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A posteriori error estimates for a finite element discretization of interior point methods for an elliptic optimization problem with state constraints

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Abstract In this paper we are concerned with a posteriori error estimates for the solution of some state constraint optimization problem subject to an elliptic PDE. The solution is obtained using an interior point method combined with a finite element method for the discretization of the problem. We will derive separate estimates for the error in the cost functional introduced by the interior point parameter and by the discretization of the problem. Finally we show numerical examples to illustrate the findings for pointwise state constraints and pointwise constraints on the gradient of the state.

Keywords state constraints · gradient constraints · mesh adaptivity · finite element method · a posteriori error estimates · optimal control · interior point methods

Mathematics Subject Classification (2000) 65N30 · 65K10 · 90C51 · 65N50 · 90C59

1 Introduction

In this paper we develop a posteriori error estimates with respect to the cost functional for state constraint optimization problems governed by second order elliptic equations. For this purpose we extend the work done in [44] for pointwise constraints on the control, based on the ideas of [1, 2] to the case of constraints on the state or the gradient of the state.

It is well known that problems of this type may exhibit Lagrange multipliers that are measures, see, e.g., [7, 8, 10, 11, 16] in the presence of pointwise state constraints or [11, 12] for constraints on the gradient of the state. In the case of finitely many constraints on the state we may expect better regularity of the adjoint state in contrast to pointwise constraints, see, e.g., [11, 13, 15].

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To overcome this low regularity there are several techniques available for pointwise state constraints like augmented Lagrangians [4, 6], Lavrentiev regularization (or mixed control-state constraints) [17, 32, 34, 35, 41], Moreau-Yoshida type regularization [5, 7, 25, 26] or interior point methods [39, 40, 46]. Recently a Moreau-Yoshida type regularization for a non variational problem with gradient constraints was proposed in [23].

For some of these methods, a priori analysis for the finite element discretization of the "regularized" problem is available, see, e.g., [14, 20, 28], or [14, 19] for a direct discretization of the problem.

In the case of pointwise constraints on the gradient less is currently known. To the author's knowledge the only publication concerned with a priori error analysis is [18] which is concerned with the finite element discretization of the unregularized problem.

In the case of a posteriori estimates, preprints are available for the error with respect to the cost functional see [3, 24], and with respect to natural norms see [29] both in the case of pointwise state constraints. They tackle the discretization error for a direct discretization of the optimization problem. To the author's knowledge there are currently no publications for a posteriori estimates for problems with constraints on the gradient.

In this paper we will use an interior point method for the solution of the constraint optimization problem. This method has the special feature that the solution of the interior point method is (for fixed interior point parameter) a feasible solution with respect to the "unregularized" optimization problem.

Here we are not interested in the computation of the limiting solution on a fixed mesh, but rather link the mesh size h and the interior point parameter γ such that the errors introduced by both parameters are equilibrated. This is sensible since the solution of the linear subproblems becomes rather tedious for small values of h or γ due to ill conditioning of the Hessian matrix, see [30, 36]. To the purpose of balancing the error contributions we derive a posteriori error estimates for the error in the cost functional introduced by the interior point method as well as estimates for the error introduced by the discretization of the interior point (sub-)problem.

Even though a posteriori estimates for the remaining regularization techniques are beyond the scope of this article and are subject to further research, it should be noted that the difficulties arising from ill conditioning of the Hessian matrices are not limited to interior point methods and must be expected to come up in the other algorithms as well.

The paper is structured as follows, in Section 2 we give an abstract setting for the optimization problem under consideration, there we will keep especially the type of the constraints rather abstract. Further we discuss the interior point formulation for the constraints. In section 3 we will discuss the finite element discretization of the interior point problem. Then we will derive separated estimates for the error in the cost functional introduced by the interior point method and the discretization of the PDE. To illustrate our findings and to show that the assumptions we made in Sections 2 and 3 are fulfilled in the case of linear elliptic equations for pointwise state or gradient constraints, we discuss both types of constraints in more detail in Section 5. Finally in Section 6 we show some numerical examples to demonstrate our findings.

2 Optimization problem

In this section we give a precise formulation of the optimization problem under consideration. To incorporate different types of state constraints into our framework we keep the spaces in this section as abstract as possible. Therefore it is unavoidable to make several assumptions on the solvability of equations appearing in this section. We show later on that the assumptions are fulfilled for pointwise state constraints (Section 5.1) and pointwise constraints on the gradient of the state (Section 5.2).

Let Ω be an open bounded subset of $\mathbb{R}^n$ $(n \geq 2)$ with boundary $\Gamma = \partial\Omega$ and A be a second order linear elliptic operator in divergence form, to be precise A is of the form:

$$Au = -\nabla \cdot \mathcal{A}\nabla u + du,$$

where $d \geq 0$ and there exists $m_0 > 0$ such that for each $\xi \in \mathbb{R}^n$ the (possibly space dependent matrix) $\mathcal{A} \in \mathbb{R}^n \times \mathbb{R}^n$ fulfills

$$\xi^T \mathcal{A}\xi \geq m_0|\xi|^2 \quad \text{for almost every } x \in \overline{\Omega}.$$

For simplicity the coefficients a_{ij} of $\mathcal{A}$ are assumed to be in $\in C^{0,1}(\Omega)$ and d shall fulfill $d \in L^\infty(\Omega)$.

We consider the state equation

$$\begin{cases} Au = q & \text{in } \Omega, \\ \quad u = 0 & \text{on } \Gamma, \end{cases} \tag{2.1}$$

where we assume that the boundary Γ is such that (2.1) exhibits for every given $q \in L^t(\Omega) \subset H^{-1}(\Omega)$ (for some fixed $t \geq 2$) a unique solution u_q in the Banach space $W = W^{2,t}(\Omega) \cap W_0^{1,t}(\Omega) \subset H^2(\Omega) \cap H_0^1(\Omega)$ and there exists a constant c independent of q such that

$$\|u_q\|_W \leq c\,\|q\|_{L^t(\Omega)}.$$

Especially it holds that if $\{q_k\} \subset L^t(\Omega)$ converges to q weakly (or weakly* if $t = \infty$) in $L^t(\Omega)$, then $\{u_{q_k}\}$ converges to u_q weakly in W.

We now define the associated bilinear form $a(\,\cdot\,,\,\cdot\,)$ as:

$$a(u, \varphi) = \int_\Omega \mathcal{A}\nabla u \nabla\varphi \, dx + \int_\Omega du\varphi \, dx = (\mathcal{A}\nabla u, \nabla\varphi) + (du, \varphi).$$

Then the weak formulation of (2.1) is:
For given $q \in H^{-1}(\Omega)$ find $u \in V = H_0^1(\Omega)$ such that:

$$a(u)(\varphi) = (q, \varphi) \quad \forall \varphi \in V \tag{2.2}$$

and every solution of (2.2) is a solution of (2.1) if $q \in L^t(\Omega)$.

We are interested in minimizing the functional

$$\text{Minimize } J(q,u) := \frac{1}{2}\|u - u^d\|^2_{L^2(\Omega)} + \frac{\alpha}{r}\|q\|^r_{L^r(\Omega)}, \tag{2.3a}$$

$$\text{such that } \begin{cases} (2.2) \text{ holds,} \\ K(u) \geq 0 \text{ on } \Omega_C, \end{cases} \tag{2.3b}$$

where $u^d \in L^2(\Omega)$ is a given function, $r \geq t$, $\alpha > 0$. Thus we can choose the control space to be $Q = L^r(\Omega) \subseteq L^t(\Omega)$. The constraint mapping $K\colon W \to C(\Omega_C)$ shall be a three times differentiable mapping form the state space W to the space of continuous functions on the compact set $\Omega_C \subseteq \overline{\Omega}$. In addition, let us assume that K is also a mapping $K\colon V \to L^1(\Omega_C)$. Furthermore we require that the set $\{u \in W \,|\, K(u) \geq 0\}$ is closed with respect to weak convergence.

Remark 1 If we would not assume $K\colon V \to L^1(\Omega_C)$, then we would have to introduce another constraint mapping for the discretized problems. As we think that this would only mislead the reader we made the assumption above, which is fulfilled by pointwise constraints on the state or the gradient of the state as we will see later on.

One can show using standard arguments, that if there exists a feasible point (q, u_q) which satisfies (2.3b), then there exists a solution $(\overline{q}, \overline{u}) \in Q \times W$ to problem (2.3).

In order to write down first order necessary conditions we note that the solution operator

$$S\colon Q \to W \;;\; q \mapsto u_q \tag{2.4}$$

is linear and continuous, therefore it is of class C^1. Furthermore let us assume that the adjoint equation

$$\int_\Omega A\varphi \cdot z \, dx = \int_\Omega (u - u^d)\varphi \, dx + \int_{\Omega_C} K'(u)\varphi \, d\mu \quad \forall \varphi \in W, \tag{2.5}$$

admits a solution $z \in L^{t'}(\Omega) = Q^*$ for any given $u \in W$ and $\mu \in M(\Omega_C)$. Here $\frac{1}{t'} + \frac{1}{t} = 1$ and $M(\Omega_C)$ is the dual space of $C(\Omega_C)$.

For the interior point method we also assume that the (weak) adjoint equation

$$a(\varphi, z) = (u - u^d, \varphi) + (\hat{\mu}, K'(u)\varphi)_{\Omega_C} \quad \forall \varphi \in V, \tag{2.6}$$

exhibits for any given $u \in V$ and $\hat{\mu} \in L^\infty(\Omega_C)$ a solution $z \in V$. As $L^\infty(\Omega_C) \subset M(\Omega_C)$ this solution satisfies the equation

$$\int_\Omega A\varphi \cdot z \, dx = \int_\Omega (u - u^d)\varphi \, dx + \int_{\Omega_C} K'(u)\varphi \, d\hat{\mu} \quad \forall \varphi \in W,$$

where $(\,\cdot\,,\,\cdot\,)_{\Omega_C}$ denotes the L^2 inner product on Ω_C

Let us now assume the existence of $q^0 \in Q$ such that the following Slater condition is fulfilled:

$$K(\overline{u}) + K'(\overline{u})u^0 > 0 \quad \text{on } \Omega_C \tag{2.7}$$

where $u^0 = S(q^0 - \overline{q})$ is the solution to

$$\begin{aligned} Au^0 &= q^0 - \overline{q} \quad \text{in } \Omega, \\ u^0 &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$

With these assumptions the first order necessary conditions take the following form, c.f. [10, 11]:
There exist elements $\overline{z} \in L^{t'}(\Omega)$, $\overline{\mu} \in M(\Omega_C)$ such that

$$\int_\Omega A\overline{u}\varphi \, dx = \int_\Omega \overline{q}\varphi \, dx \qquad \forall \varphi \in L^{t'}(\Omega), \tag{2.8a}$$

$$\int_\Omega A\varphi \cdot \overline{z} \, dx + \int_\Omega (u^d - \overline{u})\varphi \, dx = \int_{\Omega_C} K'(\overline{u})\varphi \, d\overline{\mu} \quad \forall \varphi \in W, \tag{2.8b}$$

$$\int_{\Omega_C} (\varphi - K(\overline{u})) \, d\overline{\mu} \leq 0 \qquad \forall \varphi \in C(\Omega_C) : \varphi \geq 0, \tag{2.8c}$$

$$\int_\Omega (\overline{z} + \alpha|\overline{q}|^{r-2}\overline{q})q \, dx = 0 \qquad \forall q \in Q. \tag{2.8d}$$

We now introduce the following functions $l(\cdot;\gamma;o) \colon \mathbb{R}_+ \to \overline{\mathbb{R}}$, see e.g. [40]:

$$l(x;\gamma;o) = \begin{cases} -\gamma \ln(x) & o = 1, \\ \frac{\gamma^o}{(o-1)x^{o-1}} & o > 1, \end{cases}$$

and define the barrier functional $b(\,\cdot\,;\gamma;o) \colon W \to \overline{\mathbb{R}}$ for the state constraints by:

$$b(v;\gamma;o) = \int_{\Omega_C} l(K(v)(x);\gamma;o) \, dx. \tag{2.9}$$

Once again this also defines a mapping $b(\,\cdot\,;\gamma;o) \colon V \to \overline{\mathbb{R}}$ using the same definition, this is due to our assumption on K

To simplify notation we introduce

$$b'(v;\gamma;o) = \frac{-\gamma^o}{K(v)^o},$$

then $\frac{\partial}{\partial v} b(v;\gamma;o)\delta v = (b'(v;\gamma;o), K'(v)\delta v)_{\Omega_C}$ by the chain rule. As the order o of the barrier functional is arbitrary but fixed it will be omitted. Thus we write $b'(v;\gamma)$ instead of $b'(v;\gamma;o)$, etc.

Now we are able to define a family of problems depending on the parameter $\gamma > 0$:

$$\text{Minimize } J_\gamma(q,u) := J(q,u) + b(u;\gamma) \tag{2.10a}$$

$$\text{such that(2.2) holds.} \tag{2.10b}$$

It can be shown, using similar arguments as in [38, 40] that if there exists one parameter γ_0 such that (2.10) admits a solution $(\overline{q}_{\gamma_0}, \overline{u}_{\gamma_0})$, then it admits a solution $(\overline{q}_\gamma, \overline{u}_\gamma)$ for every $\gamma \in (0, \gamma_0]$. In addition one can show that the solution satisfies $K(\overline{u}_\gamma) \geq c > 0$ if the order o is sufficiently large and $K(\overline{u}_\gamma) \in C^\beta(\Omega_C)$ for some $\beta > 0$.

Let us assume that o is chosen large enough to obtain $K(\overline{u}_\gamma) \geq c > 0$. Then the first order necessary conditions for (2.10) read:
There exist $\overline{z}_\gamma \in V$ such that

$$a(\overline{u}_\gamma)(\varphi) = (\overline{q}_\gamma, \varphi) \qquad \forall \varphi \in V, \tag{2.11a}$$

$$a(\varphi, \overline{z}_\gamma) + (u^d - \overline{u}_\gamma, \varphi) = (b'(\overline{u}_\gamma; \gamma), K'(\overline{u}_\gamma)\varphi)_{\Omega_C} \qquad \forall \varphi \in V, \tag{2.11b}$$

$$\int_\Omega (\overline{z}_\gamma + \alpha |\overline{q}_\gamma|^{r-2} \overline{q}_\gamma) q \, dx = 0 \qquad \forall q \in Q. \tag{2.11c}$$

It should be noted however, that as $\overline{q}_\gamma \in Q \subset L^t(\Omega)$, the state possesses the additional regularity $\overline{u}_\gamma \in W$. Thus $b'(\overline{u}_\gamma; \gamma) \in C(\Omega_C) \subset M(\Omega_C)$ and we deduce that (2.11b) is solvable with $\overline{z}_\gamma \in L^{t'}(\Omega) \cap V$. As this leads to more regular adjoint variables $\overline{z}_\gamma$ and a more regular approximation of the multiplier $\mu_\gamma = b'(\overline{u}_\gamma; \gamma)$, we refer to (2.11) as the 'regularized' problem.

For the convenience of the reader we compile a list of the assumptions we made in the preceding section:

Assumption 1 *We assume that the state equation* (2.1) *and the (weak) state equation* (2.2) *are uniquely solvable.*

Assumption 2 *We assume that the adjoint equation* (2.5) *and the (weak) adjoint equation* (2.6) *are uniquely solvable.*

Assumption 3 *We assume that the constraint mapping* $K: W \to C(\Omega_C)$ *is three times differentiable. The same shall hold if the mapping is considered as* $K: V \to L^1(\Omega_C)$. *Furthermore the set* $\{u \in W \mid K(u) \geq 0\}$ *is assumed to be closed with respect to weak convergence.*

Assumption 4 *We assume that the Slater condition* (2.7) *holds.*

Remark 2 At the end of this section we give a short list of possible generalizations of the problem described above that would allow for a similar analysis:

- Note that we could easily take more general functionals

$$J(q, u) = J_1(u) + \frac{\alpha}{r} \|q - q^d\|^r_{L^r(\Omega)}$$

  Also elliptic equations with Neumann instead of Dirichlet boundary conditions are easily obtained by simply replacing $u = 0$ on Γ with $\partial_A u = 0$ on Γ and choosing $V = H^1(\Omega)$ instead of $V = H^1_0(\Omega)$, under the additional assumption that ess $\inf(d) > 0$. Since the modifications in (2.3) and (2.8) for this are all quite obvious but may interfere with the readability we will not complicate our notation by these generalizations.

- For reasons of simplicity we consider only the case where we have one component in K. This is not sufficient for constraints of the type $a \leq u(x) \leq b$. In that case one has to consider $K(u)\colon W \to C(\Omega_C)^k$ where k is the number of inequality constraints under consideration. As this would only make the notation more involved we do not consider this case, it should be noted however that everything done here for $k = 1$ can easily be extended to arbitrary $k \in \mathbb{N}$.
- For the following a posteriori estimates it is not required that (2.1) is a linear equation. In fact it is only required that the first-order necessary conditions are fulfilled. The generalization is rather straightforward but will be omitted to simplify notation.
  Note that for a general nonlinear equation and nonlinear constraints the solution of (2.3) might not be unique. Therefore special care has to be taken during computations. The a posteriori estimates remain valid if there exists a solution to the KKT-System (2.8), that is approximated by a solution to (2.11) which has to be approximated by (3.2). Or vice versa if one has a discrete solution such that there are solutions to (2.11), (2.8) which are "near" that discrete solution the estimates remain valid. This is due to the fact that they require only stationary points of the Lagrangians introduced in section 4, which need to have the property that the remainder term is negligible.
- In the same spirit it is also possible to include the case $r < t$ into the analysis presented. In those cases it is required to take q from a closed, convex and bounded subset $Q_{\mathrm{ad}} \subset Q$. This usually leads to a variational inequality coupling control and adjoint state. If the constraint $\overline{q} \in Q_{\mathrm{ad}}$ is inactive at the optimal solution the variational inequality becomes an equality and our a posteriori estimates remain valid.
- One may also consider the case of finitely many constraints on the state. In this case Ω_C is a finite subset of $\mathbb{N}$, with the discrete topology, e.g. all functions $\Omega_C \to \mathbb{R}$ are continuous. Especially $C(\Omega_C)$ and its dual space are isomorphic to $\mathbb{R}^m$ with m the cardinality of Ω_C and integrals over Ω_C are sums.
- The conditions on the coefficients of $\mathcal{A}$ to be in $C^{0,1}$ can be weakened for some type of constraints. We keep them that restrictive to have well posedness of the problem even for pointwise constraints on the gradient of the state on $\overline{\Omega}$.
  In the same sense the space $W \subset H^2(\Omega) \cap H^1_0(\Omega)$ is far too restrictive for several possible choices of constraints, e.g. in general it doesn't allow for non convex polygonal domains. This assumption is not necessary for the following a posteriori estimates but helps to give a clear presentation that covers both state and gradient constraints.

3 Finite element discretization

In this section we discuss finite element discretization of the optimization problem (2.10).

For this let $\mathcal{T}_h$ be a triangulation of the computational domain Ω_h, for simplicity let us assume that $\Omega = \Omega_h$. The triangulation shall consist of closed cells T which are either triangles or quadrilaterals. The (maximal) smooth parts of the boundary ∂T of a cell T are called faces. The mesh parameter h is defined as a cellwise constant function by setting $h|_T = h_T$ and h_T is the diameter of T. The mesh is assumed to be shape regular. In order to ease mesh refinement we allow the cells to have nodes which lie on midpoints of faces of neighboring cells.

On the mesh $\mathcal{T}_h$ we define a finite element space $V^h \subset V = H^1_0(\Omega)$ consisting of linear or bilinear shape functions, see, e.g., [21] or [9]. In the case of hanging nodes we remark that there are no degrees of freedom corresponding to these nodes, and thus the values at these nodes are given by pointwise interpolation. This implies continuity over the faces and therefore global H^1 conformity.

For the discretization of the control space $Q = L^t(\Omega)$ we introduce a finite dimensional subspace $Q^h \subset Q$. There are several possible choices for Q^h, one may choose Q^h similar to V^h as continuous cellwise (bi-)linear functions or as (discontinuous) cellwise constant functions. A slightly different approach doesn't use discretization of the control space, but instead uses the optimality condition $\alpha|q|^{r-2}q + z = 0$ in the spirit of [27].

In the case of pointwise state constraints, a priori analysis can be found, e.g., in [14, 20, 31] for the solution to the 'unregularized' problem (2.3). An a priori analysis of the interior point discretization for pointwise state constraints can be found in [28]. Note that there is currently no a priori analysis available in the case of pointwise constraints of the gradient. Only for a mixed formulation of the state equation and constraints on the cellwise mean value of ∇u, convergence of order $\sqrt{h \log |h|}$ has been shown in [18].

The discretized optimization problem is formulated as follows:

$$\text{Minimize } J_\gamma(q^h, u^h) \quad q^h \in Q^h,\ u^h \in V^h, \tag{3.1a}$$

$$\text{such that } a(u^h, \varphi) = (q^h, \varphi) \quad \forall\, \varphi \in V^h, \tag{3.1b}$$

Remark 3 Once again it is of interest whether the discrete state is strictly feasible. To argue that this is the case, we assume for a moment that $K(u)$ is in fact of the following form: $K(u)(x) = k(x, u(x), \nabla u(x))$ for some function $k : \mathbb{R} \times \mathbb{R} \times \mathbb{R}^n \mapsto \mathbb{R}$. With this assumption we can "localize" the argument for strict feasibility.

Consider an arbitrary cell T, then the discrete state u_h is a function in $C^\infty(T)$. Then, following the arguments in [40] , we obtain that u_h is strictly feasible on T for a sufficiently high order o_T. Next we remark, that o_T depends only on the space dimension n and the regularity of u_h, which are independent of T thus we conclude that we can take the same order o for all cells.

Let as now assume, that the order of the barrier is sufficiently high to obtain strictly feasible states, then the following first order necessary conditions hold for a solution $(\overline{q}_\gamma^h, \overline{u}_\gamma^h) \in Q^h \times V^h$:
There exist $\overline{z}_\gamma^h \in V^h$ such that:

$$a(\overline{u}_\gamma^h)(\varphi) = (\overline{q}_\gamma^h, \varphi) \qquad \forall\, \varphi \in V^h, \tag{3.2a}$$

$$a(\varphi, \overline{z}_\gamma^h) + (u^d - \overline{u}_\gamma^h, \varphi) = (b'(\overline{u}_\gamma^h;\gamma), K'(\overline{u}_\gamma^h)\varphi)_{\Omega_C} \qquad \forall\, \varphi \in V^h, \tag{3.2b}$$

$$\int_\Omega (\overline{z}_\gamma^h + \alpha|\overline{q}_\gamma^h|^{r-2}\overline{q}_\gamma^h) q \, dx = 0 \qquad \forall\, q \in Q^h. \tag{3.2c}$$

4 A posteriori error estimation

In this section we derive a posteriori estimates for the regularization error as well as for the discretization error with respect to the cost functional $J(q,u)$. Unfortunately neither a solution to (2.8) provides feasible test functions for (3.2) nor is a solution to (3.2) feasible for (2.8). Therefore we split the estimation into two parts:

$$\begin{aligned} J(\overline{q},\overline{u}) - J_\gamma(\overline{q}_\gamma^h, \overline{u}_\gamma^h) &= (J(\overline{q},\overline{u}) - J_\gamma(\overline{q}_\gamma, \overline{u}_\gamma)) + (J_\gamma(\overline{q}_\gamma, \overline{u}_\gamma) - J_\gamma(\overline{q}_\gamma^h, \overline{u}_\gamma^h)) \\ &\approx \eta_{\text{hom}} + \eta_{\text{disc}}. \end{aligned}$$

Thus we estimate the error in the cost functional between the solution $(\overline{q},\overline{u})$ of (2.3) and the solution $(\overline{q}_\gamma, \overline{u}_\gamma)$ of the barrier problem (2.10), and then the discretization error between the solution of (2.10) and the solution $(\overline{q}_\gamma^h, \overline{u}_\gamma^h)$ to its discretization (3.1).

Remark 4 A short remark concerning the generalization to the case of additional control constraints, e.g. if the control q is searched for in a closed convex set Q_{ad}. In this case the equations (2.8d), (2.11c) and (3.2c) become variational inequalities. To cope with this we would have to add additional terms to the Lagrangians introduced later on as well as in the error estimators. These terms can be found in [44]. However since the approximation suggested in [44] requires sufficient regularity of the adjoint state to be rigorously justified it is not clear whether these techniques can successfully be applied to the case of state constraints. Hence the case of active control constraints is subject to further research.

4.1 Homotopy error

In order to estimate the error introduced by the homotopy parameter γ we define the Lagrangian $\mathcal{M}\colon Q \times W \times L^{t'}(\Omega) \times M(\Omega_C) \to \mathbb{R}$ by

$$\mathcal{M}(q,u,z,\mu) = J(q,u) + (q,z) - (Au,z) + \int_{\Omega_C} K(u)\, d\mu. \tag{4.1}$$

We can now formulate the following

Theorem 1 *Let* $\xi = (\overline{q}, \overline{u}, \overline{z}, \overline{\mu})$ *be a solution to the first order necessary system* (2.8) *and let* $\xi_\gamma = (\overline{q}_\gamma, \overline{u}_\gamma, \overline{z}_\gamma, b'(\overline{u}_\gamma;\gamma))$ *where* $(\overline{q}_\gamma, \overline{u}_\gamma, \overline{z}_\gamma)$ *are given as a solution to the first order necessary system* (2.11) *of the barrier problem. Then the following estimate holds:*

$$\begin{aligned} J(\overline{q}, \overline{u}) - J_\gamma(\overline{q}_\gamma, \overline{u}_\gamma) = \frac{1}{2}\int_{\Omega_C} \big(K(\overline{u}_\gamma) - K(\overline{u})\big)\, db'(\overline{u}_\gamma;\gamma) \\ - b(\overline{u}_\gamma;\gamma) + \frac{1}{2}\int_{\Omega_C} K(\overline{u}_\gamma)\, d\overline{\mu} + \mathcal{R}_{hom} \end{aligned} \tag{4.2}$$

with a remainder term $\mathcal{R}_{hom}$ *given by:*

$$\mathcal{R}_{hom} = \frac{1}{2}\int_0^1 \mathcal{M}'''(\xi_\gamma + s(\xi - \xi_\gamma))(\xi - \xi_\gamma, \xi - \xi_\gamma, \xi - \xi_\gamma) s(s-1)\, ds. \tag{4.3}$$

Proof From (2.8c) we conclude that the support of $\overline{\mu}$ is contained in the set

$$\mathcal{A} = \{\, x \in \Omega_C \mid K(\overline{u})(x) = 0 \,\}.$$

Using this and (2.8a) we obtain

$$J(\overline{q}, \overline{u}) = \mathcal{M}(\overline{q}, \overline{u}, \overline{z}, \overline{\mu}) = \mathcal{M}(\xi).$$

Unfortunately we do not have a complementarity condition for the solution to (2.11) thus utilizing (2.11a) we obtain

$$\begin{aligned} J_\gamma(\overline{q}_\gamma, \overline{u}_\gamma) =& J(\overline{q}_\gamma, \overline{u}_\gamma) + b(\overline{u}_\gamma;\gamma) \\ =& \mathcal{M}(\overline{q}_\gamma, \overline{u}_\gamma, \overline{z}_\gamma, b'(\overline{u}_\gamma;\gamma)) \\ & - \int_{\Omega_C} K(\overline{u}_\gamma) b'(\overline{u}_\gamma;\gamma)\, dx + b(\overline{u}_\gamma;\gamma) \\ =& \mathcal{M}(\xi_\gamma) - \int_{\Omega_C} K(\overline{u}_\gamma) b'(\overline{u}_\gamma;\gamma)\, dx + b(\overline{u}_\gamma;\gamma). \end{aligned}$$

Now we estimate the difference between the values of the Lagrangian $\mathcal{M}$ using the trapezoidal rule to evaluate the integral and obtain

$$\mathcal{M}(\xi) - \mathcal{M}(\xi_\gamma) = \int_0^1 \mathcal{M}'(\xi_\gamma + s(\xi - \xi_\gamma))(\xi - \xi_\gamma)\, ds \tag{4.4}$$

$$= \frac{1}{2}\mathcal{M}'(\xi)(\xi - \xi_\gamma) + \frac{1}{2}\mathcal{M}'(\xi_\gamma)(\xi - \xi_\gamma) + \mathcal{R}_{\mathrm{hom}} \tag{4.5}$$

with the remainder $\mathcal{R}_{\mathrm{hom}}$ as given in (4.3).

First we discuss $\mathcal{M}'(\xi)(\xi - \xi_\gamma)$, for that we consider the following functionals:

$$\begin{aligned} \mathcal{M}'_u(\xi)(\varphi) =& (\overline{u} - u^d, \varphi) - (A\varphi, \overline{z}) + \int_{\Omega_C} K'(\overline{u})\varphi\, d\overline{\mu}, \\ \mathcal{M}'_z(\xi)(\varphi) =& (\overline{q}, \varphi) - (A\overline{u}, \varphi), \\ \mathcal{M}'_q(\xi)(\varphi) =& \alpha(|\overline{q}|^{r-2}\overline{q}, \varphi) + (\varphi, \overline{z}), \\ \mathcal{M}'_\mu(\xi)(\varphi) =& \int_{\Omega_C} K(\overline{u})\, d\varphi. \end{aligned}$$

Using (2.8a) we obtain for the primal residual $\mathcal{M}'_z(\xi)(\overline{z} - \overline{z}_\gamma) = 0$, and from (2.8b) we get for the adjoint residual $\mathcal{M}'_u(\xi)(\overline{u} - \overline{u}_\gamma) = 0$ and from (2.8d) we deduce $\mathcal{M}'_q(\xi)(\overline{q} - \overline{q}_\gamma) = 0$ and thus

$$\mathcal{M}'(\xi)(\xi - \xi_\gamma) = \mathcal{M}'_\mu(\xi)(\overline{\mu} - b'(\overline{u}_\gamma; \gamma)),$$

where we use complementarity to get

$$\mathcal{M}'(\xi)(\xi - \xi_\gamma) = \mathcal{M}'_\mu(\xi)(-b'(\overline{u}_\gamma; \gamma)) = -\int_{\Omega_C} K(\overline{u})\, db'(\overline{u}_\gamma; \gamma).$$

Now we take a closer look on $\mathcal{M}'(\xi_\gamma)(\xi - \xi_\gamma)$. Here we have

$$\begin{aligned}
\mathcal{M}'_u(\xi_\gamma)(\varphi) =& (\overline{u}_\gamma - u^d, \varphi) - (A\varphi, \overline{z}_\gamma) + \int_{\Omega_C} K'(\overline{u}_\gamma)\varphi\, db'(\overline{u}_\gamma, \gamma),\\
\mathcal{M}'_z(\xi_\gamma)(\varphi) =& (\overline{q}_\gamma, \varphi) - (A\overline{u}_\gamma, \varphi),\\
\mathcal{M}'_q(\xi_\gamma)(\varphi) =& \alpha(|\overline{q}_\gamma|^{r-2}\overline{q}_\gamma, \varphi) + (\varphi, \overline{z}_\gamma),\\
\mathcal{M}'_\mu(\xi_\gamma)(\varphi) =& \int_{\Omega_C} K(\overline{u}_\gamma)\, d\varphi.
\end{aligned}$$

As the solution $\overline{u}_\gamma$ to (2.11a) satisfies the additional regularity $\overline{u}_\gamma \in W$ we obtain from the equivalence of the weak formulation (2.2) to the formulation (2.1) that $\mathcal{M}'_u(\xi_\gamma)(\overline{u} - \overline{u}_\gamma) = 0$. Similarly we obtain that $\mathcal{M}'_z(\xi_\gamma)(\overline{z} - \overline{z}_\gamma) = 0$ and from (2.11c) that $\mathcal{M}'_q(\xi_\gamma)(\overline{u} - \overline{u}_\gamma) = 0$. Hence we conclude that

$$\begin{aligned}
\mathcal{M}'(\xi_\gamma)(\xi - \xi_\gamma) &= \mathcal{M}'_\mu(\xi_\gamma)(\overline{\mu} - b'(\overline{u}_\gamma; \gamma))\\
&= -\int_{\Omega_C} K(\overline{u}_\gamma)\, db'(\overline{u}_\gamma; \gamma) + \int_{\Omega_C} K(\overline{u}_\gamma)\, d\overline{\mu}.
\end{aligned}$$

Summing up all terms we finally get:

$$\begin{aligned}
J(\overline{q}, \overline{u}) - J_\gamma(\overline{q}_\gamma, \overline{u}_\gamma) =& -\frac{1}{2}\int_{\Omega_C} \big(K(\overline{u}) + K(\overline{u}_\gamma)\big)\, db'(\overline{u}_\gamma; \gamma)\\
&+ \frac{1}{2}\int_{\Omega_C} K(\overline{u}_\gamma)\, d\overline{\mu}\\
&+ \int_{\Omega_C} K(\overline{u}_\gamma) b'(\overline{u}_\gamma; \gamma)\, dx - b(\overline{u}_\gamma; \gamma) + \mathcal{R}_{\mathrm{hom}}\\
=& \frac{1}{2}\int_{\Omega_C} \big(K(\overline{u}_\gamma) - K(\overline{u})\big)\, db'(\overline{u}_\gamma; \gamma)\\
&- b(\overline{u}_\gamma; \gamma) + \frac{1}{2}\int_{\Omega_C} K(\overline{u}_\gamma)\, d\overline{\mu} + \mathcal{R}_{\mathrm{hom}}.
\end{aligned}$$

This concludes the proof.

We now have to obtain a computable estimate from this error identity. We suggest two possible methods to do this.

4.1.1 Complementarity driven estimation

Using $K(u) \geq 0$ together with the definition of b' we see that

$$-\int_{\Omega_C} K(\overline{u})\, db'(\overline{u}_\gamma;\gamma) \geq 0$$

and we obtain using the fact that $(\overline{q}_\gamma, \overline{u}_\gamma)$ are feasible for (2.8)

$$\begin{aligned} 0 \geq J(\overline{q},\overline{u}) - J_\gamma(\overline{q}_\gamma,\overline{u}_\gamma) \geq & \frac{1}{2}\int_{\Omega_C} K(\overline{u}_\gamma)\, db'(\overline{u}_\gamma;\gamma) - b(\overline{u}_\gamma;\gamma) \\ & + \frac{1}{2}\int_{\Omega_C} K(\overline{u}_\gamma)\, d\overline{\mu} + \mathcal{R}_{\text{hom}}. \end{aligned}$$

Now we assume that $\int_{\Omega_C} K(\overline{u}_\gamma)\, d\overline{\mu} \approx \int_{\Omega_C} K(\overline{u}_\gamma)\, db'(\overline{u}_\gamma;\gamma)$ which is reasonable if $b'(\overline{u}_\gamma;\gamma)$ converges weakly* to $\overline{\mu}$. A discussion on this in the case of pointwise state constraints can be found in [40].

We finally suggest to take the best approximation for $\overline{u}_\gamma$ available. Thus the computable estimate reads as:

$$0 \geq J(\overline{q},\overline{u}) - J_\gamma(\overline{q}_\gamma,\overline{u}_\gamma) \gtrsim \eta^1_{\text{hom}} = (K(\overline{u}^h_\gamma), b'(\overline{u}^h_\gamma;\gamma))_{\Omega_C} - b(\overline{u}^h_\gamma;\gamma). \tag{4.6}$$

As we neglected $-\int_{\Omega_C} K(\overline{u})\, db'(\overline{u}_\gamma;\gamma)$ due to its sign we can expect this to overestimate the real error. Therefore we suggest an alternative variant.

4.1.2 Convergence driven estimation

The other suggested variant uses the idea that $\overline{u}_\gamma \to \overline{u}$ as $\gamma \to 0$, thus

$$\int_{\Omega_C} K(\overline{u}_\gamma) - K(\overline{u})\, db'(\overline{u}_\gamma;\gamma) \to 0.$$

Hence we neglect the term $\int_{\Omega_C} K(\overline{u}_\gamma) - K(\overline{u})\, db'(\overline{u}_\gamma;\gamma)$ in the error representation and approximate the multiplier $\overline{\mu}$ with $b'(\overline{u}_\gamma;\gamma)$. Then using our discrete approximation $\overline{u}^h_\gamma$ to $\overline{u}_\gamma$ we obtain:

$$J(\overline{q},\overline{u}) - J_\gamma(\overline{q}_\gamma,\overline{u}_\gamma) \approx \eta^2_{\text{hom}} = \frac{1}{2}(K(\overline{u}^h_\gamma), b'(\overline{u}^h_\gamma;\gamma))_{\Omega_C} - b(\overline{u}^h_\gamma;\gamma). \tag{4.7}$$

Remark 5 This might seem unreasonable as $J(\overline{q},\overline{u}) - J_\gamma(\overline{q}_\gamma,\overline{u}_\gamma) \to 0$. By neglecting a term due to its convergence to zero this might lead to different convergence rates of $J(\overline{q},\overline{u}) - J_\gamma(\overline{q}_\gamma,\overline{u}_\gamma)$ and η^2_{hom} thus spoiling the estimates we obtain. Our numerical experience however shows that this estimation works in fact better than the first estimator. This might be an indication for a higher convergence rate of the term $\int_{\Omega_C} K(\overline{u}_\gamma) - K(\overline{u})\, db'(\overline{u}_\gamma;\gamma) \to 0$. This should be further investigated in future work.

4.2 Discretization error

In order to estimate the discretization error in the value of the functional J_γ defined in (2.10), we define the Lagrangian $\mathcal{L}(q,u,z)\colon Q\times V\times V\to\mathbb{R}$ for the barrier problem by

$$\mathcal{L}(q,u,z) = J_\gamma(q,u) + (q,z) - a(u,z). \tag{4.8}$$

Furthermore we introduce the following residual functionals:

$$\rho_u(\overline{q}_\gamma^h,\overline{u}_\gamma^h,\overline{z}_\gamma^h)(\,\cdot\,) = (\overline{q}_\gamma^h,\,\cdot\,) - a(\overline{u}_\gamma^h,\,\cdot\,), \tag{4.9a}$$

$$\rho_z(\overline{q}_\gamma^h,\overline{u}_\gamma^h,\overline{z}_\gamma^h)(\,\cdot\,) = (\overline{u}_\gamma^h - u^d,\,\cdot\,) + (b'(\overline{u}_\gamma^h;\gamma), K'(\overline{u}_\gamma^h)\,\cdot\,)_{\Omega_C} - a(\,\cdot\,,\overline{z}_\gamma^h), \tag{4.9b}$$

$$\rho_q(\overline{q}_\gamma^h,\overline{u}_\gamma^h,\overline{z}_\gamma^h)(\,\cdot\,) = \alpha(|\overline{q}_\gamma^h|^{r-2}\overline{q}_\gamma^h,\,\cdot\,) + (\overline{z}_\gamma^h,\,\cdot\,). \tag{4.9c}$$

Then the following holds:

Theorem 2 *Let $\xi_\gamma = (\overline{q}_\gamma,\overline{u}_\gamma,\overline{z}_\gamma)$ be a solution to the first order necessary system* (2.11) *of the barrier problem and let $\xi_\gamma^h = (\overline{q}_\gamma^h,\overline{u}_\gamma^h,\overline{z}_\gamma^h)$ be the solution to its discretization* (3.2)*. Then the following estimate holds:*

$$\begin{aligned} J_\gamma(\overline{q}_\gamma,\overline{u}_\gamma) - J_\gamma(\overline{q}_\gamma^h,\overline{u}_\gamma^h) &= \frac{1}{2}\rho_u(\xi_\gamma^h)(\overline{z}_\gamma - \tilde{z}^h) + \frac{1}{2}\rho_z(\xi_\gamma^h)(\overline{u}_\gamma - \tilde{u}^h) \\ &\quad + \frac{1}{2}\rho_q(\xi_\gamma^h)(\overline{q}_\gamma - \tilde{q}^h) + \mathcal{R}_{disc} \end{aligned} \tag{4.10}$$

with arbitrary $(\tilde{q}^h,\tilde{u}^h,\tilde{z}^h)\in Q^h\times V^h\times V^h$ and a remainder term $\mathcal{R}_{disc}$ given by:

$$\mathcal{R}_{disc} = \frac{1}{2}\int_0^1 \mathcal{L}'''(\xi_\gamma^h + s(\xi_\gamma - \xi_\gamma^h))(\xi_\gamma - \xi_\gamma^h, \xi_\gamma - \xi_\gamma^h, \xi_\gamma - \xi_\gamma^h)s(s-1)\,ds. \tag{4.11}$$

Proof From the (weak) state equation (2.11a) and its discrete counterpart (3.2a) we obtain

$$J_\gamma(\overline{q}_\gamma,\overline{u}_\gamma) = \mathcal{L}(\xi_\gamma) \quad\text{and}\quad J_\gamma(\overline{q}_\gamma^h,\overline{u}_\gamma^h) = \mathcal{L}(\xi_\gamma^h).$$

To estimate the difference $\mathcal{L}(\xi_\gamma) - \mathcal{L}(\xi_\gamma^h)$ we proceed as in the proof of Theorem 1 and obtain

$$\mathcal{L}(\xi_\gamma) - \mathcal{L}(\xi_\gamma^h) = \frac{1}{2}\mathcal{L}'(\xi_\gamma)(\xi_\gamma - \xi_\gamma^h) + \frac{1}{2}\mathcal{L}'(\xi_\gamma^h)(\xi_\gamma - \xi_\gamma^h) + \mathcal{R}_{\text{disc}}$$

where $\mathcal{R}_{\text{disc}}$ is as in (4.11). As we used conforming subspaces for the discretization we see that $\xi_\gamma - \xi_\gamma^h \in Q\times V\times V$. Thus, we obtain from (2.11) that

$$\mathcal{L}'(\xi_\gamma)(\xi_\gamma - \xi_\gamma^h) = 0.$$

Using the definition of the residual functionals (4.9) we obtain

$$\mathcal{L}'(\xi_\gamma^h)(\xi_\gamma - \xi_\gamma^h) = \rho_u(\xi_\gamma^h)(\overline{z}_\gamma - \overline{z}_\gamma^h) + \rho_z(\xi_\gamma^h)(\overline{u}_\gamma - \overline{u}_\gamma^h) + \rho_q(\xi_\gamma^h)(\overline{q}_\gamma - \overline{q}_\gamma^h),$$

here we can use linearity of the residual functionals in the second argument together with (3.2) to obtain

$$\begin{aligned}\rho_u(\xi_\gamma^h)(\overline{z}_\gamma - \overline{z}_\gamma^h) &= \rho_u(\xi_\gamma^h)(\overline{z}_\gamma - \tilde{z}^h),\\ \rho_z(\xi_\gamma^h)(\overline{u}_\gamma - \overline{u}_\gamma^h) &= \rho_z(\xi_\gamma^h)(\overline{u}_\gamma - \tilde{u}^h),\\ \rho_q(\xi_\gamma^h)(\overline{q}_\gamma - \overline{q}_\gamma^h) &= \rho_q(\xi_\gamma^h)(\overline{q}_\gamma - \tilde{q}^h),\end{aligned}$$

with arbitrary $(\tilde{q}^h, \tilde{u}^h, \tilde{z}^h)$ in $Q^h \times V^h \times V^h$.

To obtain a computable error estimate from Theorem 2 we first choose $\tilde{u}^h = i^h\overline{u}_\gamma$, $\tilde{z}^h = i^h\overline{z}_\gamma$ with an interpolation operator $i^h\colon V \to V^h$. Then we have to approximate the interpolation errors $\overline{u}_\gamma - i^h\overline{u}_\gamma$ and $\overline{z}_\gamma - i^h\overline{z}_\gamma$. To do this, several heuristic techniques are known, see, e.g., [2, 42]. For our computations we assume to have an operator $\pi : V^h \to \tilde{V}^h$, with $\tilde{V}^h \neq V^h$, such that $\overline{u}_\gamma - \pi\overline{u}_\gamma^h$ and $\overline{z}_\gamma - \pi\overline{z}_\gamma^h$ have a better local asymptotic behavior than $\overline{u}_\gamma - \overline{u}_\gamma^h$ and $\overline{z}_\gamma - \overline{z}_\gamma^h$. Then we approximate:

$$\rho_u(\xi_\gamma^h)(\overline{z}_\gamma - i^h\overline{z}_\gamma) \approx \rho_u(\xi_\gamma^h)(\pi\overline{z}_\gamma^h - \overline{z}_\gamma^h) \text{ and } \rho_z(\xi_\gamma^h)(\overline{u}_\gamma - i^h\overline{u}_\gamma) \approx \rho_z(\xi_\gamma^h)(\pi\overline{u}_\gamma^h - \overline{u}_\gamma^h).$$

The term $\rho_q(\xi_\gamma^h)(\overline{q}_\gamma - \tilde{q}^h)$ requires some additional arguments. First of all, this term vanishes in some cases, e.g., if the control space is not discretized, $Q = Q^h$, or more general if $-\frac{1}{\alpha}\operatorname{sign}(\overline{z}_\gamma^h)|\overline{z}_\gamma^h|^{\frac{1}{r-1}} \in Q^h$. Thus the residual needn't to be evaluated.

If we have to evaluate the residual we define

$$\pi_Q\overline{q}_\gamma^h = \frac{-1}{\alpha}\operatorname{sign}(\pi\overline{z}_\gamma^h)|\pi\overline{z}_\gamma^h|^{\frac{1}{r-1}}.$$

Then we approximate

$$\rho_q(\xi_\gamma^h)(\overline{q}_\gamma - \tilde{q}^h) \approx \rho_q(\xi_\gamma^h)(\pi_Q\overline{q}_\gamma^h - \overline{q}_\gamma^h)$$

as proposed (for additional control constraints) in [44]. This (nonlocal) definition of $\pi_Q : Q^h \to Q$ is assumed to be locally better convergent following the results in [33].

Remark 6 The non locality introduced by the mapping $\overline{q}_\gamma^h \mapsto \overline{z}_\gamma^h$ does not introduce much additional numerical effort, as the adjoint state $\overline{z}_\gamma^h$ has to be computed anyway.

Finally we obtain the computable estimate

$$\begin{aligned}J_\gamma(\overline{q}_\gamma, \overline{u}_\gamma) - J_\gamma(\overline{q}_\gamma^h, \overline{u}_\gamma^h) &\approx \rho_u(\xi_\gamma^h)(\pi\overline{z}_\gamma^h - \overline{z}_\gamma^h) + \rho_z(\xi_\gamma^h)(\pi\overline{u}_\gamma^h - \overline{u}_\gamma^h)\\ &\quad + \rho_q(\xi_\gamma^h)(\pi_Q\overline{q}_\gamma^h - \overline{q}_\gamma^h)\\ &= \eta_{\text{disc}}.\end{aligned}$$

Remark 7 To obtain indicators suitable for mesh refinement, one has to localize this estimate to cellwise or nodewise contributions. A direct localization leads in general to local contributions of wrong order. To overcome this, one may integrate the residual terms by part, see, e.g., [2] or use a filtering operator, see [43] for details.

4.3 An adaptive algorithm

The remaining question is how to steer the values of γ and h. As we are interested in computing the value of the cost functional, it is not sensible to have γ or h too small in comparison to the other, especially as this makes the underlying problems harder to solve. Instead we try to choose both parameters in such a way, that the errors introduced by the parameters are equilibrated. To do this we choose both parameters such that the error estimators are of approximately the same size, e.g.:

$$|\eta_{\text{hom}}| \approx |\eta_{\text{disc}}|.$$

Thus we arrive at the following algorithm:

```
Initialize TOL, h, γ
repeat
    Solve problem (3.1)
    if |η_hom| > |η_disc| then
        Reduce γ
    else
        Refine mesh according to η_disc
until |η_hom| + |η_disc| < TOL
```

Remark 8 In some problems it might occur, that $\eta_{\text{disc}}\eta_{\text{hom}} < 0$, e.g., the errors introduced by both parameters have different sign. If in these cases $|\eta_{\text{hom}}| \approx |\eta_{\text{disc}}|$ we may expect that $|\eta_{\text{hom}} + \eta_{\text{disc}}| \ll |\eta_{\text{hom}}| + |\eta_{\text{disc}}|$, thus we would loose reliability of the estimate if we would simply take $\eta = \eta_{\text{hom}} + \eta_{\text{disc}}$. Therefore we suggested to use

$$|J(\overline{q}, \overline{u}) - J_\gamma(\overline{q}^h_\gamma, \overline{u}^h_\gamma)| \lesssim |\eta_{\text{hom}}| + |\eta_{\text{disc}}|$$

to obtain a more reliable estimate.

We will show later in our numerical examples that the changing sign doesn't occur only in the error estimation but can also be observed in the error $|J(\overline{q}, \overline{u}) - J_\gamma(\overline{q}^h_\gamma, \overline{u}^h_\gamma)|$. Hence we can not expect any estimation, near the zero of $|J(\overline{q}, \overline{u}) - J_\gamma(\overline{q}^h_\gamma, \overline{u}^h_\gamma)|$ or $\eta_{\text{hom}} + \eta_{\text{disc}}$ respectively, to be both reliable and efficient .

5 Illustration of the results for two specific types of constraints

In this section we are concerned to give two examples of constraints that can be treated in the framework we prepared in the Sections 2 and 3. For this we consider pointwise constraints on the state and pointwise constraints on the gradient of the state. We show that for these choices the assumptions in Section 2 are fulfilled and write down the a posteriori estimates from Section 4. Note that we won't discuss the case of finitely many state constraints in detail. However for these cases one may find the first order necessary conditions for instance in [11, 15].

5.1 State constraints

Here we choose pointwise bounds on the state, therefore our optimization problem (2.3) takes the form

$$\text{Minimize } J(q,u) := \frac{1}{2}\|u-u^d\|^2_{L^2(\Omega)} + \frac{\alpha}{r}\|q\|^r_{L^r(\Omega)}, \tag{5.1a}$$

$$\text{such that} \begin{cases} (2.2) \text{ holds}, \\ \psi - u \geq 0 \text{ on } \Omega_C, \end{cases} \tag{5.1b}$$

where Ω_C is a compact subset of $\overline{\Omega}$ and $\psi \in \mathbb{R}$. The mapping K is defined by

$$K(u) = \psi - u.$$

Remark 9 The restriction to constant bounds for the state is crucial in the following sense. For our computation we have to replace ψ by a finite dimensional approximation ψ_h, either due to interpolation as a finite element function $\psi_h \in V^h$ or by numerical integration. Our discrete problem would then use the mapping $K_h(u) = \psi_h - u$. This is only covered by our analysis if $\psi_h = \psi$.

If we restrict the dimension of the domain $\Omega \subset \mathbb{R}^n$ to $n = 2, 3$ and assume that the domain is either convex polygonal or has a smooth boundary, then we have for $W = H^2(\Omega) \cap H^1_0(\Omega)$ that the mapping $K\colon W \to C(\overline{\Omega})$ is well-defined and continuous by a well known embedding theorem. In addition we see that K is also continuous if interpreted as mapping $K\colon V \to L^2(\Omega_C) \subset L^1(\Omega_C)$. By noting that $\{u \,|\, K(u) \geq 0\}$ is closed and convex Assumption 3 on K is verified. In order to obtain $\overline{u} \in W$ it is sufficient to take $t = t' = r = 2$ in the definition of the control space.

The solvability of the adjoint equation (2.5) and the existence of $\overline{z}$ and $\overline{\mu}$ that satisfy the first order necessary condition (2.8) can be seen for linear equations in [7, 8] or in [15, 16] for semilinear equations. The first order necessary conditions (2.11) for the corresponding barrier problem can be found in [39]. Therefore the Assumptions 1 and 2 are verified for this type of equations.

For the convenience of the reader we write down the a posteriori estimates derived in Section 4.1 for this setting:

$$\begin{aligned} J(\overline{q},\overline{u}) - J_\gamma(\overline{q}_\gamma,\overline{u}_\gamma) = \frac{\gamma^o}{2}\int_{\Omega_C} \frac{(\overline{u}_\gamma - \overline{u})}{(\psi - \overline{u}_\gamma)^o}\,dx + \frac{1}{2}\int_{\Omega_C} (\psi - \overline{u}_\gamma)\,d\overline{\mu} \\ - b(\overline{u}_\gamma;\gamma) + \mathcal{R}_{\text{hom}}. \end{aligned}$$

The residual ρ_z from (4.9b) of the adjoint equation takes the form

$$\rho_z(\xi^h_\gamma)(\,\cdot\,) = (\overline{u}^h_\gamma - u^d, \,\cdot\,) - \gamma^o((\psi - \overline{u}_\gamma)^{-o}, \,\cdot\,)_{\Omega_C} - a(\,\cdot\,, \overline{z}^h_\gamma).$$

5.2 Gradient constraints

Here we choose pointwise bounds on the gradient of the state and the optimization problem takes the form

$$\text{Minimize } J(q,u) := \frac{1}{2}\|u-u^d\|^2_{L^2(\Omega)} + \frac{\alpha}{r}\|q\|^r_{L^r(\Omega)}, \tag{5.2a}$$

$$\text{such that} \begin{cases} (2.2) \text{ holds,} \\ \psi - |\nabla u|^2 \geq 0 \text{ on } \Omega_C, \end{cases} \tag{5.2b}$$

where once again Ω_C is a compact subset of $\overline{\Omega}$ and $\psi > 0$ is a constant. The mapping K is defined by

$$K(u) = \psi - |\nabla u|^2.$$

Here we need $W \subset C^1(\Omega_C)$ to obtain that K differentiable as mapping $K\colon W \to C(\Omega_C)$. Therefore we have to consider $W = W^{2,t}(\Omega) \cap W^{1,t}_0(\Omega)$ with $t > n$ ($\Omega \subset \mathbb{R}^n$). In addition we see that the interpretation of $K\colon V \to L^1(\Omega_C)$ makes sense. Once again the set $\{u \mid K(u) \geq 0\}$ is closed and convex hence Assumption 3 is verified.

However to obtain that the control to state mapping maps $L^t(\Omega)$ into W we have to require that $n = 2$ and Ω is convex polygonal or that the boundary of Ω is sufficiently smooth. For the last condition on the boundary of Ω the solvability of the adjoint equation (2.5) and the existence of $\overline{z}$ and $\overline{\mu}$ satisfying the first order necessary condition (2.8) has be investigated in [11,12] for semilinear equations. The first order necessary conditions (2.11) for the corresponding barrier problem can be obtained using similar techniques as in [39] for pointwise state constraints. This gives us the Assumptions 1 and 2.

For the convenience of the reader we write down the a posteriori estimates derived in Section 4.1 for this setting:

$$\begin{aligned} J(\overline{q},\overline{u}) - J_\gamma(\overline{q}_\gamma,\overline{u}_\gamma) = \frac{\gamma^o}{2}\int_{\Omega_C} \frac{\left(|\nabla \overline{u}_\gamma|^2 - |\nabla \overline{u}|^2\right)}{(\psi - |\nabla \overline{u}_\gamma|^2)^o}\,dx + \frac{1}{2}\int_{\Omega_C}\left(\psi - |\nabla \overline{u}_\gamma|^2\right)d\overline{\mu} \\ - b(\overline{u}_\gamma;\gamma) + \mathcal{R}_{\text{hom}}. \end{aligned}$$

The residual ρ_z from (4.9b) of the adjoint equation takes the form

$$\rho_z(\xi^h_\gamma)(\,\cdot\,) = (\overline{u}^h_\gamma - u^d, \,\cdot\,) + 2\gamma^o((\psi - |\nabla \overline{u}^h_\gamma|^2)^{-o}\nabla \overline{u}^h_\gamma, \nabla\,\cdot\,)_{\Omega_C} - a(\,\cdot\,, \overline{z}^h_\gamma).$$

6 Numerical examples

In this section we demonstrate our findings for two example configurations taken from other publications. All computations where made using the software packages RoDoBo [37] and Gascoigne [22]. The Visualizations where obtained using VisuSimple [45]. In both examples bilinear finite elements were used for the discretization of the space for the state and control variable.

6.1 State Constraints

Here we consider an example taken from [24]. There the following problem was considered:

$$\min_{q\in L^2(\Omega)} J(q,u) := \frac{1}{2}\|u-0.5\|^2_{L^2(\Omega)} + \frac{1}{2}\|q-60\|^2_{L^2(\Omega)}$$

$$\text{such that } \begin{cases} -\Delta u + u = q & \text{in } \Omega, \\ \partial_n u = 0 & \text{on } \partial\Omega, \end{cases}$$

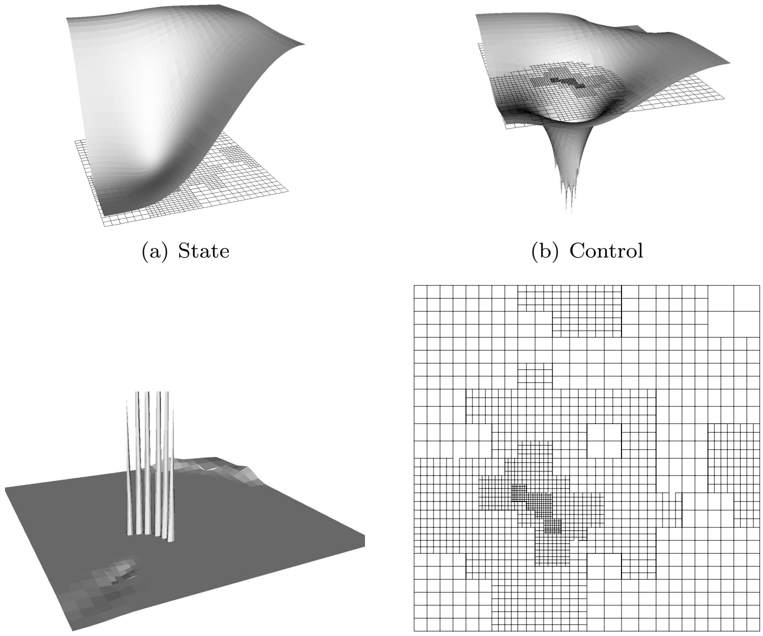
$$\text{and } 0.45 \le u(x) \le \psi(x) \quad \forall\, x \in \overline{\Omega}$$

on the domain $\Omega = (0,1)^2 \subset \mathbb{R}^2$ with the upper bound

$$\psi(x) = \min\bigl(1, \max\bigl(0.5, 50((x_1-0.3)^2 + (x_2-0.3)^2)\bigr)\bigr).$$

An approximation $J^* \approx 1759.04733$ for the optimal value of the cost functional is given in [24] where it was obtained on a equidistant mesh with 557^2 nodes.

In Figure 1 we show a computed approximation of the state, the control, and the approximated multiplier on the mesh in Figure 1(d). For these and the following computations we have chosen $o = 4$ as order of our barrier function.



(a) State (b) Control

(c) Multiplier approximation (d) Mesh

Fig. 1 Computed solutions and corresponding mesh

Remark 10 It should be noted, that this example doesn't exactly fit into our framework, as the upper bound for u is not constant, see the discussion in Section 5.1. Here we neglect the error introduced by the discretization of the upper bound and see that we still get satisfactory results for this example. However the question of estimating the error introduced by discretization of the bounds is subject to further research.

Table 1 Comparison of effectivity indices for the homotopy error

(a) Global refinement with η^1_{hom}

γ	N = 625	2401	9409
$3 \cdot 10^{-1}$	0.36	0.36	0.36
$1 \cdot 10^{-1}$	0.65	0.62	0.65
$3 \cdot 10^{-2}$	0.11	0.21	0.64
$1 \cdot 10^{-2}$	1.89	1.82	0.29
$3 \cdot 10^{-3}$	5.82	7.12	3.29
$1 \cdot 10^{-3}$	10.5	16.2	10.0

(b) Global refinement with η^2_{hom}

γ	N = 625	2401	9409
$3 \cdot 10^{-1}$	0.48	0.47	0.48
$1 \cdot 10^{-1}$	0.87	0.83	0.87
$3 \cdot 10^{-2}$	0.15	0.25	0.85
$1 \cdot 10^{-2}$	2.36	2.35	0.38
$3 \cdot 10^{-3}$	6.74	8.74	4.19
$1 \cdot 10^{-3}$	11.1	18.3	12.0

We start the discussion of this example with a comparison of the effectivity of the two proposed variants to estimate the error introduced by the barrier parameter γ. The effectivity indices

$$I_{\text{eff}} = \frac{|J^* - J_\gamma(\overline{q}^h_\gamma, \overline{u}^h_\gamma)|}{|\eta_{\text{disc}}| + |\eta_{\text{hom}}|}$$

for the choice $\eta_{\text{hom}} = \eta^1_{\text{hom}}$ can be found in Table 1(a) whereas those for $\eta_{\text{hom}} = \eta^2_{\text{hom}}$ can be found in Table 1(b) where they are depicted for a sequence of globally refined meshes.

Here we can see the expected behavior of the indices, especially for η^1_{hom} we do not get effectivities near 1. Note that for the smallest values of γ both indicators give almost the same value, which is due to the fact, that the error in the cost functional is then dominated by the discretization error. For dominant discretization error we see, that the effectivity indices become rather large. This can be explained by the fact, that we used nonconstant bounds. Thus we had to use an interpolation of the bounds which leads to the problem, that the discrete solutions are no longer feasible with respect to the continuous bounds. To substantiate this we introduce the following transformation:

$$v = \frac{\psi - u}{\psi - 0.45}.$$

Then v solves the problem:

$$\min_{q\in L^2(\Omega)} J(q,u) := \frac{1}{2}\|(0.45-\psi)v+\psi-0.5\|^2_{L^2(\Omega)} + \frac{1}{2}\|q-60\|^2_{L^2(\Omega)}$$

$$\text{such that} \begin{cases} -\Delta((0.45-\psi)v+\psi) + ((0.45-\psi)v+\psi) = q & \text{in } \Omega, \\ \partial_n v = 0 & \text{on } \partial\Omega, \end{cases}$$

$$\text{and } 0 \le v(x) \le 1 \ \ \forall x \in \overline{\Omega}$$

The results for this computation are depicted in Table 2. Here we can

Table 2 Comparison of effectivity indices for the homotopy error

(a) Transformed example with η^1_{hom}

γ	N = 625	2401	9409
$3\cdot10^{-1}$	0.29	0.52	0.71
$1\cdot10^{-1}$	0.00	0.26	0.57
$3\cdot10^{-2}$	1.24	1.47	0.10
$1\cdot10^{-2}$	1.50	2.23	0.96
$3\cdot10^{-3}$	1.58	2.55	1.50
$1\cdot10^{-3}$	1.60	2.65	1.70

(b) Transformed example with η^2_{hom}

γ	N = 625	2401	9409
$3\cdot10^{-1}$	0.36	0.67	0.94
$1\cdot10^{-1}$	0.00	0.31	0.72
$3\cdot10^{-2}$	1.29	1.60	0.12
$1\cdot10^{-2}$	1.52	2.30	1.03
$3\cdot10^{-3}$	1.58	2.58	1.54
$1\cdot10^{-3}$	1.60	2.66	1.71

see that the effectivities are far better. However even for the in the case of non constant bounds we obtain remarkably good results if local refinement is used as can be seen in the following tables. Since the estimation of the error introduced by the homotopy methods is better if η^2_{hom} is used we used this estimator for the results in Table 3 and Figure 2.

Reasons for the very small effectivity indices for the choices $\gamma = 1\cdot10^{-1}$ and $\gamma = 3\cdot10^{-2}$ will be discussed in the next example.

Table 3 Effectivity indices for locally refined meshes

(a) Local refinement balanced with η^2_{hom}

N	I_{eff}	γ	$\lvert J^* - J_\gamma(\overline{q}^h_\gamma, \overline{u}^h_\gamma)\rvert$
169	0.48	$2\cdot10^{-2}$	$1.5\cdot10^{-1}$
281	3.83	$4\cdot10^{-3}$	$1.9\cdot10^{-1}$
401	1.27	$8\cdot10^{-3}$	$1.1\cdot10^{-1}$
1057	1.56	$4\cdot10^{-3}$	$4.7\cdot10^{-2}$
1981	0.65	$3\cdot10^{-3}$	$1.6\cdot10^{-2}$

(b) Local refinement for $\gamma \to 0$

N	I_{eff}	$\lvert J^* - J_\gamma(\overline{q}^h_\gamma, \overline{u}^h_\gamma)\rvert$
169	1.98	$3.4\cdot10^{-1}$
269	7.80	$2.2\cdot10^{-1}$
401	3.45	$1.7\cdot10^{-1}$
1045	3.90	$6.7\cdot10^{-2}$
1749	2.09	$3.2\cdot10^{-2}$

In Table 3(a) we see the behavior of the effectivity index for a sequence of locally refined meshes where γ was chosen in such a way that the discretization error is of the same size as the error introduced by the interior point parameter

γ. Furthermore we see that apparently the influence of the bad estimation for the discretization error as seen in 1(a) and 1(b) doesn't have great influence on the estimation for the values of γ obtained from our balancing strategy.

In addition, the value of γ to have equilibrated error contributions is given as well as the total error obtained from discretization and interior penalty is shown. As a comparison we show in Table 3(b) the values obtained for local refinement where γ was driven towards zero as an estimate for the error obtained without an interior point method. These values are in good correspondence to those shown in [24].

We now compare the development of the estimated errors in the cost functional in Figure 2. Here we compared global and local refinement for γ chosen

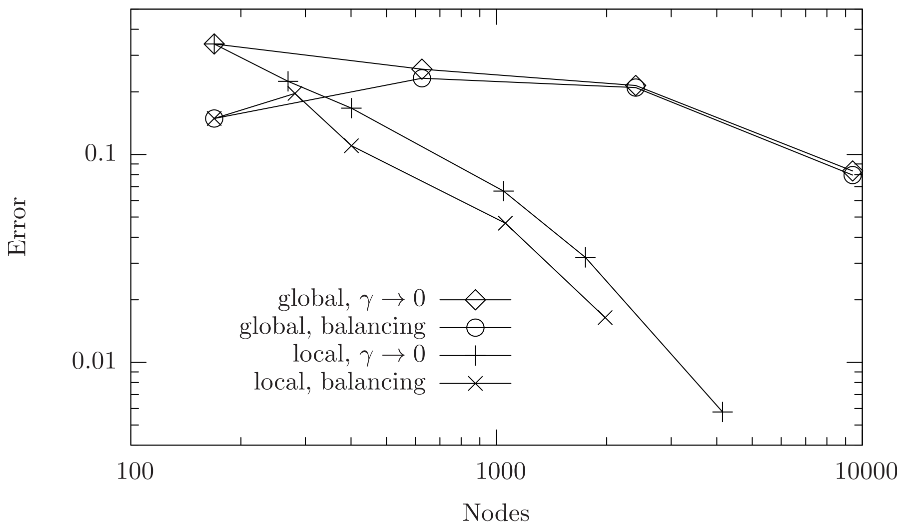


Fig. 2 Error in J for different refinement strategies

to equilibrate the error contributions and for the choice $\gamma \to 0$. The choice $\gamma \to 0$ is made to simulate the computation without 'regularization'. In that case we stopped the computation once the value of J_γ was unchanged in the first four digits by changing γ.

Especially we can see that there is no real difference in the error between the 'unregularized' discretization simulated by $\gamma \to 0$ and the error obtained for γ chosen to equilibrate the error contributions, except for the fact that the solutions in the latter case are easier to compute.

6.2 Gradient Constraints

Here we consider the example given in [18]. The problem reads as follows:

$$\min_{q \in Q_{\mathrm{ad}}} J(q,u) = \frac{1}{2}\|u - u^d\|^2_{L^2(\Omega)} + \frac{1}{2}\|q\|^2_{L^2(\Omega)}$$

$$\text{such that } \begin{cases} -\Delta u = f + q & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

$$\text{and } \frac{1}{4} - |\nabla u(x)|^2 \geq 0 \;\; \forall x \in \overline{\Omega}$$

on the domain $\Omega = \{ x \in \mathbb{R}^2 \mid |x| \leq 2 \}$ with the admissible set

$$Q_{\mathrm{ad}} = \{ q \in L^2(\Omega) \mid -2 \leq q \leq 2 \text{ a.e. in } \Omega \}$$

for the controls. With the desired state

$$u^d(x) = \begin{cases} \frac{1}{4} + \frac{1}{2}\ln 2 - \frac{1}{4}|x|^2, & |x| \leq 1 \\ \frac{1}{2}\ln 2 - \frac{1}{2}\ln|x|, & \text{otherwise} \end{cases}$$

and the right-hand side

$$f(x) = \begin{cases} 2, & |x| \leq 1 \\ 0, & \text{otherwise} \end{cases}$$

this problem admits the unique solution

$$\overline{u} = u^d \quad \text{and} \quad \overline{q} = \begin{cases} -1, & |x| \leq 1 \\ 0, & \text{otherwise.} \end{cases}$$

The optimal value of the cost functional is $\frac{\pi}{2}$ and in addition the control constraints are inactive at the solution $(\overline{u}, \overline{q})$. The order of the barrier is chosen to be $o = 6$.

We note that the introduction of the admissible set for the controls is necessary to ensure existence of a solution following standard arguments, as they are inactive at the optimal solution, the first order necessary conditions have the same form as proposed in Section 2 and Section 3, thus our estimates are applicable, see also Remark 2.

In Figure 3 we can see that the error in the value of the cost functional has indeed a sign change. This verifies Remark 8. Especially we can expect that the effectivity index

$$I_{\mathrm{eff}} = \frac{|0.5\pi - J\gamma(\overline{q}^h_\gamma, \overline{u}^h_\gamma)|}{|\eta_{\mathrm{disc}}| + |\eta_{\mathrm{hom}}|}$$

can go to zero for some values of γ.

In Table 4(a) the effectivity indices for $\eta_{\mathrm{disc}} = \eta^1_{\mathrm{disc}}$ and in Table 4(b) the effectivity indices for $\eta_{\mathrm{disc}} = \eta^2_{\mathrm{disc}}$ are shown. First of all we can see that for some value of γ the effectivity index is rather small, e.g., less than 0.1, which

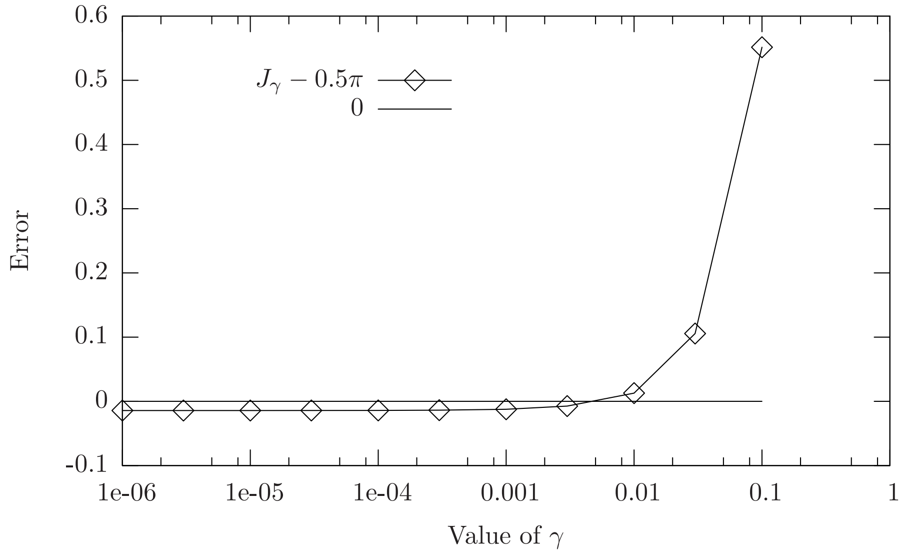


Fig. 3 Error in J for different γ

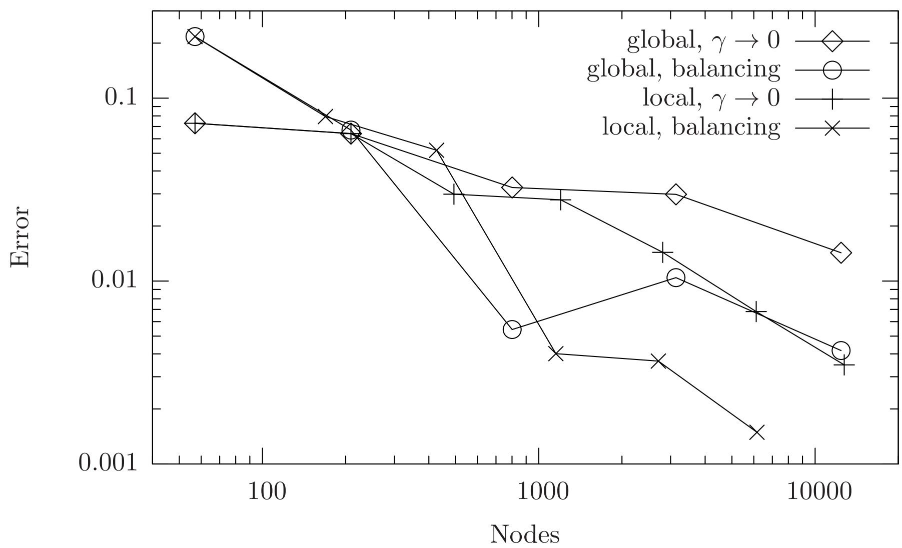


Fig. 4 Error in J for different refinement strategies

is in accordance with our observation, that $0.5\pi - J_\gamma(\overline{q}_\gamma^h, \overline{u}_\gamma^h)$ is zero for an appropriate choice of γ. Furthermore we can see, that for large values of γ the estimation is of less good quality which is due to the fact, that $\overline{u}_\gamma$ is still a bad approximation to $\overline{u}$. As these values do not change with grid refinement we can assume that this effect is not caused by the discretization. In addition we note that in contrast to the previous example the effectivity indices are of moderate size for dominant discretization error.

Table 4 Comparison of effectivity indices for the homotopy error

(a) Global refinement with η^1_{hom}

γ	N = 801	3137	12417
$3 \cdot 10^{-1}$	0.39	0.38	0.38
$1 \cdot 10^{-1}$	0.74	0.80	0.83
$3 \cdot 10^{-2}$	0.43	0.62	0.81
$1 \cdot 10^{-2}$	0.07	0.09	0.31
$3 \cdot 10^{-3}$	0.25	0.79	0.29
$1 \cdot 10^{-3}$	0.31	1.10	0.55

(b) Global refinement with η^2_{hom}

γ	N = 801	3137	12417
$3 \cdot 10^{-1}$	0.52	0.52	0.52
$1 \cdot 10^{-1}$	0.97	1.07	1.12
$3 \cdot 10^{-2}$	0.52	0.79	1.07
$1 \cdot 10^{-2}$	0.08	0.11	0.37
$3 \cdot 10^{-3}$	0.26	0.83	0.32
$1 \cdot 10^{-3}$	0.31	1.12	0.56

In Table 5(a) the effectivity indices are shown for a locally refined mesh where γ was chosen in order to balance the error contributions, also for each mesh size the value of γ obtained in the iteration, rounded to one decimal, is shown. Finally, in Table 5(b) the effectivity indices are shown for a locally refined mesh where $\gamma \to 0$ was taken to simulate the results one would obtain if the optimal control problem was discretized without further regularization.

Table 5 Effectivity indices for locally refined meshes

(a) Local refinement balanced with η^2_{hom}

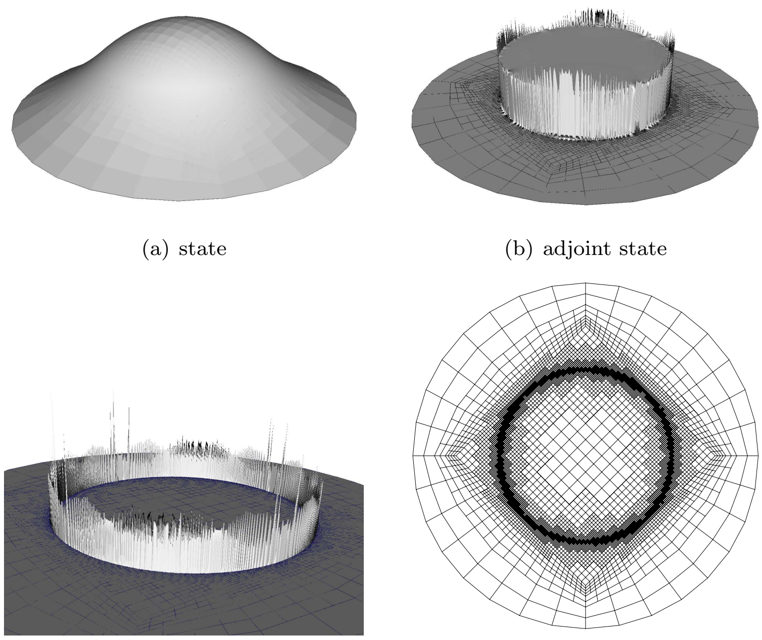
N	I_{eff}	γ
169	0.33	$4 \cdot 10^{-2}$
427	0.41	$2 \cdot 10^{-2}$
1153	0.11	$8 \cdot 10^{-3}$
2709	0.14	$5 \cdot 10^{-3}$
6161	0.13	$3 \cdot 10^{-3}$
12885	0.33	$3 \cdot 10^{-3}$

(b) Local refinement for $\gamma \to 0$

N	I_{eff}
200	0.30
493	0.30
1201	1.37
2809	0.76
6121	0.95
12745	1.02

A comparison of the development of the error in the cost functional is depicted in Figure 4. Here we compare global and local refinement as well as the choice of γ to balance the error contributions with $\gamma \to 0$. Note that the kink in the graphs for the case of balanced error contributions are due to cancellation effects between the error components. The kinks are larger than in the previous example because there the estimate of the discretization error was of lower quality due to the non constant bound.

The computed state $\overline{u}^h_\gamma$, the control $\overline{q}^h_\gamma$ and the approximation to the multiplier for the state constraints obtained by local refinement with γ chosen to balance the error contributions are depicted in Figure 5 together with the mesh on which they were obtained.



(a) state (b) adjoint state

(c) multiplier approximation (d) mesh

Fig. 5 computed solutions and corresponding mesh

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