In what follows we shall regard the generalized equation (4.2) with the set-valued map $F(u)$ associated to the normal cone $N^\varepsilon(u)$. In view of Theorem 5.2 on Lipschitz-stability, the preceding investigations ensure the strong stability of this generalized equation at $\bar{w} = (\bar{y}, \bar{p}, \bar{u})$.

6 The Sequential Quadratic Programming method

Let $w_1 = (y_1, p_1, u_1)$ be a starting triplet (we shall assume that w_1 is close to $\bar{w} = (\bar{y}, \bar{u}, \bar{p})$). Then the Sequential Quadratic Programming (SQP) method determines a sequence $w_n = (y_n, p_n, u_n)$ as follows. Let $\varepsilon > 0$ be given according to Lemma 5.1. Initiating from w_n, the next iterate w_{n+1} is obtained from solving

$$(\boldsymbol{QP}^n) \qquad \varphi'(y_n, u_n)(y - y_n, u - u_n) + \frac{1}{2}\mathcal{L}''(y_n, u_n, p_n)[(y - y_n, u - u_n)]^2 = \min! \quad (6.1)$$

subject to

$$\begin{aligned} y_t &= \Delta y \\ y(0) &= y_0 \\ \partial_n y &= b(y_n) + b'(y_n)(y - y_n) + u, \quad u \in U_{ad}^\varepsilon, \end{aligned} \qquad (6.2)$$

while p_{n+1} is the associated Lagrange multiplier. First of all, we have to make sure that (QP^n) is uniquely solvable. This property cannot be derived from the convergence theorem 4.1 for Newton's method: It might happen that (QP^n) has more solutions than the solution $w_{n+1} = (y_{n+1}, p_{n+1}, u_{n+1})$ of (4.3). The existence of at least one solution of (QP^n) follows by the arguments used at the end of the proof of Lemma 5.1 (note that

$$\begin{aligned} \frac{1}{2}\mathcal{L}''(y_n, u_n, p_n)[y - y_n, u - u_n] &= \int\limits_\Omega (y(T) - y_n(T))^2 \, dx \\ &+ \int\limits_\Sigma (p_n b''(y_n)(y - y_n)^2 + \lambda(u - u_n)^2) \, dS dt \end{aligned}$$

is convex w.r. to u and u appears linearly in (6.2).) If $w_n = (y_n, p_n, u_n) \in B_\rho(\bar{w})$ is sufficiently close to $\bar{w} = (\bar{y}, \bar{p}, \bar{u})$ and ε is taken sufficiently small, then any solution u_{n+1} of (QP^n) satisfies $u_{n+1} = \bar{u}$ on I_σ, hence $u_{n+1} \in \overline{U_{ad}}$. This is shown in the same way as

Corollary 5.2, since $\mathcal{L}_u(y_n, u_n, p_n)(t,x)$ has on I_σ the same sign as $\mathcal{L}_u(\bar{y}, \bar{u}, \bar{p})(t,x)$. On the other hand, the quadratic form $\mathcal{L}''(y_n, u_n, p_n)$ is then coercive on the linear subspace of all (y, u), which satisfy the parabolic equation (6.2) and $u = 0$ on I_σ. This permits to derive uniqueness (any difference of solutions u_{n+1}, $\hat{u}_{n+1}$ of (QP^n) satisfies $u_{n+1} - \hat{u}_{n+1} = 0$ on I_σ). We should underline that "ε is small" can be defined independently of $w_n \in B_\rho(\bar{w})$. We refer for the details to the forthcoming paper [30], as the methods are completely analogous to the proofs of Theorems 5.1, 5.2 and Corollary 5.2. Summarizing up, we have obtained:

Theorem 6.1 *Let $0 < \bar{\rho} \leq \rho_N$ and $\varepsilon > 0$ be sufficiently small. Then the SQP-method generates for any starting point $(y_1, p_1, u_1) \in B_{\rho_N}(\bar{w})$ a unique sequence $\{(y_n, p_n, u_n)\}$ such that*

$$\|(y_{n+1}, p_{n+1}, u_{n+1}) - (\bar{y}, \bar{p}, \bar{u})\|_{C(\bar{Q})^2 \times L^\infty(\Sigma)} \leq c_N \|(y_n, p_n, u_n) - (\bar{y}, \bar{p}, \bar{u})\|^2_{C(\bar{Q})^2 \times L^\infty(\Sigma)} \quad (6.3)$$

$(n = 1, 2, \ldots)$.

We should underline that we have applied Theorem 4.1 for the normal cone $N^\varepsilon(u)$. (6.3) shows the quadratic convergence of the SQP method in U^ε_{ad}.

The restriction of U_{ad} to U^ε_{ad} seems to contradict the experience with the SQP method in $\mathbb{R}^n$, where this is not necessary. In finite dimensions, the constraints contain only finitely many inequalities. The active inequalities are assumed to be known in the attraction region of the method. Then the SQP method is nothing more than the Newton method for a system of equations, where the iterates do not leave the region. In our setting, we cannot assume that the active set is known after finitely many steps.

To motivate the need for the additional constraint in U^ε_{ad} we consider the following example:

$$\begin{aligned} min \quad & -x^2 \\ x \quad & \in \quad [-2, 1]. \end{aligned} \quad (6.4)$$

This nonconvex quadratic problem has stationary solutions at -2, 0, and 1. The points -2, and 1 are strict local minima at which first order sufficient conditions are satisfied. Therefore, (SSC) is trivially fulfilled. Choose $\bar{x} = 1$ to be our reference solution. (QP^n) is identical to (6.4) and will always deliver the global minimum at $x_{n+1} = -2$, independently on how close x_n is taken to $\bar{x} = 1$. Convergence to $\bar{x}$ can only be guaranteed by restriction to a neighborhood of $\bar{x} = 1$. We cannot do better in our framework.

A different method of Newton type, presented by Kelley and Sachs [20] for the control of ordinary differential equations, is able to avoid this restriction to a neighborhood. However, the authors have to impose some structural assumptions on the active set and conditions on the slope of the switching function at the junction points.

There remained an other unsatisfactory point for the application: U_{ad}^{ε} depends on the unknown control $\bar{u}$. Define $U_{ad}^1 := \{u \in U_{ad} | \, \|u - u_1\|_{L^\infty(\Sigma)} \leq \frac{2}{3}\varepsilon\}$ and assume that $\|w_1 - \bar{w}\|_W \leq min(\frac{\varepsilon}{3}, \rho_N)$. Then $U_{ad}^1 \subset U_{ad}^{\varepsilon}$. Moreover, the closed ball of radius $\|\bar{u} - u_1\|_{L^\infty(\Sigma)}$ is contained in U_{ad}^1. According to the preceding theorem, this ball is an attraction region for the SQP-method. Therefore the iterates do not leave the set U_{ad}^1 and the SQP method converges in U_{ad}^1.

Remark 6.1 *If the second order condition (3.7) holds for* all $u \in L^2(\Sigma)$ *(this corresponds to the formal setting $I_\sigma := \emptyset$), then the restriction to U_{ad}^{ε} or U_{ad}^1 is not necessary. In this case, (QP^n) admits a unique globally optimal control in U_{ad}.*

In our computational examples, (QP^n) was solved on the whole region U_{ad}.

7 Some computational results

Our convergence result is more or less of theoretical value only. Any implementation has to be linked with some discretization. We solve a discretized version of (QP^n). This result is taken to define (QP^{n+1}), which is discretized again. In this way the accuracy of the SQP-method depends on that for solving the quadratic subproblems. Let h denote a mesh size parameter describing the discretization of the quadratic subproblems and let w_n^h denote the current solution obtained from $(\mathrm{QP}_h^{(n-1)})$, the discretization of $(\mathrm{QP}^{(n-1)})$ with mesh size h. The problem (QP^n) is discretized with parameter h^+ and has the solution $w_{n+1}^{h^+}$. It is obvious that the quadratic convergence of the SQP method can only be observed during the computation, if the accuracy of solving (QP^n) is compatible with the precision reached in the preceding SQP-step, i.e. h^+ has to be chosen such that

$$\|w_{n+1} - w_{n+1}^{h^+}\|_W \leq c \, \|w_n^h - \bar{w}\|_W^2,$$

where w_{n+1} denotes the exact solution of (QP^n). In other words, the mesh size has to be adapted to the progress of precision of the SQP method. In particular, this refers to the numerical method for the partial differential equation. Therefore, this successive refinement of the mesh size leads after a few steps to astronomical dimensions of the discretized problems.

Aiming to find a compromise between verification of fast convergence and acceptable dimensions of the discretized problems, we decided to solve our quadratic sub–problems by a fine discretization, where the difference to the exact (linear-quadratic) control is at least not visible in the plotted pictures, cf. Figure 1. We found that 400 node-points for the controls were sufficient for this purpose and had to solve problems of dimension greater than $640,000$ of variables in this case.

We avoid any table of computed results, as an accuracy beyond 10^{-2} was not compatible with the accuracy chosen for solving the heat equation.

Nevertheless, establishing (QP^n) and its solution by a standard QP–method will need very high storage capacity. Therefore, we applied a multigrid method of the second kind due to Hackbusch [12] combined with the Bertsekas projection method [6]. We refer to the authors paper [11] for the details. Similar techniques have already been successfully applied by different authors. We only mention Hackbusch and Will [13], Heinkenschloss and Sachs [15], and Kelley and Sachs [19], [20].

Test examples:

To illustrate the strong dependence of the computed optimal control on the discretization, we first discuss the numerical treatment of the following linear–quadratic problem due to Schittkowski [26]:

$$0.5\int_0^1 [y(T,x) - y_T(x)]^2\,dx + 0.5\lambda\int_0^T u^2(t)\,dt = \min! \tag{7.1}$$

subject to

$$\begin{array}{rcll} y_t(t,x) & = & y_{xx}(t,x) & \text{on} \quad (0,T]\times(0,1) \\ y(0,x) & = & 0 & \text{on} \quad (0,1) \\ y_x(t,0) & = & 0 & \text{in} \quad (0,T] \\ y_x(t,1) & = & u(t) - y(t,1) & \text{in} \quad (0,T], \end{array} \tag{7.2}$$

and

$$-1 \le u(t) \le 1 \qquad \text{a.e. at} \quad [0,T], \tag{7.3}$$

where $y_T(x) = 0.5(1-x^2)$, $\lambda = 0.001$ and $T = 1.58$. Let n_t, n_x and n_u denote the number of subintervals used for the discretization of $[0,T]\times[0,1]$ in the PDE and of $[0,T]$ with respect to u. Figure 1 shows the plots of the computed controls for the following triplets of (n_t, n_x, n_u): $(100,100,50)$, $(400,400,200)$, $(800,800,400)$.

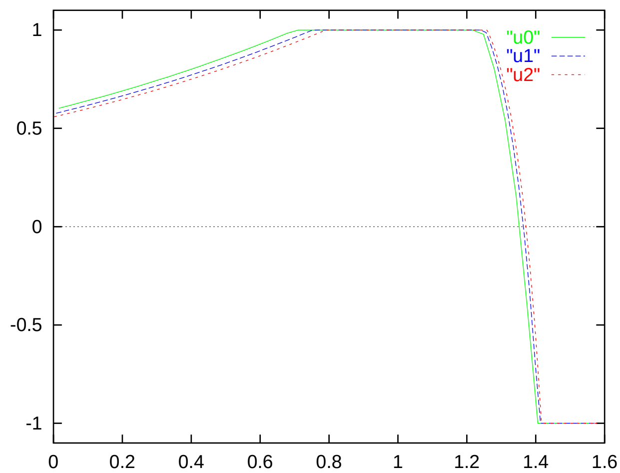

Figure 1

The figure shows that the controls are very sensitive with respect to the discretization. Hence a fine discretization should be used to verify the gain of accuracy given by the SQP method at least in the first steps (cf. the arguments at the beginning of section 7).

The next example is a nonlinear problem with almost the same data as above, but with the boundary condition

$$y_x(t,1) = u(t) - y(t,1)^2.$$

This boundary condition does not directly fit into our assumptions, as $b(y) = -y^2$ is monotone increasing for $y < 0$. If we put $b(y) = y^2$ for $y < 0$, then the assumptions are satisfied. In the computational example, the state y remained positive in all iterations. Hence this formal change does not influence the result in this test example.

The initial SQP iterate was taken as $(y_0, u_0, p_0) = (0,0,0)$, $(n_t, n_x, n_u) = (800, 800, 400)$. In Figure 2 the first iterates are represented. A continuation of the iteration process after the 5. iteration was appearently not meaningful.

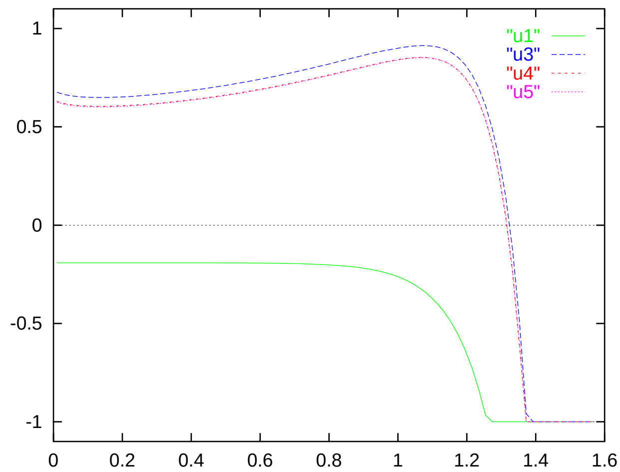

Figure 2

Computations with coarser discretizations exhibited the same behaviour. In this way, all of our test examples confirmed the mesh–independence principle of Alt [3].

In the test example the restriction to a neighborhood around $\bar{u}$ was not necessary. Moreover, the method converged, although the starting element was far from the solution. This behaviour cannot be expected in general. To make Newton type methods practicable, a globalization technique has to be used.

Acknowledgement: The authors are grateful to W. Alt, W. Hackbusch, M. Heinkenschloss and E.W. Sachs for helpful discussions during the work on this paper.

References

[1] W. Alt. The Lagrange–Newton method for infinite–dimensional optimization problems. *Numer. Funct. Anal. and Optim.*, 11:201–224, 1990.

[2] W. Alt. The Lagrange Newton method for infinite-dimensional optimization problems. *Control and Cybernetics*, 23:87–106, 1994.

[3] W. Alt. Discretization and mesh independence of Newton's method for generalized equations. To appear.

[4] W. Alt and K. Malanowski. The Lagrange–Newton method for nonlinear optimal control problems. *Computational Optim. and Appl.*, 2:77–100, 1993.

[5] W. Alt, R. Sontag, and F. Tröltzsch. An SQP Method for Optimal Control of a Weakly Singular Hammerstein Integral Equation. *Appl. Math. Optim.*, 33:227–252, 1996.

[6] D. B. Bertsekas. Projected Newton methods for optimization problems with simple constraints. *SIAM J. Control Optim.*, 20:221–246, 1982.

[7] E. Casas, A. Unger, and F. Tröltzsch. Second order sufficient optimality conditions for a nonlinear elliptic control problem. *J. Analysis and its Appl. (ZAA)*, 15, No.3:687–707, 1996.

[8] A.L. Dontchev. Local analysis of a Newton–type method based on partial linearization. In *Proc. of the Summer Seminar "Mathematics of numerical analysis: Real Number algorithms*, Park City, UT July 17– August 11, 1995, Eds. J. Renegar, M. Shub, and S. Smale. To appear.

[9] A.L. Dontchev. Uniform convergence of the Newton method for Aubin continuous maps. *To appear.*

[10] A.L. Dontchev, W.W. Hager, A.B. Poore, and B. Yang. Optimality, stability, and convergence in optimal control. *Appl. Math. Optim.*, 31:297–326, 1995.

[11] H. Goldberg and F. Tröltzsch. On a SQP–multigrid technique for nonlinear parabolic boundary control problems. Faculty of Mathematics, TU Chemnitz, Rep. 97–11. To appear.

[12] W. Hackbusch. On the fast solving of parabolic boundary control problems. *SIAM J. Control Optim.*, 17, No. 2:231–244, 1979.

[13] W. Hackbusch and Th. Will. A numerical method for a parabolic bang–bang problem. *Control and Cybernetics*, 12, No. 3–4:100–116, 1983.

[14] M. Heinkenschloss. The numerical solution of a control problem governed by a phase field model. *Optimization Methods and Software*, 7, 1997. To appear.

[15] M. Heinkenschloss and E. W. Sachs. Numerical solution of a constrained control problem for a phase field model. *Control and Estimation of Distributed Parameter Systems, Int. Ser. Num. Math.*, 118:171–188, 1994.

[16] M. Heinkenschloss and F. Tröltzsch. Analysis of the Lagrange-SQP-Newton method for the control of a phase field equation. Technical Report No. 03–01, Virginia Polytechnic Institute and State Unversity, ICAM report, 1995. To appear.

[17] K. Ito and K. Kunisch. Augmented Lagrangian-SQP methods for nonlinear optimal control problems of tracking type. *SIAM J. Control Optim.*, 34:874–891, 1996.

[18] K. Ito and K. Kunisch. Augmented Lagrangian-SQP methods in Hilbert spaces and application to control in the coefficients problems. *SIAM J. Optim.*, 6:96–125, 1996.

[19] C.T. Kelley and E.W. Sachs. Multilevel algorithms for constrained compact fixed point problems. *SIAM J. Scientific and Stat. Computing*, 15:645–667, 1994.

[20] C.T. Kelley and E.W. Sachs. Solution of optimal control problems by a pointwise projected Newton method. *SIAM J. Control Optim.*, 33:1731–1757, 1995.

[21] S.-F. Kupfer and E. W. Sachs. Numerical solution of a nonlinear parabolic control problem by a reduced SQP method. *Computational Optim. and Appl.*, 1:113–135, 1992.

[22] J.L. Lions and E. Magenes. *Problèmes aux limites non homogènes et applications*, volume 1–3. Dunod, Paris, 1968.

[23] K. Machielsen. Numerical solution of optimal control problems with state constraints by sequential quadratic programming in function space. CWI Tract, 53, Amsterdam, 1987.

[24] J.P. Raymond and H. Zidani. Hamiltonian Pontryagin's principles for control problems governed by semilinear parabolic equations. *Preprint* 1995. To appear.

[25] S.M. Robinson. Strongly regular generalized equations. *Mathematics of Operations Research*, 5:43–62, 1980.

[26] K. Schittkowski. Numerical solution of a time–optimal parabolic boundary-value control problem. *J. Optim. Theor. Appl.*, 27:271–290, 1979.

[27] F. Tröltzsch. Semidiscrete Ritz–Galerkin approximation of nonlinear parabolic boundary control problems. *Int. Ser. Num. Math.*, 111:57–68, 1993.

[28] F. Tröltzsch. Convergence of an SQP – method for a class of nonlinear parabolic boundary control problems. In *Control and Estimation of Distributed Parameter Systems: Nonlinear Phenomena.* W. Desch, F. Kappel, K. Kunisch (Eds.), *Int. Ser. Num. Math.* Vol. 118: 343–358, 1994.

[29] F. Tröltzsch. An SQP method for the optimal control of a nonlinear heat equation. *Control and Cybernetics*, 23(1/2):267–288, 1994.

[30] F. Tröltzsch. On the Lagrange–Newton method for the optimal control of semilinear parabolic equations. 1997, to appear.