

A short step method designed for solving linear quadratic optimal control problems with hp finite elements

D. Wachsmuth, * J.-E. Wurst *

July 11, 2014

Abstract

We consider linear quadratic optimal control problems with elliptic PDEs. The problem is solved with an interior point method in the control variable. We prove convergence of the short step method in function space by employing a suitable smoothing operator. As discretization we choose hp -FEM based on local estimates on the smoothness of functions. A fully adaptive algorithm is implemented and a-posteriori error estimators are derived for the central path and the Newton system. The theoretical results are complemented by numerical examples.

Keywords. Optimal control, control constraints, interior point method, hp -finite elements, adaptive refinement.

MSC classification. 49M37, 90C51, 65K05, 65N30

Acknowledgment. This work was funded by the Austrian Science Fund (FWF) grant P23484-N18.

1 Introduction

Let $\Omega \subset \mathbb{R}^2$ be a polygonal domain and denote by $U \subset \bar{\Omega}$ the domain where the control acts. We investigate the linear quadratic optimal control problem

$$(P) \quad \begin{cases} \text{minimize } J(u, y) := \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\nu}{2} \|u\|_{L^2(U)}^2 \\ \text{subject to} \\ Ay = Bu, \\ u \in U_{ad}, \end{cases}$$

with $U_{ad} = \{u \in L^2(U) \mid u_a \leq u \leq u_b \text{ a.e. on } U\}$. The box constraints are assumed to satisfy $u_a, u_b \in L^\infty(U)$ with $|u_a - u_b| \geq \vartheta > 0$ almost everywhere. The domain Ω is supposed to have Lipschitz boundary $\Gamma := \partial\Omega$. Furthermore, the operator A represents a partial differential equation (PDE) in its weak formulation

$$A : Y := H^1(\Omega) \rightarrow Y^*$$

*Institut für Mathematik, Universität Würzburg, 97074 Würzburg, Germany
D. Wachsmuth: daniel.wachsmuth@mathematik.uni-wuerzburg.de
J.-E. Wurst: jan-eric.wurst@mathematik.uni-wuerzburg.de

and A^* shall denote its adjoint. We assume that A is continuously invertible. This problem formulation conveniently covers the case of distributed controls

$$U = \Omega, \quad B : L^2(\Omega) \ni u \mapsto (u, \cdot)_{L^2(\Omega)} \in Y^*.$$

The framework can be extended to problems with Dirichlet boundary conditions ($Y = H_0^1(\Omega)$), or Neumann boundary controls

$$U = \Gamma, \quad B : L^2(\Gamma) \ni u \mapsto (u, \cdot)_{L^2(\Gamma)} \in Y^*.$$

Problem **(P)** has been intensively studied in literature. Projected gradient methods, semi-smooth Newton methods (primal dual active set methods) or SQP methods for non-linear problems are well understood and can solve the non-smooth first order necessary conditions (see e.g. [3, 19, 20, 24, 36]). Many error estimates for different types of discretizations are available. Usually, finite elements with constant polynomial degree are used (h -FEM) (see e.g. [2, 6, 7, 17, 18, 28]). Higher order methods for an integral control constraint were investigated in [8, 9, 15]. To the best of our knowledge, there are no available references about the application of adaptive hp -FEM to control constrained problems with pointwise inequality constraints.

The optimization methods mentioned above directly solve the inequality constrained problem. A different approach is the solution via interior point methods where the control constraints are dropped and barrier terms in the cost functional enforce feasibility. A control reduced algorithm has been successfully been applied in [31, 34, 40]. Here, the control is eliminated from the optimality system, which is similar to the concept of variational discretization [17]. Additionally, superlinear convergence in problem specific norms is proven. This approach is also suitable for treating state constraints, see [41, 33, 32].

Interior point methods working with primal and dual variables and projection or smoothing steps are explored in [39]. We also mention [27] for a problem with mixed control and state constraints. In [38] an affine scaling method is augmented by a smoothing step to prove super-linear convergence, which is related to semi-smooth Newton methods in function space [37]. All authors use h -FEM with a fixed polynomial degree (usually linear elements) as discretization.

This paper is concerned with developing an interior point method using higher order finite elements in regions where the optimal control is smooth and fine discretizations otherwise. Such a discretization is referred to as hp -FEM and has already been applied to optimal control problems with boundary control (see [4, 5]). Here, we mainly focus on distributed controls, although all results remain valid for Neumann controls. In addition, we use adaptive mesh hp -refinement. Here, we explore the fact that the necessary optimality conditions of the barrier problems can be written as a smooth system of equations.

In the following section we rigorously define the barrier problem and provide main results, such as existence of the central path and first order necessary optimality conditions. Within section 3 we formulate the short step method and prove convergence in function space. We use the general framework of [39], which allows solutions that touch the bounds at isolated points.

In section 4 we explain the implementation of a discrete version of the short step method. Adaptive updates for the barrier parameter and mesh refinement will ensure that the iterates stay within the area of convergence for Newton's method. After that, we derive a-posteriori error estimators for the central path as well as the Newton system, which is the core problem of the short step method. Both rely on residual based error estimators of the underlying PDE.

Finally, in section 6, we solve a test problem with known solution, where the convergence radius for Newton's method is large around the central path. Here, the hp -character of our method will be the center of investigation. Then, a problem with very small regularization parameter ν is solved. The adaptivity in the path-following algorithm successfully manages to stay within the region of attraction of Newton's method, which is very sensitive to reductions in the homotopy parameter μ .

Notation Let us briefly provide the notation for some function spaces. We denote by $L^p(\Omega)$ the set of p -times Lebesgue integrable functions for $1 \leq p < \infty$ and by $L^\infty(\Omega)$ functions that are essentially bounded. The Sobolev space $H^k(\Omega)$ comprises all functions in $L^2(\Omega)$ whose k -th weak derivative is square integrable ($k \in \mathbb{N}$). The subspace of $H^1(\Omega)$ consisting of functions with vanishing trace is $H_0^1(\Omega)$ with $H^{-1}(\Omega)$ as its dual space. The general dual space of a function space V is denoted by V^* with the duality pairing $\langle \cdot, \cdot \rangle_{V^*, V}$. If V has an inner product, it is denoted by $(\cdot, \cdot)_V$. Finally, $\bar{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\}$.

2 The barrier problem and central path

We follow [31] to introduce barrier functionals and their most important properties. Proofs and further references can be found in [31, chapter 2].

Definition 2.1. Let $B \subset U \times \mathbb{R}$ be measurable, such that $B(x) := \{u \in \mathbb{R} \mid (x, u) \in B\}$ is closed, convex with non-empty interior for all $x \in U$. A function $l(x, u) : U \times \mathbb{R} \rightarrow \bar{\mathbb{R}}$ is called barrier function if it fulfills

- $l(\cdot, u)$ is measurable for any $u \in \mathbb{R}$.
- $l(x, \cdot)$ is convex, continuous and differentiable on $\text{int}(B(x))$.
- $u \in \partial B(x) \Leftrightarrow l(x, u) = \infty$ and $\text{dist}(\partial B(x), u) \geq d > 0 \Leftrightarrow l(x, u) < L$ for $L \in \mathbb{R}$ depending only on d .
- $l(x, u)$ can be minorized by $a(x) - c|u|$ with $a \in L^1(U)$.

The minorizing criterion guarantees that $\int_U l(x, u(x)) \, dx > -\infty$ for $u \in L^1(U)$. A barrier function generates a barrier functional with the following definition.

$$b_\mu : L^1(U) \rightarrow \bar{\mathbb{R}}, \quad u \mapsto \mu \int_U l(x, u(x)) \, dx.$$

Theorem 2.2. For $1 \leq p \leq \infty$ the barrier functional $b_\mu : L^p(U) \rightarrow \bar{\mathbb{R}}$ is convex and lower semi-continuous. Furthermore, $b_\mu(u) < \infty \Rightarrow u \in \text{int}(B)$ a.e.

See e.g. [31, Corollary 2.1.6]. As the barrier functional suffers from reduced regularity, it is necessary to apply subdifferential calculus.

Definition 2.3. Let $f : V \rightarrow \bar{\mathbb{R}}$ be a convex function. We define the set valued mapping

$$\begin{aligned} \partial : V &\rightrightarrows V^* \\ v &\mapsto \{\partial f(v)\} \end{aligned}$$

where the image of v contains all linear and bounded functionals $m \in V^*$, such that

$$f(v + \delta v) + \langle m, \delta v \rangle_{V^*, V} \leq f(v)$$

In other words, the subdifferential $\partial f(v)$ contains the slope of all affine minorants that are exact at v .

Definition 2.4. We say $u \in U_{ad}$ is strictly feasible if and only if there is an $\varepsilon > 0$ such that

$$|u(x) - u_a(x)| + |u_b(x) - u(x)| > \varepsilon \quad \text{a.e. in } U.$$

Theorem 2.5. Consider $b : L^p(U) \rightarrow \bar{\mathbb{R}}$ with $1 \leq p \leq \infty$. If $p < \infty$ or u is strictly feasible, then

$$\partial b_\mu(u) \neq \emptyset \quad \Rightarrow \quad \partial b_\mu(u) = \{b'_\mu(u)\}$$

with the first variation

$$b'_\mu(u)\delta u = \mu \int_U \partial_u l(x, u(x)) \delta u(x) \, dx.$$

For $p < \infty$ we have $b'_\mu(u) \in L^p(U)^*$.

The result is proved in [31, Lemma 2.1.10, 2.1.11] and will be applied for the first order necessary conditions of the barrier problem.

In this work, we will work with $B(x) = [u_a(x), u_b(x)] \subset \mathbb{R}$ a.e. on U and use the logarithmic barrier function

$$l(x, u(x)) = -\ln(u(x) - u_a(x)) - \ln(u_b(x) - u(x)), \quad x \in U.$$

We enforce $u \in U_{ad}$ by adding a barrier functional to J . This leads to the problem (P_μ) :

$$(P_\mu) \quad \begin{cases} \text{minimize } J_\mu(u, y) := J(u, y) + b_\mu(u) \\ \text{subject to} \\ Ay = Bu, \\ u \in U_{ad}. \end{cases}$$

First, we have to assure that our homotopy approach makes sense insofar as the subproblem (P_μ) admits a solution.

Theorem 2.6. The problem (P_μ) admits a solution (u_μ, y_μ) for all $\mu > 0$. Its value of the objective functional is finite.

The assumptions on u_a, u_b imply that there is a \tilde{u} with $u_a < \tilde{u} < u_b$ a.e. Then, the proof is standard (see e.g. [31, Lemma 2.2.2]) and basically builds on the minima of convex functions (see [14, Proposition II.1.2]). For a more general setting, see [39].

In order to characterize the solution, we derive optimality conditions.

Theorem 2.7. The first order necessary optimality system for (P_μ) reads

$$Ay_\mu = Bu_\mu, \tag{2.1a}$$

$$A^*q_\mu = y_\mu - y_d \tag{2.1b}$$

$$\nu u_\mu + B^*q_\mu + b'_\mu(u_\mu) = 0. \tag{2.1c}$$

These conditions are also sufficient for a minimizer (u_μ, y_μ) .

Proof. We eliminate the state from the objective function by inverting the state equation. Take a minimizer u_μ from Theorem 2.6 and observe

$$J_\mu(u) \geq J_\mu(u_\mu) = J_\mu(u_\mu) + \langle 0, u - u_\mu \rangle \quad \forall u \in U_{ad}.$$

So we conclude $0 \in \partial J_\mu(u^*) \neq \emptyset$ and compute the derivative with the sum and chain rule ([14, Proposition I.5.6, I.5.7]). The fact that $b'_\mu(u_\mu) \in L^2(U)$ follows from Theorem 2.5 and the representation theorem of Riesz. As the optimization problem is convex, the necessary conditions are also sufficient. \square

Definition 2.8. For notational convenience, we set

$$Y := Q := H^1(\Omega).$$

The solution (u_μ, y_μ) together with the corresponding adjoint variable q_μ are referred to as the central path

$$(u, y, q)_\mu \in L^2(U) \times Y \times Q.$$

Because of the bounds on the control and the boundedness of the solution operators for the state and adjoint equation, we get for all $\mu \in (0, \mu_0]$

$$\|(u, y, q)_\mu\|_{L^2(U) \times Y \times Q} \leq C_{\mu_0}.$$

Remark 2.9. As the operators A, A^* are boundedly invertible, we can write down an equivalent formulation of the optimality system: $(u, y, q)_\mu \in L^2(U) \times Y \times Q$ solves (2.1) if and only if

$$F_\mu(u) = \nu u_\mu + B^* A^{-*} (A^{-1} B u_\mu - y_d) + b'_\mu(u_\mu) = 0. \quad (2.2)$$

This equation holds a.e. in U .

Theorem 2.10. The central path is Hölder continuous with index $1/2$, i.e.

$$\|(u, y, q)_\mu - (u, y, q)_\eta\|_{U \times Y \times Q} \leq L_c \sqrt{|\mu - \eta|}$$

for all $\mu, \eta \in (0, \mu_0]$. Moreover, $(u^*, y^*, q^*) = \lim_{\mu \searrow 0} (u, y, q)_\mu$ exists and is the global solution of P .

For the proof we refer the reader to [39, Lemma 9].

Remark 2.11. If the controls on the central path have positive distance to the bounds u_a, u_b in the L^∞ sense, the central path is differentiable (see e.g. [31, 39]) and admits the bound

$$\|\partial_\mu(u, y, q)_\mu\| \leq C\mu^{-1/2}.$$

3 The interior point method

Interior point methods can be regarded as methods that systematically solve a perturbed optimality system of the original minimization problem. This perturbed system is itself the exact optimality system for a barrier problem, which is characterized by an additional term in the cost functional that penalizes the violation of constraints. This strategy allows to deal with control and/or state constraints where the resulting equations have the advantage of being smooth.

3.1 An abstract short step method

Let the first order necessary conditions of the central path be given by $\mathcal{F}_\mu(x) = 0$ with a mapping

$$\mathcal{F}_\mu : X \rightarrow Y \quad (3.1)$$

and spaces X, Y , which will be specified later. A general short step algorithm in function space tries to solve (3.1) with Newton's method and drives $\mu \searrow 0$ at the same time.

Algorithm 1 Short Step Method in Function Space

- 1: Choose initial point x_0 and barrier parameter $\mu_0 > 0$.
- 2: $k := 0$.
- 3: Solve the Newton system

$$\partial \mathcal{F}_{\mu_k}(x_k) \delta x = -\mathcal{F}_{\mu_k}(x_k).$$

- 4: $\tilde{x}_{k+1} := x_k + \delta x$.
 - 5: Apply a smoothing step $x_{k+1} := Z(\tilde{x}_{k+1})$.
 - 6: Choose $\sigma_k \in [\sigma_{min}, 1)$ and set $\mu_{k+1} := \sigma_k \mu_k$.
 - 7: $k := k + 1$ and go to **3**.
-

We remark that the smoothing step is not always necessary for convergence of the algorithm. Note that more details and investigations are essential for implementing this short step algorithm in practice.

3.2 Well posedness and convergence in function space

We take $\mathcal{F}_\mu(u)$ from Algorithm 1 as $F_\mu(u)$ from (2.2) and investigate the Newton system

$$\partial F_{\mu_k}(u_k) \delta u_k = -F_{\mu_k}(u_k). \quad (3.2)$$

Let $\mu_k > 0$ and u_k denote an iterate of the short step method. Moreover, let $1 \leq p \leq \infty$ and

$$D^p := \{u \in U_{ad} \cap L^p(U) \mid (u - u_a)^{-1}, (u_b - u)^{-1} \in L^p(U)\}. \quad (3.3)$$

A formal derivation at $u_k \in D_p$ in the direction h for $2 \leq p \leq \infty$ yields

$$\partial F_\mu(u_k)h = \nu h + B^* A^{-*} A^{-1} B h + \frac{\mu h}{(u_k - u_a)^2} + \frac{\mu h}{(u_b - u_k)^2}. \quad (3.4)$$

In order to guarantee that the Newton system can be solved at the new iterate $u_k + \delta u_k$, the smoothing operator is designed accordingly.

Lemma 3.1. *The μ -dependent function*

$$\beta : (u_a, u_b) \rightarrow \mathbb{R}, \quad x \mapsto \nu x - \frac{\mu}{x - u_a} + \frac{\mu}{u_b - x}. \quad (3.5)$$

is invertible and gives rise to a Lipschitz continuous superposition operator

$$\beta^{-1} : L^p(U) \rightarrow \{v \in L^p(U) \mid u_a < v < u_b\} =: \tilde{U}_{ad}$$

where $p \in [2, \infty)$ and the Lipschitz constant is $1/\nu$.

Note that we identify the generating function with its associated superposition operator. The lemma is proved in [39]. We set

$$W^p := L^p(U) \times Y \times Q \times L^p(U) \times L^p(U), \text{ with} \\ w := (w_u, w_y, w_q, w_a, w_b) \in W^p$$

to address each component. Furthermore, we use the notation $y(u) := A^{-1}Bu$ for the solution of the state equation and $q(u) = q(y(u))$ for the solution to the adjoint equation, respectively. At this point, we need an additional regularity assumption for the constraint $Ay = Bu$.

Assumption 3.2. Assume that there is a $\delta \in (0, 1]$ such that the differential operators A, A^* allow solutions which belong to the Sobolev-Slobodeckij space $H^{1+\delta}(\Omega)$ (as defined in [16]). That is $A^{-1}, A^{-*} \in \mathcal{L}(L^2(\Omega), H^{1+\delta}(\Omega))$. Furthermore, we assume that $2 \leq p < q \leq \infty$ with the continuous embedding

$$H^{1+\delta}(\Omega) \hookrightarrow L^q(U).$$

Definition 3.3. The smoothing operators $z_u : L^p(U) \rightarrow L^q(U)$ and $Z : W^p \rightarrow W^q$ are defined as

$$Z(w) := \begin{pmatrix} z_u(w_u) \\ z_y(w_u) \\ z_q(w_u) \\ z_a(w_u) \\ z_b(w_u) \end{pmatrix} = \begin{pmatrix} \beta^{-1}(q(w_u)) \\ y(z_u(w_u)) \\ q(w_u) \\ \mu/(z_u(w_u) - u_a) \\ \mu/(u_b - z_u(w_u)) \end{pmatrix} \quad (3.6)$$

For the convergence of the short step method, it is essential that the smoothing step satisfies a Lipschitz property.

Lemma 3.4. Let Assumption 3.2 hold and $u \in L^p(U)$. Let $s := (u_\mu, y_\mu, q_\mu, z_a(u_\mu), z_b(u_\mu))$ be a solution to P_μ . Then the smoothing operators z_u, Z are well defined and there exist constants $L_u, L > 0$ such that

$$\|z_u(w_u) - s_u\|_{L^q(\Omega)} \leq L_u \|w_u - s_u\|_{L^p(\Omega)}, \quad (3.7)$$

$$\|Z(w) - s\|_{W^q} \leq L \|w - s\|_{W^p}, \quad \forall w \in W^p. \quad (3.8)$$

Moreover,

$$z_u(w_u) \in D^q.$$

Proof. Obviously, $s \in W^q$ and $s = Z(s)$ due to the first order necessary conditions. Lemma 3.1 and the invertibility of A, A^* yield

$$\|z_u(w_u) - z_u(s_u)\|_{L^q(U)} \leq \frac{1}{\nu} \|q(w_u) - q(s_u)\|_{L^p(U)} \leq \frac{C}{\nu} \|w_u - s_u\|_{L^p(U)}.$$

This proves the first claim. Similarly, we find

$$\|z_y(w_u) - z_y(s_u)\|_Y \leq C \|u - u_\mu\|_{L^p(U)}, \quad \|z_q(w_u) - z_q(s_u)\|_Q \leq C \|w_u - s_u\|_{L^p(U)}.$$

The remaining components of Z can be treated as in the proof of [39, Theorem 2] and we obtain with constants L_a, L_b

$$\|z_a(w_u) - z_a(s_u)\|_{L^q(U)} \leq L_a \|w_u - s_u\|_{L^p(\Omega)} \quad (3.9)$$

$$\|z_b(w_u) - z_b(s_u)\|_{L^q(U)} \leq L_b \|w_u - s_u\|_{L^p(\Omega)}. \quad (3.10)$$

Thus, we can bound $\|Z(w) - Z(s)\|_{W^q}$ by $\|w_u - s_u\|_{L^p(U)} \leq \|w - s\|_{W^p}$. It holds

$$\|Z(w) - s\|_{W^q} \leq \max\{L_u, C, L_a, L_b\} \|w - s\|_{W^p}.$$

It remains to show the last claim, i.e. $z_u(w_u) \in D^q$.

From the definition of z_u we get $\beta(z_u(w_u)) = q(w_u)$. Writing out the terms of β yields

$$\nu z_u(w_u) + z_a(z_u(w_u)) + z_b(z_u(w_u)) = q(w_u).$$

As $z_u(w_u) \in U_{ad}$ it follows that $\nu z_u(w_u)$ is essentially bounded. With $q(w_u) \in H^{1+\delta}(\Omega)$, we conclude

$$z_a(z_u(w_u)) + z_b(z_u(w_u)) \in L^q(U).$$

The possible singularities of the two addends do not interfere because $|u_a - u_b| \geq \vartheta > 0$. Consequently, each of them is q -times integrable and $z_u(w_u)$ belongs to D^q . \square

Finally, we establish the invertibility of the Newton system (see also [39, chapter 5]).

Theorem 3.5. *Let $\mu_k > 0$ and Assumption 3.2 be fulfilled. For any $u_k \in D^q$ and $r \in L^q(U)^*$, there is a $\delta u : U \rightarrow \mathbb{R}$ such that*

$$\partial F_\mu(z_u(u_k))\delta u_k = r \quad \text{a.e. on } U \quad (3.11)$$

If $r \in L^q(U)$ we also have $\|\delta u\|_{L^t(U)} \leq C\|r\|_{L^p(U)}$ for all $t \in [p, q]$ where the constant C can be chosen uniformly on bounded subsets $(\mu, u) \in \mathbb{R} \times D^q$.

Proof. The result follows from the proof of [39, Lemma 4] if we show that $Z(u_k)$ lies in

$$\begin{aligned} N_{-\infty, q}(\mu) := \{ & (u, y, q, w_a, w_b) \in W_q \mid u \in U_{ad}, (u - u_a)w_a \geq \gamma\mu, (u_b - u)w_b \geq \gamma\mu, \\ & w_a|_{u > (u_a + u_b)/2} \leq \Theta_\mu, w_a|_{u < (u_a + u_b)/2} \leq \Theta_\mu, \\ & \min\{w_a, w_b\}|_{u = (u_a + u_b)/2} \leq \Theta_\mu \} \end{aligned}$$

with $\theta_\mu = 2 \max\{\mu_{-\infty}, \mu/\gamma\}/\vartheta$.

Remember that $u_b - u_a \geq \vartheta > 0$ almost everywhere. The values of $\gamma \in (0, 1)$ and $\mu_{-\infty}$ are arbitrary. From the definition of the smoothing operator Z it is clear that $z_u(u_k) \in U_{ad}$ and

$$(z_u(u_k) - u_a)z_a(u) = \mu \geq \gamma\mu, \quad (u_b - z_u(u_k))z_b(u) = \mu \geq \gamma\mu.$$

Define $U_k^+ := \{x \in U \mid z_u(u_k) > \frac{u_a + u_b}{2}\}$. Then,

$$z_a(u_k)|_{U_k^+} = \frac{\mu}{(z_u(u_k) - u_a)}|_{U_k^+} \leq \frac{2\mu}{u_b - u_a}|_{U_k^+} \leq \frac{2\mu}{\vartheta} \leq \Theta_\mu.$$

The same estimate yields $z_b(u)|_{U_k^-} \leq \Theta_\mu$ with $U_k^- := \{x \in U \mid z_u(u_k) < \frac{u_a + u_b}{2}\}$.

For $z_u(u_k) = (u_a + u_b)/2$ we directly get

$$z_a(u_k) = z_b(u_k) = \frac{2\mu}{u_b - u_a} \leq \Theta_\mu,$$

which implies $Z(u_k) \in N_{-\infty, q}(\mu)$. □

3.3 Convergence of the short step method

In this section we show that the Algorithm 1 converges. The Lipschitz continuity of Z , which was proved in Lemma 3.4, is vital because it closes a $p - q$ gap in the convergence analysis of the short step method.

Theorem 3.6. *Let $\mu_0, \rho_0 > 0$ be fixed. Assume that $u^* = \lim_{\mu \searrow 0} u_\mu$ satisfies strict complementarity (as in [39, Definition 2]). Then there exists a sequence $\sigma_{min, k} \leq \sigma_{max} < 1$ with $\sigma_k \in [\sigma_{min, k}, \sigma_{max}]$ such that the iterates u_k generated by Algorithm 1 with the smoothing operator z_u are well defined and satisfy*

$$\|u_k - u_\mu\|_{L^q(U)} \leq C\sqrt{\mu_{k-1}} \quad (3.12)$$

$$\|u_k - u^*\|_{L^q(U)} \leq (C + L_c)\sqrt{\mu_{k-1}}. \quad (3.13)$$

where C is some constant and L_c the Hölder constant of the central path (see Theorem 2.10) on $(0, \mu_0]$.

Proof. The proof of convergence is achieved by showing equivalence of Algorithm 1 with the short step method of [39]. The latter is designed for iterates in W^q . By choosing μ_0 large enough we can launch the algorithms with

$$u_0 := \frac{u_a + u_b}{2} \in D^q,$$

respectively

$$w_0 := (u_0, y(u_0), q(u_0), \mu(u_a - u_0)^{-1}, \mu(u_b - u_0)^{-1})^\top \in W^q$$

sufficiently close to the central path.

It suffices to show that the iterates u_k of Algorithm 1 (smoothed under z_u) have a corresponding sequence w_k with $u_k = w_{k,u}$ that is generated by the interior point method of [39] (smoothed under Z). Convergence then follows from [39, Theorem 3] because the projection operator Z satisfies a Lipschitz property (due to Lemma 3.4)

The iterates in W_q are given by $w_{k+1} = Z(w_k + \delta w_k)$ with the Newton update

$$\begin{pmatrix} \nu & 0 & B^* & -I & I \\ 0 & I & A^* & 0 & 0 \\ B & A & 0 & 0 & 0 \\ w_{k,a} & 0 & 0 & (w_{k,u} - u_a) & 0 \\ -w_{k,b} & 0 & 0 & 0 & (u_b - w_{k,u}) \end{pmatrix} \delta w_k = - \begin{pmatrix} w_{k,y} - y_d + A^* w_{k,q} \\ \nu w_{k,u} + w_{k,q} - w_{k,a} + w_{k,b} \\ A w_{k,y} - B w_{k,u} \\ w_{k,a}(w_{k,u} - u_a) - \mu \\ w_{k,b}(u_b - w_{k,u}) - \mu \end{pmatrix} \quad (3.14)$$

Now we show that $\delta w_{k,u} = \delta u_k$ for $k \geq 0$. By construction, we have $u_k = (w_k)_u$ and

$$A w_{k,y} - B w_{k,u} = 0, \quad w_{k,a}(w_{k,u} - u_a) = \mu, \quad w_{k,b}(u_b - w_{k,u}) = \mu w_{k,b} \quad (3.15)$$

for $k = 0$.

Assume by induction that these equalities hold for $k \geq 0$. From (3.15) we deduce that the last three components of the right hand side of (3.14) are zero. Eliminating $\delta w_{k,q}, \delta w_{k,a}, \delta w_{k,b}$ from the first row of (3.14) yields (3.2) and proves that $\delta w_{k,u} = \delta u_k$.

As the projection operator only depends on $(w_k)_u = u_k$ we find

$$u_{k+1} = z_u(u_k + \delta u_k) = z_u(w_k + \delta w_k) = Z(w_k + \delta w_k)_u = w_{k+1,u}.$$

The construction of Z guarantees that (3.15) remains valid. Thus, the induction is complete and the short step algorithm equivalent to the one of [39], where all claims are established. \square

4 Discretization

First, we explain the discretization of the optimality system by finite elements. We develop our ideas starting with the discretization of (2.1) and end up with a fully discrete version for solving (2.2). This shows why some diligence is necessary for the treatment of the non-linear optimality system when using higher order elements. After that, we present an implementable short step algorithm, which adaptively controls the homotopy parameter, the area of convergence for Newton's method, and the discretization errors.

4.1 The optimality system

In the following, we suppress the dependence on μ in (2.1). We start by discretizing the state/adjoint equation with hp -FEM. As usual in finite element methods, we replace the function space in the weak formulation of $Ay = Bu$ by a N -dimensional subspace $S^p(\Omega, \tau)$ for a shape-regular mesh τ being a collection of open cells K such that $\bigcup_{K \in \tau} \bar{K} = \bar{\Omega}$. Each element $K \in \tau$ has an associated polynomial degree p_K . The diameter of an element $K \in \tau$ is denote by h_K . The local polynomial degrees p_K are collected in a polynomial degree vector \mathbf{p} . More details on the definition and efficient design of hp -spaces, its basis functions $\text{span}\{\Phi_1, \dots, \Phi_N\} = S^p(\Omega, \tau)$ and underlying triangulations can be found in [10, 21, 25, 35] and references therein. The numerical results in section 6 were obtained with a conform discretization on quadrilateral elements that allow hanging nodes.

We utilize the standard notation for elliptic PDEs and denote by $y^h \in S^{\mathbf{P}}(\Omega, \tau)$ the finite element function that solves

$$a(y^h, v^h) = (u_\mu^h, v^h)_{L^2(U)}, \quad \forall v^h \in S^{\mathbf{P}}(\Omega, \tau).$$

There is a one-to-one correspondence between y^h as a function in $H^1(\Omega)$ and the coefficients of the representation $y^h = \sum_{i=1}^N \tilde{y}_i^h \Phi_i$, which is why we implicitly change between the two.

The discrete version of (2.1a),(2.1b) of the optimality system reads

$$Ky_\mu^h - Mu_\mu^h = 0, \quad (4.1)$$

$$K^*q_\mu^h - My_\mu^h + \bar{y}_d = 0, \quad (4.2)$$

with M being the mass matrix $M_{ij} = \int_U \Phi_i \Phi_j \, dx$. K, K^* shall represent the matrices corresponding to the differential operator A, A^* . If $A = \Delta = A^*$, this is the stiffness matrix with $K_{ij} = \int_\Omega \nabla \Phi_i \cdot \nabla \Phi_j \, dx$. The load vector is denoted by $\bar{y}_d := \int_\Omega y_d \Phi_i \, dx$.

The main question is how to discretize the control in (2.1c). If we used a finite element function $u^h \in S^{\mathbf{P}}(\Omega, \tau)$, it would be hard to check whether a new Newton iterate $u_{k+1}^h = u_k^h + \delta u_k^h$ is feasible and produces finite integrals

$$\int_U \mu(u_{k+1}^h - u_a)^{-1} \, dx, \quad \int_U \mu(u_b - u_{k+1}^h)^{-1} \, dx.$$

An implementation has to ensure that the values at the integration points x_j lie in $(u_a(x_j), u_b(x_j))$. But this is challenging for polynomials of degree greater than one.

This issue is solved by representing the control not as a member of $S^{\mathbf{P}}(\Omega, \tau)$, but as a vector consisting of values at the integration points, which are also used for the evaluation of the barrier terms.

We approximate

$$\int_U u \Phi_i \, dx \approx \sum_{j=1}^M u(x_j) \Phi_i(x_j) \omega_j \quad (4.3)$$

where x_j are integration points in U with weights ω_j . We set

$$R^\top = \Phi_i(x_j), \quad D = \text{diag}(\omega_j), \quad i = 1, \dots, N, \quad j = 1, \dots, M. \quad (4.4)$$

and use u_j^h , $j = 1, \dots, M$ as a discrete control variable. Finding the values of $v^h \in S^{\mathbf{P}}(\Omega, \tau)$ at x_j is achieved by

$$v_j^h := v^h(x_j) = (Rv^h)_j.$$

The discrete version of the first order necessary optimality condition only enforces (2.2) at each integration point, i.e.

$$\nu u_j^h + (Rq^h)_j - \frac{\mu}{u_j^h - u_a} + \frac{\mu}{u_b - u_j^h} = 0, \quad \forall j = 1, \dots, M.$$

We take the values of u^h as a column vector (and understand non-linear terms as vectors as well) and rewrite the last equation as

$$\nu u^h + Rq^h - \frac{\mu}{u^h - u_a} + \frac{\mu}{u_b - u^h} = 0.$$

If we correct (4.1) according to the conventions in (4.3),(4.4), we have to solve the discrete optimality system

$$F_\mu^h(u^h, y^h, q^h) := \begin{pmatrix} Ky^h - R^\top Du^h \\ K^*p^h - My^h + \bar{y}_d \\ \nu u^h + Rq^h - \frac{\mu}{u^h - u_a} + \frac{\mu}{u_b - u^h} \end{pmatrix} = 0$$

It can easily be verified that this is the exact optimality system of the following discrete problem.

$$(\mathbf{P}_\mu^h) \quad \left\{ \begin{array}{l} \text{minimize } J_\mu^h(y^h, u^h) := \frac{1}{2} \|y^h - y_d\|_{L^2(\Omega)}^2 + \frac{\nu}{2} \sum_{i=1}^N \omega_i (u_i^h)^2 \\ \quad - \mu \sum_{i=1}^N \omega_i (\ln(u_i^h - u_a) + \ln(u_b - u_i^h)) \\ \text{subject to} \\ Ky^h = R^\top Du^h, \end{array} \right.$$

This non-linear system of equations is to be solved with Newton's method. The linearization reads

$$\partial F_\mu^h(u^h, y^h, p^h) = \begin{pmatrix} \nu I + \mu \text{diag}((u_i^h - u_a)^{-2} + (u_b - u_i^h)^{-2}) & 0 & R \\ 0 & M & -K \\ R^\top D & -K & 0 \end{pmatrix}$$

If we multiply the first row by D , the discretized optimality system in the variables (u^h, y^h, q^h) is symmetric. It can be solved either with direct methods or an iterative solver such as MINRES.

Completely analogously to the continuous case, where we eliminated the state and adjoint variable, we can invert K, K^* and get a discrete equation only in the variable u_k^h . We find

$$\begin{aligned} \partial F_\mu^h(u_k^h) \delta u_k^h &:= (\nu I + \mu \text{diag}((u_k^h - u_a)^{-2} + (u_b - u_k^h)^{-2}) + RK^{*-1}MK^{-1}R^\top D) \delta u_k^h = \\ &\quad - \nu u + \mu(u_k^h - u_a)^{-1} - \mu(u_b - u_k^h)^{-1} - RK^{*-1}(MK^{-1}R^\top Du - \bar{y}_d) =: -F_\mu^h(u_k^h). \end{aligned}$$

which is a discretization of the continuous Newton system (3.4). Multiplying this equation with $D = D^\top$ from the left yields

$$\begin{aligned} (\nu D + \mu D \text{diag}((u_k^h - u_a)^{-2} + (u_b - u_k^h)^{-2}) + DRK^{*-1}MK^{-1}R^\top D) u_{k+1}^h = \\ \mu D(u_k^h - u_a)^{-1} - \mu D(u_b - u_k^h)^{-1} + \mu D((u_k^h - u_a)^{-2} + D(u_b - u_k^h)^{-2}) + DRK^{*-1}MK^{-1}\bar{y}_d. \end{aligned}$$

For the addends of the left hand side of the system, we now have

- $\nu D > 0$, if we use an integration scheme with positive weights only.
- $\text{diag}((u_k^h - u_a)^{-2} > 0$ and $\text{diag}(u_b - u_k^h)^{-2} > 0$, if $u_k^h(x_j) \in (u_a, u_b)$.
- $DRK^{*-1}MK^{-1}R^\top D > 0$ because of $M, K, K^* > 0$.

The symmetry of the left hand side is obvious. Thus, the system can be inverted by a PCG-Solver.

The pointwise smoothing operator Z calls for numerical solutions of the cubic equation (3.5), which can be implemented in a numerically stable way (see [31]). It guarantees that the values u_j^h are feasible making the numerical algorithm well-defined.

The adaptive short step method will have to control the discretization error and perform hp mesh refinements. There are different strategies to guide between a finer triangulation and higher order elements. We choose the estimate of the smoothness of u_k based on the expansion in a Legendre series ([13]). Several modifications are possible because the variables $y_k(u_k)$ and/or $q_k(u_k)$ can also be examined and included in the decision process.

Let us now comment on the estimation of the smoothness of u_k^h , which is complicated by the fact that u_k^h is represented by the values at the integration points and, therefore, does not fit into the framework of [13]. Assume that $U = \Omega$ (the case of boundary control is analogously) and let $K \in \tau$ be an element with polynomial degree $p_K \geq 1$. As we want to assemble element mass and stiffness matrix on K without

errors, we work with Gaussian quadrature, which is at least exact for polynomials of order $2p_K$. Hence, we tensorize a one dimensional integration scheme with $p_K + 1$ points and obtain $(p_K + 1)^2$ points. A vector of values at these integration points uniquely determines a polynomial of order p_K . We therefore obtain a one to one mapping Ψ_K

$$\Psi_K : \mathbb{R}^{(p_K+1)^2} \rightarrow Q(p_K) := \left\{ v : K \rightarrow \mathbb{R} \mid v = \sum_{i,j} a_{i,j} x_1^i x_2^j, \quad 0 \leq i, j \leq p_K, \quad a_{i,j} \in \mathbb{R}, \quad x \in K \right\}. \quad (4.5)$$

Let u_K^h be the vector that consists of all u_j^h with $x_j \in K$ ordered by the value of j . The transformation of u^h to a finite element function is realized by

$$\Psi : \mathbb{R}^N \rightarrow S^{\mathbf{p}}(\Omega, \tau) \quad (4.6)$$

$$u^h \mapsto \min_{u \in S^{\mathbf{p}}(\Omega, \tau)} \| u - \sum_{K \in \tau} \chi_K \Psi_K(u_K^h) \|_{L^2(\Omega)}. \quad (4.7)$$

It is obvious that $\Psi(R^T v) = v$ for every v from the image space of Ψ .

In order to obtain sensible estimates of the smoothness of approximate solutions, the initial mesh consists of piecewise quadratic or cubic functions. Based on the decay of the Legendre coefficients of $\Psi(u_k^h)$, the smoothness of the control is estimated in the numerical implementation of Algorithm 1.

4.2 A fully adaptive short step method

The implementation of Algorithm 1 is done as described in [31]. We borrow ideas from [33, 32] as regards the adaptive update of μ , which builds on general results about Newton and homotopy methods in [11]. The ideas are formulated for iterates u_k of Newton's method, which intends to solve the optimality conditions of the central path u_μ , i.e. the non-linear equation $F_\mu(u_\mu) = 0$.

A numerical realization of the homotopy method can only compute an inexact Newton step in function space, i.e.

$$\delta u_k = -\partial F_\mu(u_k)^{-1} F_\mu(u_k) + e_k.$$

In order to ensure that the inexact method converges, the error e_k and the contraction

$$\theta_k(\mu) := \frac{\| \partial F_\mu(u_k)^{-1} [\partial F_\mu(u_k)(u_k - u_\mu) - (F_\mu(u_k) - F_\mu(u_\mu))] \|}{\| u_k - u_\mu \|} \quad (4.8)$$

are controlled. The simple calculation

$$\begin{aligned} \| u_{k+1} - u_\mu \| &= \| u_k + \delta u_k - u_\mu \| = \| u_k - \partial F_\mu^{-1} F_\mu(u_k) + e_k - u_\mu \| \\ &\leq \| \partial F_\mu^{-1}(u_k) [\partial F_\mu(u_k)(u_k - u_\mu) - (F_\mu(u_k) - F_\mu(u_\mu))] \| + \| e_k \| \\ &\leq \theta_k(\mu) \| u_k - u_\mu \| + \| e_k \|. \end{aligned} \quad (4.9)$$

shows that linear convergence

$$\| u_{k+1} - u_\mu \| \leq \gamma \| u_k - u_\mu \| \quad (4.10)$$

with a factor $\gamma \in (0, 1)$ is achieved if

$$\theta_k(\mu) + \| e_k \| / \| u_k - u_\mu \| \leq \gamma. \quad (4.11)$$

The estimates (4.10) and (4.11) describe the interaction of discretization error and non-linearity of the barrier problem. For mildly non-linear problems (first example in Section 6) we have $\theta_k \ll 1$ and the relative discretization error is the main contribution in (4.11). Highly non-linear problems (second

example in Section 6), on the other hand, may allow the algorithm to perform several short steps without refining the mesh, because θ_k dominates in (4.11).

For obtaining a numerical estimate of θ_k , we assume $e_k = 0$, and insert u_{k+1} in (4.8) as the best possible guess for the unknown u_μ . This leads to

$$\begin{aligned}\theta_k(\mu) \approx [\theta_k(\mu)] &:= \frac{\|\partial F_\mu(u_k)^{-1}[\partial F_\mu(u_k)(u_k - u_{k+1}) - (F_\mu(u_k) - F_\mu(u_{k+1}))]\|}{\|u_k - u_{k+1}\|} \\ &= \frac{\|u_k - u_{k+1} - \partial F_\mu(u_k)^{-1}(F_\mu(u_k) - F_\mu(u_{k+1}))\|}{\|u_k - u_{k+1}\|} = \frac{\|u_k - \bar{u}_{k+1}\|}{\|u_k - u_{k+1}\|}\end{aligned}\quad (4.12)$$

with the simplified Newton iterate

$$\bar{u}_{k+1} := u_{k+1} + \Delta u_k := u_{k+1} - \partial F_\mu(u_k)^{-1} F_\mu(u_{k+1}). \quad (4.13)$$

The short step method, as describe in Algorithm 1, uses a smoothing step $u_{k+1} := z_u(u_k + \delta u_k)$. Inserting this into (4.12) and (4.13) yields

$$[\theta_k(\mu)] = \frac{\|u_k - (z_u(u_k + \delta u_k) - \partial F_\mu(u_k)^{-1} F_\mu(z_u(u_k + \delta u_k)))\|}{\|z_u(u_k + \delta u_k) - u_k\|}. \quad (4.14)$$

The discretization error e_k is estimated with a robust a-posteriori error estimator (see section 5). If the distance of u_{k+1} to the central path u_{μ_k} is below a certain accuracy tol_d and the contraction is below a critical threshold (e.g. $[\theta_k(\mu_k)] \leq \theta_t = 0.5$), the Newton corrector is considered successful and a new homotopy parameter is computed. Otherwise, more Newton steps might be necessary. The simplified Newton step can be added to the current iterate in order to reduce the distance to the central path. If the contraction is beyond a critical value (e.g. $[\theta_k(\mu_k)] > \theta_c = 0.8$), a more conservative value for μ_k is computed and the Newton corrector is relaunched.

An adaptive choice of σ_k as an update of the barrier parameter μ_k shall ensure that the iterates do not leave the area of convergence of Newton's method. The two main ingredients are slope information about the central path and estimates of an affine covariant Lipschitz constant.

If the central path u_μ is differentiable, we approximate the slope η_k at the current iterate u_k by

$$\partial_\mu u_\mu \approx [\eta_k(\mu)] := -\partial F_\mu^{-1}(u_k) \partial_\mu F_\mu(u_k). \quad (4.15)$$

Here and in the following, we stay consistent with our notation but remark that $\partial_\mu u_\mu$ is the derivative of the central path with respect to μ evaluated at the point μ , which is more commonly written as $\partial_\mu u(\mu)$. If u_k is close to the central path, we expect this inexact quantity to be a good estimate.

We use the approximation of the slope for the termination criterion of the short step algorithm. The fundamental theorem of calculus yields

$$u_{\mu_k} - u^* = \lim_{\substack{\mu \searrow 0 \\ \mu}} \int_{\mu}^{\mu_k} \partial_\mu u_\mu \, d\mu.$$

From the result of Remark 2.11, i.e. $\|\partial_\mu u_\mu\| \in \mathcal{O}(\mu^{-1/2})$ we construct the approximation

$$\frac{\partial_\mu u_\mu}{\partial_\mu u_{\mu_k}} \approx \sqrt{\frac{\mu_k}{\mu}}.$$

We approximate the distance by

$$\|u_{\mu_k} - u^*\| \lesssim \lim_{\substack{\mu \searrow 0 \\ \mu}} \int_{\mu}^{\mu_k} \left\| \sqrt{\frac{\mu_k}{\mu}} \partial_\mu u_{\mu_k} \right\| d\mu = 2\mu_k [\eta_{k+1}] =: [\|u_{\mu_k} - u^*\|]. \quad (4.16)$$

Note the offset $[\eta_{k+1}]$ because u_{k+1} is the best estimate for u_{μ_k} . As soon as a global tolerance tol is reached, the algorithm stops.

Assuming a linear model for the contraction we have

$$\theta_k(\mu) \leq \omega_k(\mu) \|u_k - u_\mu\|. \quad (4.17)$$

For $\mu = \mu_k$ the best available guess for the central path is u_{k+1} and leads us the the estimate

$$\omega_k(\mu_k) \approx [\omega_k(\mu_k)] := [\theta_k(\mu_k)] / \|u_k - u_{k+1}\|. \quad (4.18)$$

The numerical estimates of the contraction also provides an estimate for the error in the central path via (4.9)

$$\|u_{k+1} - u_{\mu_k}\| \approx [\theta_k(\mu_k)] \|u_k - u_{\mu_k}\| + \|e_k\| \leq [\theta_k(\mu_k)] (\|u_k - u_{k+1}\| + \|u_{k+1} - u(\mu_k)\|) + \|e_k\|.$$

Hence,

$$\|u_{k+1} - u_{\mu_k}\| \approx [\|u_{k+1} - u_{\mu_k}\|] := \frac{[\theta_k(\mu_k)]}{1 - [\theta_k(\mu_k)]} \|u_{k+1} - u_k\| + \|e_k\|. \quad (4.19)$$

In Section 5.2 we develop an a-posteriori error estimator for the error in the newton step $[\|e_k\|] \approx \|e_k\|$. As as an alternative to (4.19) one could also use the a-posteriori error estimator of section 5.1 to estimate $\|u_{k+1} - u_{\mu_k}\|$.

An adaptive step size selection aims at achieving

$$\omega_k(\mu) \|u_k - u_\mu\| \approx \theta_d \in [0.1; 0.75].$$

Assuming the model $\omega_k(\mu) \in \mathcal{O}(\mu^{-1/2})$ leads us to

$$[\omega_k(\mu)] := [\omega_k(\mu_k)] \sqrt{\frac{\mu_k}{\mu}}$$

Proceeding as in [30], we are lead to the to the step size rule

$$[\omega_k(\mu_k)] \sigma^{-1/2} (\|x_k - x(\mu_k)\| + [\eta_k] 2\mu_k (1 - \sqrt{\sigma})) = \theta_d. \quad (4.20)$$

If the Newton corrector was not successful, we use same equation for computing a more conservative μ_k . We simply replace $[\eta_k]$ and $\|x_k - x(\mu_k)\|$ by the estimates of the previous (successful) iterate (see also [32]). In detail, the conservative step size selection reads

$$[\omega_k(\mu_k)] \sigma^{-1/2} (\|x_{k-1} - x(\mu_k)\| + [\eta_{k-1}] 2\mu_k (1 - \sqrt{\sigma})) = \theta_d. \quad (4.21)$$

Now we have everything at hand to implement a version of Algorithm 1.

Algorithm 2 Short Step Method in Finite Dimensional Space

```
1: Choose parameters  $\Lambda_d, \sigma_{min}, \sigma_{max}, \theta_c, \theta_d, \theta_t, tol_d, tol$ .
2: Choose  $(u_0, \mu_0)$ 
3:  $k := 0$ 
4:  $\varepsilon_k := tol + 1$ 
5: do
6:    $(\tilde{u}, success) := \text{NEWTON\_CORRECTOR}(u_k, \mu_k)$ 
7:   if success then ▷ Implementing Algorithm 1 line 6
8:     compute  $[\eta_k]$  ▷ see (4.15)
9:     compute  $\sigma_k \in [\sigma_{min}, \sigma_{max}]$  ▷ see (4.20)
10:     $\mu_{k+1} := \sigma_k \mu_k$ 
11:     $u_{k+1} := \tilde{u}$ 
12:     $k := k + 1$ 
13:    compute  $[\|u_k - u^*\|] =: \varepsilon_k$  ▷ see (4.16)
14:  else
15:    if  $k > 0$  then
16:      compute conservative  $\sigma_k \in [\sigma_{min}, \sigma_{max}]$  ▷ see (4.21)
17:       $\mu_k := \sigma_k \mu_{k-1}$ 
18:      restore mesh
19:    else
20:      terminate: 'bad initial guess  $(\mu_0, u_0)$ '
21:    end if
22:  end if
23: while  $\varepsilon_k > tol$ 
```

The value of σ_{min} is motivated by the best error reduction we can expect from uniform h -refinements. For elliptic equations on convex domains, the error decays like h^2 . As the central path is Hölder continuous with index $1/2$, we set $\sigma_{min} = 1/16$ to facilitate an error reduction of $1/4$. If the mesh is refined r times during one Newton corrector step, we set $\sigma_{min} = 1/16^r$.

Algorithm 3 Newton corrector in Finite Dimensional Space with Mesh Refinement

```
1: procedure NEWTON_CORRECTOR( $u_k, \mu_k$ ) ▷ Implementing Algorithm 1 line 3,5
2:   do ▷ Newton Step
3:     do ▷ Adaptive Refinement
4:       refine marked elements
5:       solve  $\partial F_{\mu_k}(u_k) \delta u_k = -F_{\mu_k}(u_k)$ 
6:       compute  $[\|e_k\|]$  ▷ see Theorem 5.2
7:       mark elements
8:       while  $[\|e_k\|] / \|\delta u_k\| < tol_d$ 
9:         compute  $[\theta_k(\mu_k)]$  ▷ see (4.12)
10:         $\tilde{u} := z_u(u_k + \delta u_k)$  ▷ see (3.6)
11:        compute  $[\|\tilde{u} - u_{\mu_k}\|]$  ▷ see (4.19)
12:        success :=  $([\|\tilde{u} - u_{\mu_k}\|] < \Lambda_d \|\tilde{u} - u_k\| \wedge [\theta_k(\mu_k)] < \theta_t) ?$ 
13:        failure :=  $([\theta_k(\mu_k)] < \theta_c) ?$ 
14:         $u_k := z_u(u_k + \delta u_k)$  ▷ see (3.6)
15:      while not(success  $\vee$  failure)
16:    return  $(\tilde{u}, success)$ 
17: end procedure
```

5 A-posteriori error estimators

The following error estimators exploit the structure of the optimality system. For treating more problems one can proceed as in [22, 23]. A different approach was taken in [29] to obtain a-posteriori error estimates for problems with additional state constraints.

5.1 Error to the central path

Let now an approximate solution (y^h, u^h, q^h) of (\mathbf{P}_μ^h) be given. We will derive an upper bound of $\|u_\mu - u^h\|_{L^2(U)}$, which will be amenable for numerical realizations, see Section 5.3 below.

Theorem 5.1. *Let (y_μ, u_μ) be the solution of (P_μ) , $\mu > 0$. Let a discrete point (y^h, u^h, q^h) be given that satisfies $b'_\mu(u_h) \in L^2(U)$. Then there is a constant $c > 0$ independent of μ , h , and (y^h, u^h, q^h) , such that*

$$\|u_\mu - u^h\|_{L^2(U)}^2 \leq c \left(\|r_y\|_{Y^*}^2 + \|r_q\|_{Y^*}^2 + \|r_u\|_{L^2(U)}^2 \right)$$

with

$$\begin{aligned} r_u &:= \nu u^h + B^* q^h + b'_\mu(u^h), \\ r_y &:= A y^h - B u^h, \\ r_q &:= A^* q^h - (y^h - y_d). \end{aligned}$$

Proof. Let q_μ be the adjoint state such that (2.1) is satisfied. Subtracting $\nu u^h + B^* q^h + b'_\mu(u^h)$ from both sides of (2.1c), multiplying with $u^h - u_\mu$, and integrating on U yields

$$\nu \|u^h - u_\mu\|_{L^2(U)}^2 + \int_U (b'_\mu(u^h) - b'_\mu(u_\mu))(u^h - u_\mu) \, dx + \int_U B^*(q^h - q_\mu)(u^h - u_\mu) \, dx = \int_U r_u(u_\mu - u^h) \, dx.$$

Due to monotonicity of the subdifferential, the second term is non-negative. Using equations (2.1a) and (2.1b) we obtain

$$\begin{aligned} \int_U B^*(q^h - q_\mu)(u^h - u_\mu) \, dx &= \langle A(y^h - y_\mu), q^h - q_\mu \rangle_{Y^*, Y} - \langle r_y, q^h - q_\mu \rangle_{Y^*, Y} \\ &= \langle A^*(q^h - q_\mu), y^h - y_\mu \rangle_{Y^*, Y} - \langle r_y, q^h - q_\mu \rangle_{Y^*, Y} \\ &= \|y^h - y_\mu\|_{L^2(\Omega)}^2 + \langle r_q, y^h - y_\mu \rangle_{Y^*, Y} - \langle r_y, q^h - q_\mu \rangle_{Y^*, Y}. \end{aligned}$$

Combining with the previous estimate, we find

$$\nu \|u^h - u_\mu\|_{L^2(U)}^2 + \|y^h - y_\mu\|_{L^2(\Omega)}^2 \leq \int_U r_u(u_\mu - \tilde{u}) \, dx - \langle r_q, y^h - y_\mu \rangle_{Y^*, Y} + \langle r_y, q^h - q_\mu \rangle_{Y^*, Y}.$$

It remains to estimate $y^h - y_\mu$ and $q^h - q_\mu$. Due to invertibility of A it follows

$$\|y^h - y_\mu\|_{H_0^1(\Omega)} \leq c \|A y^h - A y_\mu\|_{Y^*} \leq c (\|r_y\|_{Y^*} + \|u^h - u_\mu\|_{L^2(U)}).$$

Similarly, we obtain

$$\|q^h - q_\mu\|_{H_0^1(\Omega)} \leq c (\|r_q\|_{Y^*} + \|y^h - y_\mu\|_{L^2(\Omega)}).$$

Collecting all these estimate, we arrive at

$$\begin{aligned} \nu \|u^h - u_\mu\|_{L^2(U)}^2 + \|y^h - y_\mu\|_{L^2(\Omega)}^2 &\leq \|r_u\|_{L^2(U)} \|u_\mu - \tilde{u}\|_{L^2(U)} + \|r_q\|_{Y^*} \|y^h - y_\mu\|_{H_0^1(\Omega)} + \|r_y\|_{Y^*} \|q^h - q_\mu\|_{H_0^1(\Omega)} \\ &\leq (\|r_u\|_{L^2(U)} + c \|r_q\|_{Y^*}) \|u_\mu - \tilde{u}\|_{L^2(U)} + c \|r_y\|_{Y^*} (2 \|r_q\|_{Y^*} + \|y^h - y_\mu\|_{L^2(\Omega)}). \end{aligned}$$

The claim follows now with Young's inequality. \square

5.2 Error in the Newton system

In addition to the results in the previous section, we will now derive an error estimator for the discretization error of the Newton step. Recall that the first-order necessary conditions (2.2) (or equivalently (2.1)) of (\mathbf{P}_μ) are solved with Newton's method.

Let an iterate (y_k, u_k, q_k) be given. Then the Newton step $(\delta u, \delta y, \delta q)$ is computed as the solution of the system

$$A\delta y = B\delta u - (Ay_k - Bu_k), \quad (5.1a)$$

$$A^*\delta q = \delta y - (A^*q_k - (y_k - y_d)) \quad (5.1b)$$

$$\nu\delta u + B^*\delta q + b''_\mu(u_k)\delta u = -(\nu u_k + B^*q_k + b'_\mu(u_k)) \quad (5.1c)$$

This Newton system (3.2) is itself the optimality system of the following quadratic subproblem under linearized constraints:

$$(\mathbf{P}_\mu^q) \left\{ \begin{array}{l} \text{minimize } J_\mu^q(\delta y, \delta u) := (\nu u_k + B^*q_k + b'_\mu(u_k), \delta u)_{L^2(U)} + (-A^*q_k + y_k - y_d, \delta y)_{L^2(\Omega)} \\ \quad + \frac{1}{2}(\|\delta y\|_{L^2(\Omega)}^2 + \nu\|\delta u\|_{L^2(U)}^2 + b''_\mu(\delta u, \delta u)) \\ \text{subject to} \\ A\delta y - B\delta u = -(Ay_k - Bu_k), \\ \delta u \in U_{ad}. \end{array} \right.$$

Since b''_μ is non-negative, the necessary conditions (5.1) are also sufficient. Solvability of the Newton system (Theorem 3.5) automatically proves the existence of a minimizer $(\delta y, \delta u)$ of (\mathbf{P}_μ^q) .

Let a discrete approximation $(\delta y^h, \delta u^h, \delta p^h)$ of $(\delta u, \delta y, \delta q)$ be given. We will now derive an a-posteriori error estimator for $\|\delta u^h - \delta u\|_{L^2(U)}$.

In the notation of Section 4, we want to compute an estimate $\|e_k\|$ with $\|\delta u - \delta u^h\|_{L^2(U)} \leq c\|e_k\|$.

Theorem 5.2. *Let (y_k, u_k, q_k) be given such that $b'_\mu(u_k) \in L^2(U)$. Let $(\delta u, \delta y, \delta q)$ be the solution of (5.1), and let $(\delta y^h, \delta u^h, \delta p^h)$ be a discrete approximation. Then there is a constant $c > 0$ independent of μ , h , and (y^h, u^h, q^h) , $(\delta u, \delta y, \delta q)$, such that*

$$\|\delta u - \delta u^h\|_{L^2(U)}^2 \leq c \left(\|r_{\delta y}\|_{Y^*}^2 + \|r_{\delta q}\|_{Y^*}^2 + \|r_{\delta u}\|_{L^2(U)}^2 \right)$$

with

$$r_{\delta u} := \nu(u_k + \delta u^h) + B^*(q_k + \delta q^h) + b'_\mu(u_k) + b''_\mu(u_k)\delta u^h,$$

$$r_{\delta y} := A(y_k + \delta y^h) - B(u_k + \delta u^h),$$

$$r_{\delta q} := A^*(q_k + \delta q^h) - (y_k + \delta y^h - y_d).$$

Proof. The claim can be proven with similar arguments as Theorem 5.1. It exploits the non-negativity of b''_μ . \square

Remark 5.3. *The solution algorithm in the previous section strongly relies on the smoothing operator Z . The latter guarantees that the current iterate u_k of the interior point method lies in D_2 and that the Newton system is invertible. Thus, $b'_\mu(u_k) \in L^2(U)$, and Theorems 5.1 and 5.2 are applicable for Algorithm 2.*

5.3 Residual based hp error estimates

Let us explain the estimates of Y^* -norms of residuals in state and adjoint equations as they appear in Theorems 5.1 and 5.2. We exemplarily show the derivation for the residual $r_y = Ay^h - Bu^h \in Y^*$ of the state equation with operator A chosen to be $Ay = -\Delta y + y$.

Let now y^h be the solution of the discrete equation (4.1) to the control u^h . Then it holds

$$\langle r_y, v^h \rangle_{Y^*, Y} = \langle Ay^h - Bu^h, v^h \rangle_{Y^*, Y} = 0 \quad \forall v^h \in S^{\mathbf{P}}(\Omega, \tau).$$

Let $v \in H^1(\Omega)$, $v^h \in S^{\mathbf{P}}(\Omega, \tau)$ be given. Then we obtain using integration by-parts

$$\begin{aligned} \langle r_y, v \rangle_{Y^*, Y} &= \langle r_y, v - v^h \rangle_{Y^*, Y} \\ &= \int_{\Omega} \nabla y^h \nabla (v - v^h) + y^h (v - v^h) - u^h (v - v^h) \, dx \\ &= \sum_{K \in \tau} \int_K (-\Delta y^h + y^h - u^h) (v - v^h) \, dx + \int_{\partial K \setminus} \partial_n y^h (v - v^h) \, ds \\ &= \sum_{K \in \tau} \left(\int_K (-\Delta y^h + y^h - u^h) (v - v^h) \, dx + \frac{1}{2} \sum_{e \in \partial K} \int_e [\partial_n y^h] (v - v^h) \, ds \right), \end{aligned} \quad (5.2)$$

where $e \in \partial K$ is an abbreviation for the iteration over the set of all edges of an element K that are not part of $\partial\Omega$. Moreover, $[\phi]$ denotes the jump of the quantity ϕ across an edge e .

We will now choose $v^h := I_h v$, where I_h is an Clément type interpolation operator taken from [26]. Let us briefly introduce some notation to describe the approximation properties of I_h . For a vertex V of the triangulation τ , let us define the patches

$$\begin{aligned} \omega_V^0 &:= \{V\}, \\ \omega_V^j &:= \cup \{ \bar{K} \mid K \in \tau, \bar{K} \cap \omega_V^{j-1} \neq \emptyset \}, \quad j \geq 1, \end{aligned}$$

and set

$$\begin{aligned} h_V &:= \min \{ h_K \mid V \in \bar{K}, K \in \tau \}, \\ p_V &:= \max \{ p_K + 1 \mid V \in \bar{K}, K \in \tau \}. \end{aligned}$$

Then the interpolation operator I_h of [26] satisfies

$$\| I_h(v) - v \|_{L^2(\omega_V^1)} + \frac{h_V}{p_V} \| \nabla I_h(v) \|_{L^2(\omega_V^1)} + \sqrt{\frac{h_V}{p_V}} \| I_h(v) - v \|_{L^2(e)} \leq C \frac{h_V}{p_V} \| \nabla v \|_{L^2(\omega_V^s)}, \quad (5.3)$$

where $e \subset \bar{K}$ is an edge with one of its endpoints being V . For an element $K \in \tau$, let V_K denote a vertex of K . Then it holds $h_{V_K} \leq h_K$ and $p_{V_K} \geq p_K$. Using the interpolation operator I_h in (5.2) and employing (5.3) we estimate

$$\begin{aligned} \langle r_y, v \rangle_{Y^*, Y} &\leq C \sum_{K \in \tau} \left(\frac{h_K}{p_K} \| -\Delta y_h + y^h - u^h \|_{L^2(K)} + \frac{1}{2} \sum_{e \in \partial K \setminus \partial\Omega} \left(\frac{h_K}{p_K} \right)^{1/2} \| [\partial_n y_h] \|_{L^2(e)} \right) \| \nabla v \|_{L^2(\omega_{V_e}^s)} \\ &\leq C \left(\sum_{K \in \tau} \eta_K^2 \right)^{1/2} \| v \|_{H^1(\Omega)} \end{aligned}$$

where

$$\eta_K^2 := \frac{h_K^2}{p_K^2} \| -\Delta y^h + y^h - u^h \|_{L^2(K)}^2 + \frac{1}{2} \sum_{e \subset \partial K \cap \partial\Omega} \frac{h_K}{p_K} \| [\partial_n y^h] \|_{L^2(e)}^2. \quad (5.4)$$

As $v \in H^1(\Omega)$ was arbitrary, this implies

$$\|r_y\|_{Y^*} = \|Ay^h - Bu^h\|_{Y^*} \leq C \left(\sum_{K \in \tau} \eta_K^2 \right)^{1/2}.$$

Due to the construction, this error estimator is reliable, thus providing an upper bound on the error. For results regarding local efficiency of the estimator, see [26].

The residual in the adjoint equation, $r_q = A^*q - (y^h - y_d)$, can be estimated using similar arguments. For general y_d one has to take integration error into account, leading to estimates involving data oscillation term.

Remark 5.4. *The above error estimators would profit from an enhanced L^2 a-posteriori error estimators. If the problem is H^2 -regular, i.e. $A, A^{-*} \in \mathcal{L}(L^2(\Omega), H^2(\Omega))$, then Theorems 5.1 and 5.2 are valid if the Y^* -norms of the residuals are replaced by $(Y \cap H^2(\Omega))^*$ norms. These then could be estimated by $L^2(\Omega)$ -error estimators, due to $\|r_y\|_{(Y \cap H^2(\Omega))^*} \leq c \|A^{-1}r_y\|_{L^2(\Omega)}$. Unfortunately, no L^2 -error estimators are available so far. In h -FEM, they are constructed with the Aubin-Nitsche trick and estimates of the type*

$$\|v - I(v)\|_{L^2(K)} \leq Ch_K^2 |v|_{H^2(K)}, \quad \|v - I(v)\|_{L^2(\partial K)} \leq Ch_K^{3/2} |v|_{H^2(K)},$$

see [1] for details. Only suboptimal hp -equivalents are available (see [35, Remark 4.70]) and the estimates

$$\|v - I(v)\|_{L^2(K)} \leq C \left(\frac{h_K}{p_K} \right)^2 |v|_{H^2(K)}, \quad \|v - I(v)\|_{L^2(\partial K)} \leq C \left(\frac{h_K}{p_K} \right)^{3/2} |v|_{H^2(K)}.$$

are expected to be true but remain to be proven.

6 Numerical examples

In the following we test Algorithm 2 for two problems on convex domains. As a faster convergence in the L^2 -norm has been observed in numerical experiments (see also [5, 4, 12]), we modified η_K in (5.4) to contain the weights $(h_K/p_K)^4, (h_K/p_K)^3$ instead of $(h_K/p_K)^2, (h_K/p_K)$. This mimics an enhanced a-posteriori estimator as mentioned in Remark 5.4.

For the visualization of results, we used a software library developed at the TU Chemnitz.¹

6.1 Testing hp -adaptivity

The problem under consideration is taken from [36] and is equivalent to (P) with the data

$$\nu = 1, \quad u_a = 0, \quad u_b = 1.$$

The underlying PDE reads

$$\begin{aligned} -\Delta y + y &= u + e_y && \text{in } \Omega, \\ \partial_n y &= 0 && \text{on } \Gamma, \end{aligned}$$

with $\Omega = (0, 1)^2$. The objective function is

$$J(u, y) = \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\nu}{2} \|u\|_{L^2(\Omega)}^2 + (e_q, y)_{L^2(\Gamma)}$$

¹<http://www-user.tu-chemnitz.de/~pester/graf2d/>

with $y_d = -142/3 + 12 \operatorname{dist}(x - x_0)^2$ and $e_q = -12$. The optimal solution is radially symmetric with origin in $x_0 = (0.5, 0.5)$ and reads

$$\begin{aligned} u^* &= P_{U_{ad}}(-\nu^{-1}q^*), \\ y^* &\equiv 1, \\ q^* &= -12 \operatorname{dist}(x - x_0)^2 + 1/3. \end{aligned}$$

if the inhomogeneity e_y is set to $e_y = 1 - u^*$. The parameters of the algorithm are

$$\theta_d = 0.1, \quad \theta_t = 0.5, \quad \theta_c = 0.8, \quad \sigma_{max} = 0.9, \quad \sigma_{min} = 1/16.$$

with the tolerances

$$tol_d = 0.5, \quad tol = 10^{-4}, \quad \Lambda_d = 0.6.$$

We start path-following method with the homotopy parameter $\mu_0 = 1/16$.

The problem turns out to have a large region of convergence for Newton's method, which in addition is relatively robust with respect to changes in the homotopy parameter μ . That is why the method rapidly decreases μ_k and finds the solution in only 3 iterates. This fast convergence implies that many refinements are necessary during the Newton corrector iteration (algorithm 3). Due to the observed quadratic convergence of the norm of the updates $\|\delta u_k\|$, the mesh is refined several times until the relative error $[\|e_k\|]/\|\delta u_k\| < tol_d$ is small, see steps 3-8 in algorithm 3. This enforced refinement ensures that the discretization error does not prevail, and that linear convergence is achieved in function space.

If the algorithm decides to reduce the discretization error, we either p or h refine an element. The hp refinement method judges the smoothness of the control iterate u_k by expanding it in a Legendre series and estimating the decay of the Legendre coefficients ([13]). If the coefficients decay fast enough, the element will be p -refined otherwise it will be h -refined.

This strategy performs very well and nicely captures the interface γ where the optimal control is non-smooth, namely

$$\gamma = \{\operatorname{dist}(x - x_0) = 1/6\} \cup \{\operatorname{dist}(x - x_0) = 1/6\}.$$

In Figure 1 we depicted the mesh for the last iterate with $\mu_3 \approx 9.5 \cdot 10^{-7}$. In addition the interface γ drawn as white circles.

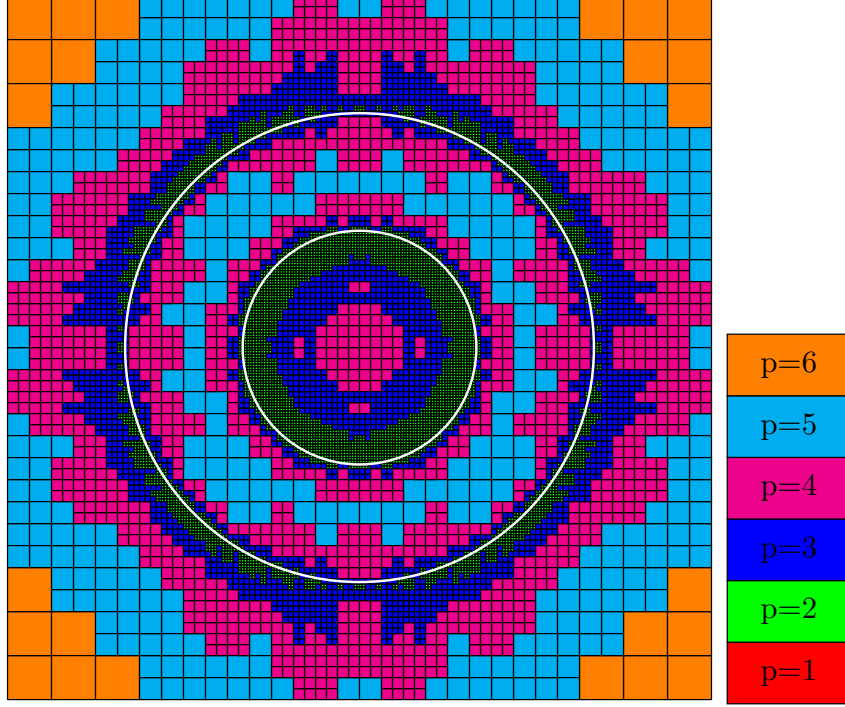


Figure 1: Discretization for $\mu_3 \approx 9.5 \cdot 10^{-7}$.

6.2 Testing adaptive path-following

This test case is taken from [31] and turns out to be numerically challenging because of the very small regularization parameter ν . Unlike the previous example, the radius of convergence around the central path is small and very sensitive with respect to changes in μ . The data of **(P)** reads

$$\nu = 10^{-6}, \quad u_a = 0, \quad u_b = 1.$$

with the underlying PDE

$$\begin{aligned} -\frac{1}{10}\Delta y + y &= u && \text{in } \Omega, \\ y &= 0 && \text{on } \Gamma, \end{aligned}$$

and $\Omega = (0, 1)^2$. The desired state is rough with patch-wise behavior

$$y_d = 0.01 \cdot \chi_{(-1,0.2) \times (-1,0.6)} - 0.01 \cdot \chi_{(-1,0.2) \times (-0.6,1)} + 0.02 \cdot \chi_{(0.2,1) \times (-0.6,1)}.$$

We choose the contraction parameters stricter than in the previous example

$$\theta_d = 0.1, \quad \theta_t = 0.3, \quad \theta_c = 0.5, \quad \sigma_{max} = 0.9, \quad \sigma_{min} = 1/16.$$

Similar as before,

$$tol_d = 0.5, \quad tol = 10^{-2}, \quad \Lambda_d = 0.6.$$

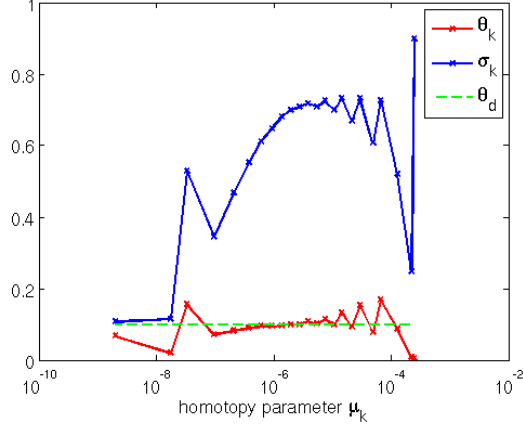


Figure 2: Stepsize and contraction factors during the short step method.

The path-following method is launched with $\mu_0 = 2.44140625 \cdot 10^{-4}$.

As the error estimators of section 5 suffer from small ν , we rescaled them to prohibit extensive mesh refinement at the beginning of the algorithm. If a mesh refinement is necessary, we adaptively refine the mesh according to a standard mean value strategy (see [26]).

The algorithm manages to stay inside the convergence radius of Newton's method by choosing relatively large values for σ . This behavior occurs because of the high non-linearity of the problem and the small convergence area for Newton's method resulting from a very small ν . The desired contraction rate θ_d is achieved nicely. The optimal state and adjoint are shown in Figure 3, while the optimal control and the final mesh is shown in Figure 4.

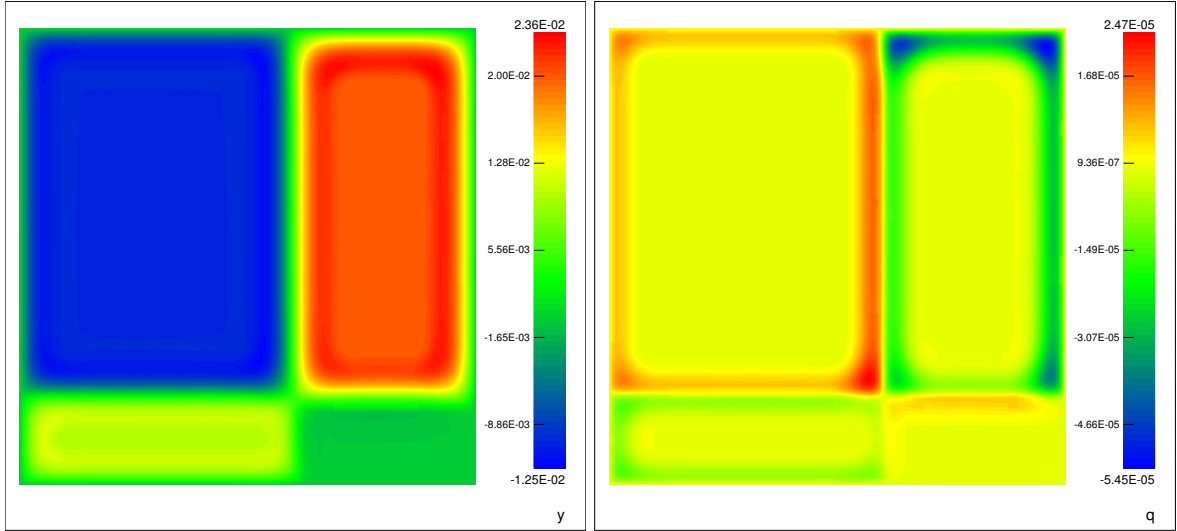


Figure 3: Optimal state (left) and adjoint (right) variable.

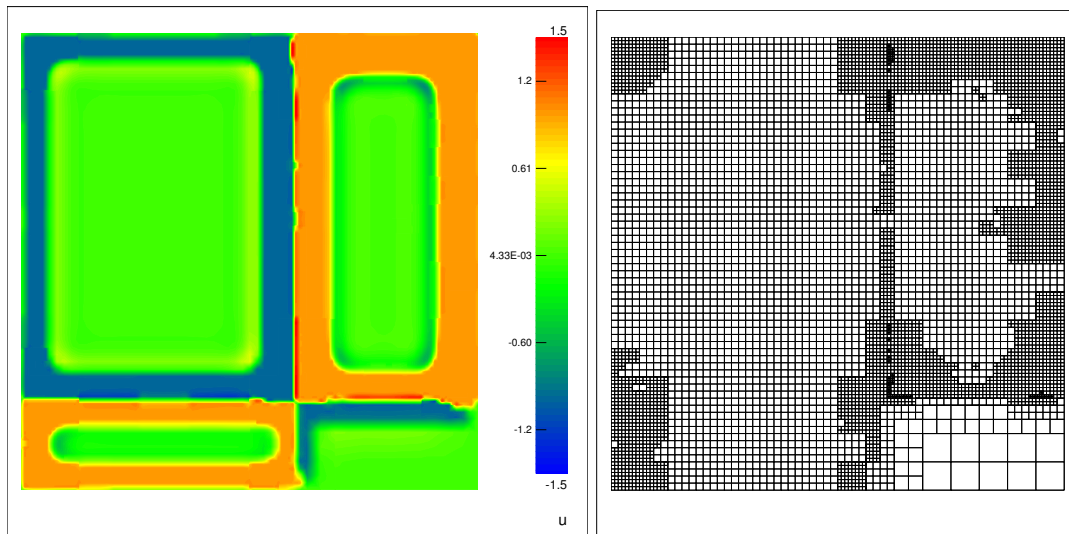


Figure 4: Optimal control (left) and corresponding mesh.

These examples clearly show that the adaptive hp -refinement can be successfully integrated within a Newton short-step method to solve the inequality constrained control problem.

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