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GOAL-ORIENTED ADAPTIVITY IN CONTROL CONSTRAINED OPTIMAL CONTROL OF PARTIAL DIFFERENTIAL EQUATIONS

M. HINTERMÜLLER AND R.H.W. HOPPE

ABSTRACT. Dual-weighted goal-oriented error estimates for a class of pointwise control constrained optimal control problems for second order elliptic partial differential equations are derived. It is demonstrated that the constraints give rise to a primal-dual weighted error term representing the mismatch in the complementarity system due to discretization. Also, for the new error estimate a posteriori error estimators for the L^2 -norm of the solution and its adjoint are derived.

1. INTRODUCTION

In many computations involving the discretization of (partial) differential equations or variational inequalities one is interested in the accurate evaluation of some target quantity. This might be the value of the solution of a partial differential equation (PDE) at some reference point in the domain of interest, a physically relevant quantity such as the drag in airfoil design, or, in optimal control, the value of the objective function at the solution of the underlying minimization problem. Highly accurate numerical evaluations of these targets can be guaranteed by using uniform meshes with a small mesh size h . This, however, usually represents a significant computational challenge due to the resulting large scale of the discrete problems. Therefore, one seeks to adaptively refine the meshes with the goal of achieving a desired accuracy in the evaluation of the output quantity of interest while keeping the computational cost as small as possible.

For this purpose, recently for (systems of) partial differential equations an approach based on dual weighted residual-based error estimates was proposed. Here we point to the pioneering work summarized in [1, 3] and the references therein; see also [4] for related literature. It essentially relies on employing the dual problem of the underlying system with the target on the right hand side. In fact, let A denote some possibly nonlinear partial

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differential operator and let f be some fixed data. Then, in some abstract form, the primal problem (or PDE) is given by

$$(1) \quad A(y) = f.$$

Let y_h be the result of a Galerkin finite element discretization of the underlying problem. If $G(\cdot)$ represents some desired target quantity (or goal), then the dual approach consists in considering

$$(2) \quad A'(y_h)^* p_h = G(\cdot)$$

from which an a posteriori error estimate of the type

$$|G(y) - G(y_h)| \leq \sum_{T \in \mathbb{T}_h} \mathfrak{p}_T(y_h) \mathfrak{d}_T(p_h)$$

is derived. Above, $A'(\cdot)^*$ is the dual operator of the Frechét-derivative $A'(\cdot)$ of $A(\cdot)$. Further, $\mathbb{T}_h = \{T\}$ denotes a computational mesh consisting of elements T , and \mathfrak{p}_T and \mathfrak{d}_T stand for the primal residual and the dual weight on each cell T , respectively.

In [2] this concept was transferred to PDE-constrained optimal control problems of the type

$$(P_0) \quad \text{minimize } J(y, u) \quad \text{subject to } A(y) = f + B(u)$$

where (y, u) denotes the state-control pair and B models the control impact. The first order optimality system of (P_0) can be formally written as

$$(3a) \quad A(y) - B(u) = f,$$

$$(3b) \quad J_y(y, u) + A'(y)^* p = 0,$$

$$(3c) \quad J_u(y, u) - B'(u)^* p = 0.$$

Here, J_y and J_u are the partial derivatives of J with respect to y and u , respectively. The variable p is called the adjoint state. Often, (3c) results in an algebraic equation, while (3a)–(3b) forms a primal-dual pair of PDEs similar to (1)–(2). Since (3a)–(3b) represents a system of PDEs the dual weighted approach can be readily carried over to this optimal control setting.

The situation, however, changes significantly if, in addition to the PDE constraint in (P_0) , one has to account for pointwise almost everywhere constraints on the control variable. In this case, the resulting problem becomes

$$(P_c) \quad \begin{cases} \text{minimize} & J(y, u) \\ \text{subject to} & A(y) = f + B(u), \\ & a \leq u \leq b \quad \text{almost everywhere (a.e.) on } \Omega_C \subset \Omega, \end{cases}$$

where $\Omega \subset \mathbb{R}^n$ denotes some suitable domain with $\Omega_C \neq \emptyset$ a measurable subset, and where $a < b$ are given bounds. The corresponding first order necessary optimality system now involves a variational inequality:

$$(4a) \quad A(y) - B(u) = f,$$

$$(4b) \quad J_y(y, u) + A'(y)^* p = 0,$$

$$(4c) \quad \langle J_u(y, u) - B'(u)^* p, v - u \rangle \geq 0 \quad \forall v \in U^{\text{ad}}, u \in U^{\text{ad}},$$

where the set

$$U^{\text{ad}} = \{v : a \leq v \leq b\}$$

represents the feasible controls, and $\langle \cdot, \cdot \rangle$ denotes a suitable duality pairing. The variational inequality induces some nonsmoothness in the first order optimality system. This can be seen best when defining the Lagrange multiplier λ pertinent to the pointwise constraints via

$$(5) \quad J_u(y, u) - B'(u)^*p + \lambda = 0$$

and, assuming that λ permits a pointwise interpretation,

$$(6) \quad \lambda \geq 0 \quad \text{a.e. on } \{u = b\}, \quad \lambda \leq 0 \quad \text{a.e. on } \{u = a\}, \quad \lambda = 0 \quad \text{else.}$$

The conditions in (6) represent the so-called *complementarity system*. It can be written equivalently as

$$(7) \quad \lambda = \min\{0, \lambda + \sigma(u - a)\} + \max\{0, \lambda + \sigma(u - b)\},$$

where $\sigma > 0$ is an arbitrarily fixed real and the max- and min-operations are understood in the pointwise sense. From (7) the nonsmoothness involved in the first order necessary optimality conditions becomes apparent. Of course, suitable a posteriori error concepts have to reflect this situation in order to accurately resolve the influence of the constraints on the solution of the optimal control problem.

In this paper, our starting point will be a sufficiently general model problem class of the type (P_c). Based on the Lagrange function

$$\mathcal{L}(y, u, p, \lambda) = J(y, u) + \langle A(y) - f - B(u), p \rangle + (u - b, \lambda)$$

of (P_c), for convenience written here for a unilaterally constrained version of the minimization problem, and with the objective function as the goal, we derive an error representation of the type

$$J(y, u) - J(y_h, u_h) = -\frac{1}{2} \langle \nabla_{xx} \mathcal{L}(x_h, \lambda_h)(x_h - x), x_h - x \rangle + (u_h - b, \lambda) + \text{osc}_h + r(x_h, x)$$

with $x = (p, y, u)$ and its discretized version $x_h = (p_h, y_h, u_h)$, respectively, and (\cdot, \cdot) some inner product. Further, osc_h represents data oscillations and r is the remainder term resulting from a Taylor expansion of \mathcal{L} . In a second step we then estimate the term due to the inequality constraints and utilize the a posteriori error estimators derived in [5] in order to obtain a computable error representation.

The rest of the paper is organized as follows: In the next section we derive our new dual-weighted residual-based error estimator for a representative control constrained optimal control model problem. Section 3 is devoted to possible extensions. In fact, we study the bilaterally constrained case, a class of nonlinear governing equations, and alternative concepts for obtaining a posteriori estimates pertinent to the complementarity system. In the appendix, for our constrained optimal control problem we derive a new a posteriori error estimate with respect to the L^2 -norm.

Notation. Throughout we use $\|\cdot\|_{0,\Omega}$ and $(\cdot, \cdot)_{0,\Omega}$ for the usual $L^2(\Omega)$ -norm and $L^2(\Omega)$ -inner product, respectively. For convenience, with respect to the notation we shall not distinguish between the norm, respectively inner product, for scalar-valued or vector-valued arguments. We also use $(\cdot, \cdot)_{0,\mathcal{S}}$, which is the $L^2(\mathcal{S})$ -inner product over a (measurable) subset $\mathcal{S} \subset \Omega$. By $|\cdot|_{1,\Omega}$ we denote the $H^1(\Omega)$ -seminorm $|y|_{1,\Omega} = \|\nabla y\|_{0,\Omega}$, which, by the Poincaré-Friedrichs-inequality, is a norm on $H_0^1(\Omega)$. The norm in $H^1(\Omega)$ is written as $\|\cdot\|_{1,\Omega}$. By $\mathbb{T}_h = \mathbb{T}_h(\Omega)$ we denote a shape regular finite element triangulation of the domain Ω . The subscript $h = \max\{\text{diam}(T) | T \in \mathbb{T}_h\}$ indicates the mesh size of \mathbb{T}_h .

2. RESIDUAL BASED ERROR ESTIMATE

For deriving the structure of the new error estimate due to the inequality constraints, we consider the model problem

$$(P) \quad \begin{cases} \text{minimize } J(y, u) := \frac{1}{2}\|y - z\|_{0,\Omega}^2 + \frac{\alpha}{2}\|u\|_{0,\Omega}^2 \\ \text{over } (y, u) \in H_0^1(\Omega) \times L^2(\Omega) \\ \text{subject to } -\Delta y = u + f, \\ \quad \quad \quad u \leq b \quad \text{a.e. in } \Omega, \end{cases}$$

which is a particular instance of (P_c) . The domain $\Omega \in \mathbb{R}^2$ is assumed to be bounded and polygonal with boundary $\Gamma := \partial\Omega$. For the data we suppose $z, b, f \in L^2(\Omega)$ and $\alpha > 0$. It is well-known that (P) admits a unique solution $(y^*, u^*) \in H_0^1(\Omega) \times L^2(\Omega)$. Moreover, the optimal solution is characterized by the existence of an adjoint state $p^* \in H_0^1(\Omega)$ and a Lagrange multiplier $\lambda^* \in L^2(\Omega)$ which satisfy the first order necessary (and in this case also sufficient) conditions

$$\begin{aligned} (8a) \quad & -\Delta y^* = u^* + f, \\ (8b) \quad & -\Delta p^* + y^* = z, \\ (8c) \quad & \alpha u^* + \lambda^* - p^* = 0, \\ (8d) \quad & u^* \leq b, \lambda^* \geq 0, (u^* - b, \lambda^*)_{0,\Omega} = 0. \end{aligned}$$

We define the Lagrange functional $\mathcal{L} : H_0^1(\Omega) \times L^2(\Omega) \times H_0^1(\Omega) \times L^2(\Omega) \rightarrow \mathbb{R}$ pertinent to (P) as

$$(9) \quad \mathcal{L}(y, u, p, \lambda) = J(y, u) + (\nabla y, \nabla p)_{0,\Omega} - (u + f, p)_{0,\Omega} + (u - b, \lambda)_{0,\Omega}.$$

For convenience we use $x := (p, y, u)$, $x^* = (p^*, y^*, u^*)$ and $X = P \times Y \times L = H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega)$. Obviously, the weak form of (8a)–(8b) and (8c) of the optimality system (8) is equivalent to

$$(10) \quad \nabla_x \mathcal{L}(x^*, \lambda^*)(\varphi) = 0 \quad \forall \varphi \in X.$$

Let $X_h \subset X$, with $X_h = P_h \times Y_h \times L_h$, denote a finite dimensional subspace with the subscript h indicating the mesh size of discretization obtained

by a standard Galerkin method, and let $\lambda_h \in L_h \subset L^2(\Omega)$ denote the discrete (finite dimensional) counterpart of λ (analogously for λ^*). The finite dimensional version of (8) reads

$$(11a) \quad \nabla_x \mathcal{L}_h(x_h^*, \lambda_h^*)(\varphi_h) = 0 \quad \forall \varphi_h \in X_h,$$

$$(11b) \quad u_h^* \leq b_h, \quad \lambda_h^* \geq 0, \quad (u_h^* - b_h, \lambda_h^*)_{0,\Omega} = 0,$$

where the discrete Lagrange function is given by

$$(12) \quad \begin{aligned} \mathcal{L}_h(x_h, \lambda_h) &= J_h(y_h, u_h) + (\nabla y_h, \nabla p_h)_{0,\Omega} - (u_h + f_h, p_h)_{0,\Omega} \\ &\quad + (u_h - b_h, \lambda_h)_{0,\Omega} \end{aligned}$$

with $J_h(y_h, u_h) = \frac{1}{2} \|y_h - z_h\|_{0,\Omega}^2 + \frac{\alpha}{2} \|u_h\|_{0,\Omega}^2$. Observe that the pointwise representation (8c) in the discrete setting reads

$$(13) \quad \alpha u_h^* + \lambda_h^* - M_h p_h^* = 0,$$

where M_h represents a projection operator from P_h onto L_h .

Further note that for $x \in X$, $\lambda \in L^2(\Omega)$ and $x_h \in X_h$, $\lambda_h \in L_h$

$$(14) \quad \mathcal{L}(x, \lambda_h) = \mathcal{L}(x, \lambda) + (u - b, \lambda_h - \lambda)_{0,\Omega},$$

$$(15) \quad \nabla_x \mathcal{L}(x_h, \lambda_h)(\varphi_h) = \nabla_x \mathcal{L}(x_h, \lambda)(\varphi_h) + (\delta u_h, \lambda_h - \lambda)_{0,\Omega}$$

for all $(\delta p_h, \delta y_h, \delta u_h) = \varphi_h \in X_h$. Moreover, for our model problem (P) the second derivative of \mathcal{L} with respect to x does not depend on x and λ . Thus, we can write $\nabla_{xx} \mathcal{L}(\varphi, \hat{\varphi})$ instead of $\nabla_{xx} \mathcal{L}(x, \lambda)(\varphi, \hat{\varphi})$. Similar observations hold true for \mathcal{L}_h . Due to $X_h \subset X$, we have for $\varphi_h = (\delta p_h, \delta y_h, \delta u_h) \in X_h$

$$(16) \quad \begin{aligned} 0 &= \nabla_x \mathcal{L}(x^*, \lambda^*)(\varphi_h) \\ &= \nabla_x \mathcal{L}(x_h^*, \lambda^*)(\varphi_h) + \nabla_{xx} \mathcal{L}(x^* - x_h^*, \varphi_h) \\ &= \nabla_x \mathcal{L}(x_h^*, \lambda_h^*)(\varphi_h) + (\delta u_h, \lambda^* - \lambda_h^*)_{0,\Omega} + \nabla_{xx} \mathcal{L}(x^* - x_h^*, \varphi_h) \\ &= \nabla_x \mathcal{L}_h(x_h^*, \lambda_h^*)(\varphi_h) - (f - f_h, \delta p_h)_{0,\Omega} - (z - z_h, \delta y_h)_{0,\Omega} \\ &\quad + (\delta u_h, \lambda^* - \lambda_h^*)_{0,\Omega} + \nabla_{xx} \mathcal{L}(x^* - x_h^*, \varphi_h) \\ &= (\delta u_h, \lambda^* - \lambda_h^*)_{0,\Omega} + \nabla_{xx} \mathcal{L}(x^* - x_h^*, \varphi_h) - (f - f_h, \delta p_h)_{0,\Omega} \\ &\quad - (z - z_h, \delta y_h)_{0,\Omega}. \end{aligned}$$

From this we further derive the relations

$$(17) \quad \begin{aligned} \nabla_{xx} \mathcal{L}(x_h^* - x^*, x_h^* - x^*) &= \\ &= \nabla_{xx} \mathcal{L}(x_h^* - x^*, x_h^* - x^* + \varphi_h) - (\delta u_h, \lambda^* - \lambda_h^*)_{0,\Omega} \\ &\quad + (f - f_h, \delta p_h)_{0,\Omega} + (z - z_h, \delta y_h)_{0,\Omega}, \end{aligned}$$

$$(18) \quad \nabla_x \mathcal{L}(x_h^*, \lambda^*)(x^* - x_h^* - \varphi_h) = \nabla_{xx} \mathcal{L}(x_h^* - x^*, x^* - x_h^* - \varphi_h)$$

and also

$$(19) \quad \begin{aligned} \nabla_x \mathcal{L}(x_h^*, \lambda_h^*)(x^* - x_h^* - \varphi_h) &= \\ &= \nabla_x \mathcal{L}(x^*, \lambda_h^*)(x^* - x_h^* - \varphi_h) + \nabla_{xx} \mathcal{L}(x_h^* - x^*, x^* - x_h^* - \varphi_h) \\ &= (\lambda_h^* - \lambda^*, u^* - u_h^* - \delta u_h)_{0,\Omega} + \nabla_{xx} \mathcal{L}(x_h^* - x^*, x^* - x_h^* - \varphi_h). \end{aligned}$$

These preliminary results are now used to prove the following theorem.

Theorem 2.1. *Let $(x^*, \lambda^*) \in X \times L^2(\Omega)$ and $(x_h^*, \lambda_h^*) \in X_h \times L_h$ denote the solution of (8) and its finite dimensional counterpart (11). Then*

$$(20) \quad \begin{aligned} J(y^*, u^*) - J_h(y_h^*, u_h^*) &= -\frac{1}{2} \nabla_{xx} \mathcal{L}(x_h^* - x^*, x_h^* - x^*) \\ &\quad + (u_h^* - b, \lambda^*)_{0,\Omega} + \text{osc}_h(x_h^*), \end{aligned}$$

where the oscillations $\text{osc}_h(x_h^*)$ are given by

$$\text{osc}_h(x_h^*) = (y_h^* - z_h, z_h - z)_{0,\Omega} + \frac{1}{2} \|z - z_h\|_{0,\Omega}^2 + (f_h - f, p_h^*)_{0,\Omega}.$$

Proof. Observe that $J(y^*, u^*) = \mathcal{L}(x^*, \lambda^*)$ and $J_h(y_h^*, u_h^*) = \mathcal{L}_h(x_h^*, \lambda_h^*)$. Using Taylor expansions and (14)-(15) we obtain

$$\begin{aligned} J(y^*, u^*) - J_h(y_h^*, u_h^*) &= \mathcal{L}(x^*, \lambda^*) - \mathcal{L}_h(x_h^*, \lambda_h^*) = \\ &= \mathcal{L}(x^*, \lambda^*) - \mathcal{L}_h(x^*, \lambda_h^*) - \nabla_x \mathcal{L}_h(x^*, \lambda_h^*)(x_h^* - x^*) \\ &\quad - \frac{1}{2} \nabla_{xx} \mathcal{L}_h(x_h^* - x^*, x_h^* - x^*) \\ &= J(y^*, u^*) - J_h(y^*, u^*) + (f_h - f, p^*)_{0,\Omega} - (u^* - b_h, \lambda_h^*)_{0,\Omega} \\ &\quad - \nabla_x \mathcal{L}_h(x^*, \lambda_h^*)(x_h^* - x^*) - \frac{1}{2} \nabla_{xx} \mathcal{L}_h(x_h^* - x^*, x_h^* - x^*) \\ &= \text{osc}_h(x_h^*) - (u^* - b_h, \lambda_h^*)_{0,\Omega} - \nabla_x \mathcal{L}(x^*, \lambda_h^*)(x_h^* - x^*) \\ &\quad - \frac{1}{2} \nabla_{xx} \mathcal{L}_h(x_h^* - x^*, x_h^* - x^*) \\ &= \text{osc}_h(x_h^*) - (u^* - u_h^*, \lambda_h^*)_{0,\Omega} + (\lambda^* - \lambda_h^*, u_h^* - u^*)_{0,\Omega} \\ &\quad - \frac{1}{2} \nabla_{xx} \mathcal{L}_h(x_h^* - x^*, x_h^* - x^*) \\ &= \text{osc}_h(x_h^*) + (\lambda^*, u_h^* - b)_{0,\Omega} - \frac{1}{2} \nabla_{xx} \mathcal{L}_h(x_h^* - x^*, x_h^* - x^*), \end{aligned}$$

where we also used the complementarity relations (8d) and (11b) as well as (10) and (11a). \square

Assume, for the moment, that $\lambda^* = 0$ and $\lambda_h^* = 0$, i.e., the continuous and the discrete control constraints are inactive, respectively. Then we infer from (17)

$$\begin{aligned} \nabla_{xx} \mathcal{L}(x_h^* - x^*, x_h^* - x^*) &= \nabla_{xx} \mathcal{L}(x_h^* - x^*, x_h^* - x^* + \varphi_h) \\ &\quad + (f - f_h, \delta p_h)_{0,\Omega} + (z - z_h, \delta y_h)_{0,\Omega} \end{aligned}$$

and further

$$(21) \quad \begin{aligned} J(y^*, u^*) - J_h(y_h^*, u_h^*) &= \frac{1}{2} \nabla_x \mathcal{L}_h(x_h, \lambda_h)(x^* - x_h^* - \varphi_h) \\ &\quad + \frac{1}{2} (f_h - f, p^* - p_h^*)_{0,\Omega} + \frac{1}{2} (z_h - z, y^* - y_h^*)_{0,\Omega} \\ &\quad + \text{osc}_h(x_h^*) \end{aligned}$$

due to (19). This corresponds to the result in [2, Proposition 4.1] for the unconstrained version of (P).

If $b_h \leq b$ a.e. in Ω , then (20) implies

$$J(y^*, u^*) \leq J_h(y_h^*, u_h^*) + \text{osc}_h(x^*, x_h^*).$$

Next we interpret the new, second term in the right hand side of (20). For this purpose we define the active set \mathcal{A}^* and the inactive set \mathcal{I}^* at the optimal solution (x^*, λ^*) of (P) by

$$(22) \quad \mathcal{A}^* := \{x \in \Omega : u^*(x) = b(x)\}, \quad \mathcal{I}^* := \Omega \setminus \mathcal{A}^*.$$

Analogously we define the discrete counterparts \mathcal{A}_h^* and \mathcal{I}_h^* , respectively. Obviously, $u^* < b$ a.e. in \mathcal{I}^* . By (8d), this implies $\lambda^* = 0$ a.e. in \mathcal{I}^* . Therefore, the term $(u_h^* - b, \lambda^*)_{0,\Omega}$ satisfies

$$(u_h^* - b, \lambda^*)_{0,\Omega} = (u_h^* - b_h, \lambda^*)_{0,\mathcal{A}^* \cap \mathcal{I}_h^*} + (b_h - b, \lambda^*)_{0,\mathcal{A}^*}.$$

The right hand side above reflects the *error in complementarity*. In fact, the second term represents the data oscillation in the bound in the active set weighted by the continuous Lagrange multiplier. For this term we introduce the notation

$$\text{osc}_h^{\mathcal{A}^*}(b; \lambda^*) := (b_h - b, \lambda^*)_{0,\mathcal{A}^*}.$$

The first term captures a *primal-dual weighted mismatch in complementarity in $\mathcal{A}^* \cap \mathcal{I}_h^*$* .

Let $i_h := (i_h^p, i_h^y, i_h^u)$ be an interpolation operator such that $i_h x \in X_h$ for $x \in X$. Moreover, for $y, p \in H_0^1(\Omega)$ there exist i_h^p and i_h^y such that $\max\{\|i_h^p p - p\|_{H^1}, \|i_h^y y - y\|_{H^1}\} \rightarrow 0$ for $h \rightarrow 0$. In connection with Theorem 2.1 we have the following result.

Theorem 2.2. *Let the assumptions of Theorem 2.1 be satisfied. Then*

$$(23) \quad \begin{aligned} J(y^*, u^*) - J_h(y_h^*, u_h^*) &= \\ &= -\frac{1}{2} \left((y_h^* - z_h, i_h^y y^* - y^*)_{0,\Omega} + (\nabla(i_h^y y^* - y^*), \nabla p_h^*)_{0,\Omega} \right. \\ &\quad + (\nabla(i_h^p p^* - p^*), \nabla y_h^*)_{0,\Omega} - (u_h^* + f_h, i_h^p p^* - p^*)_{0,\Omega} \\ &\quad \left. + (M_h p_h^* - p_h^*, i_h^u u^* - u^*)_{0,\Omega} \right) \\ &\quad + \frac{1}{2} [(b - u_h^*, \lambda^*)_{0,\Omega} + (b_h - u^*, \lambda_h^*)_{0,\Omega}] + \frac{1}{2} (f - f_h, p_h^* - p^*)_{0,\Omega} \\ &\quad + \frac{1}{2} (z - z_h, y_h^* - y^*)_{0,\Omega} + \text{osc}_h(x_h^*). \end{aligned}$$

Proof. Utilizing (17)–(18) and considering $\varphi_h = (\delta p_h, \delta y_h, \delta u_h) \in X_h$ we obtain

$$\begin{aligned}
J(y^*, u^*) - J_h(y_h^*, u_h^*) &= \frac{1}{2} \nabla_{xx} \mathcal{L}(x, \lambda_h^*)(x^* - x_h^*, x_h^* - x^* + \varphi_h) \\
&\quad + \frac{1}{2} (\delta u_h, \lambda^* - \lambda_h^*)_{0,\Omega} + \frac{1}{2} (f_h - f, \delta p_h)_{0,\Omega} + \frac{1}{2} (z_h - z, \delta y_h)_{0,\Omega} \\
&\quad + (u_h^* - b, \lambda^*)_{0,\Omega} + \text{osc}_h(x_h^*) \\
&= -\frac{1}{2} \nabla_x \mathcal{L}(x_h^*, \lambda_h^*)(x_h^* - x^* + \varphi_h) + \frac{1}{2} (\lambda_h^* - \lambda^*, u_h^* - u^*)_{0,\Omega} \\
&\quad + \frac{1}{2} (f_h - f, \delta p_h)_{0,\Omega} + \frac{1}{2} (z_h - z, \delta y_h)_{0,\Omega} + \text{osc}_h(x_h^*) \\
&= -\frac{1}{2} \nabla_x \mathcal{L}_h(x_h^*, \lambda_h^*)(x_h^* - x^* + \varphi_h) + \frac{1}{2} (\lambda_h^* - \lambda^*, u_h^* - u^*)_{0,\Omega} \\
&\quad + \frac{1}{2} (f - f_h, p_h^* - p^*)_{0,\Omega} + \frac{1}{2} (z - z_h, y_h^* - y^*)_{0,\Omega} + \text{osc}_h(x_h^*).
\end{aligned}$$

Choosing $\varphi_h = (i_h^p p^* - p_h^*, i_h^y y^* - y_h^*, i_h^u u^* - u_h^*) \in X_h$ and using complementary slackness, we continue

$$\begin{aligned}
J(y^*, u^*) - J_h(y_h^*, u_h^*) &= -\frac{1}{2} \nabla_x \mathcal{L}_h(x_h^*, \lambda_h^*)(i_h x^* - x^*) + \frac{1}{2} [(\lambda_h^*, b_h - u^*)_{0,\Omega} \\
&\quad + (\lambda^*, b - u_h^*)_{0,\Omega}] + \frac{1}{2} (f - f_h, p_h^* - p^*)_{0,\Omega} + \frac{1}{2} (z - z_h, y_h^* - y^*)_{0,\Omega} \\
&\quad + \text{osc}_h(x_h^*).
\end{aligned}$$

The assertion now follows from (9) and $u_h^* - M_h p_h^* + \lambda_h^* = 0$ a.e. in Ω . \square

This result is interesting in several ways:

- (i) For $\|M_h p_h - p_h\|_{0,\Omega} \rightarrow 0$ as $h \rightarrow 0$ sufficiently fast, only the convergence properties implied by i_h^p and i_h^y are required for obtaining an a posteriori error estimate based on (23). Since y^* and p^* solve elliptic partial differential equations they usually enjoy more regularity than u^* and λ^* .
- (ii) The term in brackets on the right hand side in (23) is again related to errors coming from complementary slackness. The first term of the sum can be interpreted as before, while the second term of the sum reflects the symmetric case, i.e.,

$$(b_h - u^*, \lambda_h^*)_{0,\Omega} = (b - u^*, \lambda_h^*)_{0,\mathcal{A}_h^* \cap \mathcal{I}^*} + (b_h - b, \lambda_h^*)_{0,\mathcal{A}_h^*},$$

Hence, the first term of the right hand side above represents the *primal-dual weighted mismatch in complementarity in $\mathcal{I}^* \cap \mathcal{A}_h^*$* , while the second term denotes the data oscillation on \mathcal{A}_h^* weighted by the discrete multiplier, i.e.,

$$\text{osc}_h^{\mathcal{A}_h^*}(b; \lambda_h^*) := (b_h - b, \lambda_h^*)_{0,\mathcal{A}_h^*}.$$

Of course, (23) is not immediately amenable to numerical realization since u^* and λ^* are involved. Before we tackle this point, let us first state a

posteriori error bounds for the control and the adjoint state which were derived in [5]. A coarser estimate was established in [7]. Recall that U^{ad} denotes the set of admissible controls, and let U_h^{ad} be its discretization. Then the following a posteriori error estimates hold true:

$$(24a) \quad \max(\|\lambda^* - \lambda_h^*\|_{0,\Omega}^2, \|u^* - u_h^*\|_{0,\Omega}^2) \leq C_1^2 \eta_1^2 + C_2^2 \eta_2^2 + C_b^2 \mu_h^2(b),$$

$$(24b) \quad \|p^* - p_h^*\|_{1,\Omega}^2 \leq C_2^2 \eta_2^2 + C_z^2 \text{osc}_h^2(z).$$

In what follows we also use

$$C_3^2 \eta_3^2 := C_1^2 \eta_1^2 + C_2^2 \eta_2^2 + C_b^2 \mu_h^2(b) \quad \text{and} \quad C_4^2 \eta_4^2 := C_2^2 \eta_2^2 + C_z^2 \text{osc}_h^2(z).$$

Here and below, $C_i > 0$, $i = 1, 2, 3, 4$, denote constants which depend on α , Ω and the shape regularity of \mathbb{T}_h . The error bounds η_1 and η_2 are defined as

$$(25) \quad \eta_1^2 = \sum_T \int_T h_T^2 (p_h^* - M_h p_h^*)^2,$$

$$(26) \quad \eta_2^2 = \sum_T \int_T h_T^2 (f + u_h^* + \Delta y_h^*)^2 + \sum_F \int_F h_F [\nabla y_h^* \cdot n]^2 \\ + \sum_T \int_T h_T^2 (z - y_h^* + \Delta p_h^*)^2 + \sum_F \int_F h_F [\nabla p_h^* \cdot n]^2.$$

Further the data oscillations

$$(27) \quad \mu_h^2(b) = \sum_{T \in \mathbb{T}_h} \|b - b_h\|_{0,T}^2,$$

$$(28) \quad \text{osc}_h^2(z) = \sum_{T \in \mathbb{T}_h} h_T^2 \|z - z_h\|_{0,T}^2$$

are involved.

Above, T denotes an element of the triangulation \mathbb{T}_h of Ω . Further, F denotes a face of T , and h_F is the maximal diameter of the face F . Moreover, $[\nabla y_h^* \cdot n]$ is the normal derivative jump over an interior face F . As noted before, the operator M_h represents the projection of a mesh function in P_h ($= Y_h$, typically in our context) onto L_h . If L_h is given by

$$L_h = \{u_h \in L^2(\Omega) : u_h|_T \in P_0(T), T \in \mathbb{T}_h\},$$

i.e., the function u_h is piecewise constant on \mathbb{T}_h , then the action of M_h in T is given by

$$(M_h p_h)|_T = \frac{1}{|T|} \int_T p_h(x) dx, \quad T \in \mathbb{T}_h.$$

A final observation concerns the unconstrained case, which is $U^{ad} = L^2(\Omega)$. In this situation we have $\lambda^* = 0$ a.e. in Ω . From (25)–(26) we see that the error estimator remains unaffected.

Our investigations concentrate now on the term

$$(29) \quad \frac{1}{2} [(b - u_h^*, \lambda^*)_{0,\Omega} + (b_h - u^*, \lambda_h^*)_{0,\Omega}] =: \Psi^*(\Omega),$$

which contains u^* and λ^* . A simple manipulation yields

$$\begin{aligned} \Psi^*(\Omega) &= \frac{1}{2} [(\lambda_h^* - \lambda^*, b_h - u^*)_{0,\Omega} + (\lambda^* - \lambda_h^*, b - u_h^*)_{0,\Omega} \\ &\quad + (\lambda^* - \lambda_h^*, b_h - b)_{0,\Omega}] \end{aligned}$$

From first order optimality we recall

$$(30) \quad u^* \leq b, \lambda^* \geq 0, (u^* - b, \lambda^*)_{0,\Omega} = 0, \alpha u^* - p^* + \lambda^* = 0,$$

$$(31) \quad u_h^* \leq b, \lambda_h^* \geq 0, (u_h^* - b, \lambda_h^*)_{0,\Omega} = 0, \alpha u_h^* - M_h p_h^* + \lambda_h^* = 0.$$

Obviously, we have

$$(32a) \quad \Psi^*(\mathcal{I}^* \cap \mathcal{I}_h^*) = 0,$$

$$(32b) \quad \Psi^*(\mathcal{A}^* \cap \mathcal{A}_h^*) = \frac{1}{2} (\lambda^* - \lambda_h^*, b_h - b)_{0,\mathcal{A}^* \cap \mathcal{A}_h^*},$$

where $\Psi^*(\mathcal{S}) = \frac{1}{2} [(b - u_h^*, \lambda^*)_{0,\mathcal{S}} + (b_h - u^*, \lambda_h^*)_{0,\mathcal{S}}]$. Note that if $b_h = b$ a.e. in Ω , then $\Psi^*(\mathcal{A}^* \cap \mathcal{A}_h^*) = 0$. From the structure of $\Psi^*(\mathcal{A}^* \cap \mathcal{A}_h^*)$ we can see that it represents a dual weighted data oscillation on $\mathcal{A}^* \cap \mathcal{A}_h^*$. Subsequently we use

$$(33) \quad \text{osc}_h^{\mathcal{S}}(b; \lambda^* - \lambda_h^*) := (b_h - b, \lambda_h^* - \lambda^*)_{0,\mathcal{S}}.$$

Note that $\text{osc}_h^{\mathcal{I}^* \cap \mathcal{I}_h^*}(b; \lambda^* - \lambda_h^*) = 0$.

Utilizing (30)–(33), for $\mathcal{C}_1^* = \mathcal{A}^* \cap \mathcal{I}_h^*$ and $\mathcal{C}_2^* = \mathcal{I}^* \cap \mathcal{A}_h^*$ we obtain

$$(34a) \quad \Psi^*(\mathcal{C}_1^*) = -\frac{\alpha}{2} \|u_h - u^*\|_{0,\mathcal{C}_1^*}^2 + \frac{1}{2} (p^* - M_h p_h^*, u^* - u_h^*)_{0,\mathcal{C}_1^*},$$

$$(34b) \quad \Psi^*(\mathcal{C}_2^*) = \frac{1}{2} (b_h - \alpha^{-1} p^*, \lambda_h^*)_{0,\mathcal{C}_2^*}.$$

On the respective sets we get the following estimates.

(i) In \mathcal{C}_1^* we have $u_{|\mathcal{C}_1^*}^* = b_{|\mathcal{C}_1^*}$. Thus,

$$\begin{aligned} |\Psi^*(\mathcal{C}_1^*)| &\leq \frac{1}{2} (\|M_h p_h^* - p_h^*\|_{0,\mathcal{C}_1^*} + \|p_h^* - p^*\|_{0,\mathcal{C}_1^*} + \alpha \|u_h^* - b\|_{0,\mathcal{C}_1^*}) \cdot \\ &\quad \cdot \|u_h^* - b\|_{0,\mathcal{C}_1^*}. \end{aligned}$$

Given \mathcal{C}_1^* and the discrete control u_h^* and adjoint state p_h^* , the first and third terms in parenthesis above are computable a posteriori. We therefore study $\|p_h^* - p^*\|_{0,\mathcal{C}_1^*}$ next. Since $p_h^*, p^* \in H_0^1(\Omega)$ and, for $n \geq 2$, $H_0^1(\Omega) \subset L^s(\Omega)$ for some $s \in (2, +\infty)$, from Hölder's inequality we obtain

$$(35) \quad \|p_h^* - p^*\|_{0,\mathcal{C}_1^*} \leq \text{meas}(\mathcal{C}_1^*)^{r(s)} \|p^* - p_h^*\|_{1,\mathcal{C}_1^*} \leq C_4 \text{meas}(\mathcal{C}_1^*)^{r(s)} \eta_4,$$

with $r(s) := \frac{1}{2} - \frac{1}{s} > 0$. Hence, we get

$$(36) \quad \|p_h^* - p^*\|_{0,\mathcal{C}_1^*} \leq \min \left(C_0^p \eta_{0,p}, C_4 \text{meas}(\mathcal{C}_1^*)^{r(s)} \eta_4 \right) =: C^p(\mathcal{C}_1^*),$$

where $\eta_{0,p}$ denotes the a posteriori estimator for $\|p^* - p_h^*\|_{0,\Omega}$ (see appendix A for its derivation) and $C_0^p > 0$ is a constant. This yields

$$(37) \quad |\Psi^*(\mathcal{C}_1^*)| \leq \frac{1}{2} \left(\|M_h p_h^* - p_h^*\|_{0,\mathcal{C}_1^*} + C^p(\mathcal{C}_1^*) + \alpha \|u_h^* - b\|_{0,\mathcal{C}_1^*} \right) \cdot \|u_h^* - b\|_{0,\mathcal{C}_1^*} =: \mu_1(\mathcal{C}_1^*).$$

(ii) In \mathcal{C}_2^* we use the identities $\lambda_h^* = M_h p_h^* - \alpha u_h^*$ and $p^* = \alpha u^*$. From this and assuming $b_h \in L^t(\Omega)$, $2 \leq t \leq s$, we infer

$$\begin{aligned} 2|\Psi^*(\mathcal{C}_2^*)| &= |(u_h^* - u^*, \lambda_h^*)_{\mathcal{C}_2^*}| \\ &\leq \text{meas}(\mathcal{C}_2^*)^{r(t)} \|b_h - \alpha^{-1} p^*\|_{t,\mathcal{C}_2^*} \|\lambda_h^*\|_{0,\mathcal{C}_2^*} \\ &\leq \text{meas}(\mathcal{C}_2^*)^{r(t)} \left(\|b_h - \alpha^{-1} p_h^*\|_{t,\mathcal{C}_2^*} + \alpha^{-1} \|p_h^* - p^*\|_{1,\Omega} \right) \|\lambda_h^*\|_{0,\mathcal{C}_2^*} \\ &\leq \text{meas}(\mathcal{C}_2^*)^{r(t)} \left(\|b_h - \alpha^{-1} p_h^*\|_{t,\mathcal{C}_2^*} + \alpha^{-1} C_4 \eta_4 \right) \|\lambda_h^*\|_{0,\mathcal{C}_2^*} \end{aligned}$$

with $r(t) \geq 0$. Alternatively, we may use (24a) for estimating $\|u_h^* - u^*\|_{0,\mathcal{M}_2^*}$. Hence, setting

$$C^u(\mathcal{C}_2^*) := \min \left(\text{meas}(\mathcal{C}_2^*)^{r(t)} \left(\|b_h - \alpha^{-1} p_h^*\|_{t,\mathcal{C}_2^*} + \alpha^{-1} C_4 \eta_4 \right), C_3 \eta_3 \right)$$

we obtain

$$(38) \quad |\Psi^*(\mathcal{C}_2^*)| \leq \frac{1}{2} C^u(\mathcal{C}_2^*) \|\lambda_h^*\|_{0,\mathcal{C}_2^*} := \mu_2(\mathcal{C}_2^*).$$

Since $\lambda_h^* = 0$ in \mathcal{I}_h^* we obviously have $\mu_2(\mathcal{I}_h^*) = 0$.

In both cases above we assume $\mu_1(\emptyset) = 0$ and $\mu_2(\emptyset) = 0$. Summarizing, we obtain

$$\begin{aligned} |\Psi^*(\Omega)| &= |\Psi^*(\mathcal{A}^* \cap \mathcal{A}_h^*) + \Psi^*(\mathcal{C}_1^*) + \Psi^*(\mathcal{C}_2^*)| \\ &\leq \frac{1}{2} \left| \text{osc}_h^{\mathcal{A}^* \cap \mathcal{A}_h^*}(b; \lambda^* - \lambda_h^*) \right| + \mu_1(\mathcal{C}_1^*) + \mu_2(\mathcal{C}_2^*). \end{aligned}$$

An alternative (and possibly coarse) estimate of $\Psi^*(\Omega)$ uses the error estimate η_3 and $\|\lambda_h^*\|_{0,\mathcal{A}_h^*}$ only:

$$|\Psi^*(\Omega)| = |(\lambda_h^* - \lambda^*, u_h^* - u^*)| \leq C_3^2 \eta_3^2 =: \mu_3(\Omega).$$

If the original problem is unconstrained with respect to u , then $\lambda^* = 0$. As a consequence, the first order conditions yield $\alpha u^* = p^*$, i.e., u^* inherits the regularity of $p^* \in H_0^1(\Omega)$. Then we may choose the same ansatz when discretizing p and u . Thus, we obtain $\eta_1 = 0$, since M_h becomes the identity operator, and—up to data oscillations— $\eta_2 = \eta_3$, and further $\|M_h p_h^* - p_h^*\|_{0,\mathcal{C}_1^*} = 0$ in μ_1 .

Finally, we express μ_1 and μ_2 such that we result in cell oriented error estimates. Let us first consider $\mu_1(\mathcal{C}_1^*)$. We have

$$\begin{aligned} \mu_1(\mathcal{C}_1^*) &= \frac{1}{2} \left(C^p(\mathcal{C}_1^*) + \|M_h p_h^* - p_h^*\|_{0,\mathcal{C}_1^*} + \alpha \|u_h^* - b\|_{0,\mathcal{C}_1^*} \right) \|u_h^* - b\|_{0,\mathcal{C}_1^*} \\ &= \frac{1}{2} \left(\hat{C}^p(\mathcal{C}_1^*) + \hat{C}_5(\mathcal{C}_1^*) \|M_h p_h^* - p_h^*\|_{0,\mathcal{C}_1^*}^2 + \alpha \|u_h^* - b\|_{0,\mathcal{C}_1^*}^2 \right). \end{aligned}$$

Above, we use

$$\hat{C}_0^p := \begin{cases} C_0^p \frac{\|u_h^* - b\|_{0, \mathcal{C}_1^*}}{\eta_{0,p}} & \text{if } \text{meas}(\mathcal{C}_1^*) \neq 0 \text{ and } \eta_{0,p} > 0, \\ 0 & \text{if } \text{meas}(\mathcal{C}_1^*) = 0, \end{cases}$$

as well as

$$\hat{C}_4(\mathcal{C}_1^*) := \begin{cases} C_4 \frac{\|u_h^* - b\|_{0, \mathcal{C}_1^*}}{\eta_4} & \text{if } \text{meas}(\mathcal{C}_1^*) \neq 0 \text{ and } \eta_4 > 0, \\ 0 & \text{if } \text{meas}(\mathcal{C}_1^*) = 0, \end{cases}$$

and further

$$\hat{C}_5(\mathcal{C}_1^*) := \begin{cases} \frac{\|u_h^* - b\|_{0, \mathcal{C}_1^*}}{\|M_h p_h^* - p_h^*\|_{0, \mathcal{C}_1^*}} & \text{if } \text{meas}(\mathcal{C}_1^*) \neq 0 \text{ and } \|M_h p_h^* - p_h^*\|_{0, \mathcal{C}_1^*} > 0, \\ 0 & \text{if } \text{meas}(\mathcal{C}_1^*) = 0. \end{cases}$$

We therefore have

$$\hat{C}^p(\mathcal{C}_1^*) = \min \left(\hat{C}_0^p \eta_{0,p}^2, \hat{C}_4(\mathcal{C}_1^*) \text{meas}(\mathcal{C}_1^*)^{r(s)} \eta_4^2 \right).$$

Finally, we turn to $\mu_2(\mathcal{C}_2^*)$. We obtain

$$\mu_2(\mathcal{C}_2^*) = \frac{1}{2} \hat{C}^u(\mathcal{C}_2^*),$$

with

$$\hat{C}_i(\mathcal{C}_2^*) := \begin{cases} C_i \frac{\|\lambda_h^*\|_{0, \mathcal{C}_2^*}}{\eta_i} & \text{if } \text{meas}(\mathcal{C}_2^*) \neq 0 \text{ and } \eta_i > 0, \\ 0 & \text{if } \text{meas}(\mathcal{C}_2^*) = 0. \end{cases}$$

for $i = 3, 4$, and

$$\begin{aligned} \hat{C}^u(\mathcal{C}_2^*) := \min & \left(\text{meas}(\mathcal{C}_2^*)^{r(t)} (\|b_h - \alpha^{-1} p_h^*\|_{t, \mathcal{C}_2^*} \|\lambda_h^*\|_{0, \mathcal{C}_2^*} \right. \\ & \left. + \alpha^{-1} \hat{C}_4(\mathcal{C}_2^*) \eta_4^2, \hat{C}_3(\mathcal{C}_2^*) \eta_3^2 \right). \end{aligned}$$

We summarize our above findings in the following proposition.

Proposition 2.1. *Let the assumptions of Theorem 2.1 be satisfied. Then*

$$(39) \quad |\Psi^*(\Omega)| \leq \min(\mu_1(\mathcal{C}_1^*), \mu_3(\Omega)) + \min(\mu_2(\mathcal{C}_2^*), \mu_3(\Omega)) =: \hat{\nu}.$$

In the case, where the solution of (P) satisfies $u^* < b$ a.e. on Ω , we expect that $\hat{\nu} \approx 0$. Indeed, for sufficiently small h we have $\lambda_h^* \approx 0$ (or even $\lambda_h^* = 0$). Thus, $\mu_2(\mathcal{C}_2^*) \approx 0$ (or $\mu_2(\mathcal{C}_2^*) = 0$) holds true. Further, $\mu_1(\mathcal{C}_1^*) = 0$ since $\mathcal{A}^* = \emptyset$. Then (39) yields $\hat{\nu} \approx 0$ (or $\hat{\nu} = 0$). If (P) involves no inequality constraints on u , which means that we can set $b \equiv +\infty$ on Ω , then we naturally obtain $\hat{\nu} = 0$. Hence, we recover the error estimator for unconstrained optimal control problems; compare [2, 7].

For deriving the full error estimate, it remains to consider the first term in parenthesis on the right hand side of (23) in Theorem 2.2. This term

is independent of the control constraints and corresponds to the usual expression obtain for (unconstrained) optimal control problems; see [2, 7]. A standard argument yields

$$\begin{aligned}
(40) \quad & |(\nabla y_h^*, \nabla(i_h^p p^* - p^*))_{0,\Omega} - (u_h^* + f_h, i_h^p p^* - p^*)_{0,\Omega}| \\
& \leq \sum_T \| -\Delta y_h^* - u_h^* - f_h \|_{0,T} \| p^* - i_h^p p^* \|_{0,T} \\
& \quad + \sum_F \| [\frac{\partial y_h^*}{\partial n}] \|_{0,F} \| p^* - i_h^p p^* \|_{0,F} =: \eta_2^p
\end{aligned}$$

for the primal equation,

$$\begin{aligned}
(41) \quad & |(y_h^* - z_h, i_h^y y^* - y^*)_{0,\Omega} + (\nabla(i_h^y y^* - y^*), \nabla p_h^*)_{0,\Omega}| \\
& \leq \sum_T \| -\Delta p_h^* + y_h^* - z_h \|_{0,T} \| y^* - i_h^y y^* \|_{0,T} \\
& \quad + \sum_F \| [\frac{\partial p_h^*}{\partial n}] \|_{0,F} \| y^* - i_h^y y^* \|_{0,F} =: \eta_2^d
\end{aligned}$$

for the dual equation, and

$$(42) \quad |(M_h p_h^* - p_h^*, i_h^u u^* - u^*)_{0,\Omega}| =: \eta_2^u.$$

The overall residual and complementarity based error estimate is given in the following theorem.

Theorem 2.3. *Let the assumptions of Theorem 2.1 be satisfied. Then we have the following error estimate*

$$\begin{aligned}
(43) \quad & |J(y^*, u^*) - J(y_h^*, u_h^*)| \leq \frac{1}{2}(\eta_2^p + \eta_2^d + \eta_2^u + \hat{\nu}) \\
& \quad + \frac{1}{2}[C_0^p \eta_{0,p} \|f - f_h\|_{0,\Omega} + C_0^y \eta_{0,y} \|z - z_h\|_{0,\Omega}] \\
& \quad + |\text{osc}_h(x_h^*)|.
\end{aligned}$$

with η_2^p , η_2^d , η_2^u and $\hat{\nu}$ defined by (40), (41), (42) and (39), respectively. Further, $C_0^y > 0$ is a constant and $\eta_{0,y}$ denotes an error estimate for $\|y_h^* - y^*\|_{0,\Omega}$. For the definition of $\eta_{0,p}$ and $\eta_{0,y}$ see (62) and (63) in appendix A.

The numerical evaluation of (43) depends on estimates of $\|i_h^y y^* - y^*\|_{0,T}$, $\|i_h^y y^* - y^*\|_{0,F}$ and analogously for $i_h^p p^* - p^*$. When discretizing the state and the adjoint state in 2D by continuous piecewise linear finite elements, the following averaging technique replacing η_2^p and η_2^d in (40) and (41), respectively, is appropriate:

$$\begin{aligned}
(44) \quad \eta_{2,h}^p := & \frac{1}{3} \sum_T \left(h_T \| -\Delta y_h^* - u_h^* - f_h \|_{0,T} \sum_{F(T)} h_F^{1/2} \| [\frac{\partial y_h^*}{\partial n}] \|_{0,F} \right) \\
& + \sum_F h_F \| [\frac{\partial y_h^*}{\partial n}] \|_{0,F} \| [\frac{\partial p_h^*}{\partial n}] \|_{0,F}
\end{aligned}$$

for the primal equation, and

$$(45) \quad \eta_{2,h}^d := \frac{1}{3} \sum_T \left(h_T \| -\Delta p_h^* + y_h^* - z_h \|_{0,T} \sum_{F(T)} h_F^{1/2} \| [\frac{\partial y_h^*}{\partial n}] \|_{0,F} \right) \\ + \sum_F h_F \| [\frac{\partial p_h^*}{\partial n}] \|_{0,F} \| [\frac{\partial y_h^*}{\partial n}] \|_{0,F}$$

for the dual equation, where $F(T)$ denotes the edges pertinent to triangle T . Notice that (44) and (45) yield typically sharper estimates than residual-based estimators for our model problem; compare (24) and [5]. Further observe that we can only expect boundedness of $\|i_h^u u^* - u^*\|_{0,\Omega}$, in general. However, typically $\|M_h p_h^* - p_h^*\|_{0,\Omega}$ is small, or, when using the same ansatz for discretizing u^* as well as p^* , it is even zero.

For the numerical evaluation of $\hat{\nu}$ observe that $\mathcal{I}_h^* \setminus \mathcal{A}^* \subset \mathcal{I}^*$ and hence $\lambda_h^* = 0$ and $\lambda^* = 0$ on this set. Consequently, we obtain

$$\Psi^*(\mathcal{I}_h^* \setminus \mathcal{A}^*) = 0.$$

Next observe that $\mathcal{I}_h^* = \mathcal{C}_1^* \dot{\cup} (\mathcal{I}_h^* \setminus \mathcal{A}^*)$. Therefore, we have

$$(46) \quad \Psi^*(\mathcal{C}_1^*) = \Psi^*(\mathcal{I}_h^*) - \Psi^*(\mathcal{I}_h^* \setminus \mathcal{A}^*) = \Psi^*(\mathcal{I}_h^*).$$

If $b_h = b$, then we obtain $\Psi^*(\mathcal{A}_h^* \setminus \mathcal{I}^*) = 0$ and further

$$(47) \quad \Psi^*(\mathcal{C}_2^*) = \Psi^*(\mathcal{A}_h^*) - \Psi^*(\mathcal{A}_h^* \setminus \mathcal{I}^*) = \Psi^*(\mathcal{A}_h^*).$$

The estimates $\mu_1(\mathcal{C}_1^*)$ and $\mu_1(\mathcal{C}_2^*)$, however, do not satisfy relations analogous to (46)–(47) even when $b_h = b$. Hence, $\hat{\nu}$ is not a posteriori. In order to have a fully a posteriori estimate we replace $\hat{\nu}$ in (43) by

$$(48) \quad \hat{\nu}^a = \min(\mu_1(\mathcal{I}_h^*), \mu_3(\Omega)) + \min(\mu_2(\mathcal{A}_h^*), \mu_3(\Omega)).$$

An alternative technique based on set estimation is the subject of section 3.3.

3. EXTENSIONS

Now we consider possible extensions of the concept derived in the previous section. We focus on three aspects: (i) Modifications for bilateral constraints; (ii) effects due to nonlinear PDEs; and (iii) alternative ways of making $\hat{\nu}$ fully a posteriori.

3.1. Bilateral constraints. We start by considering the bilaterally constrained version of (P):

$$(P_b) \quad \begin{cases} \text{minimize } J(y, u) := \frac{1}{2} \|y - z\|_{0,\Omega}^2 + \frac{\alpha}{2} \|u\|_{0,\Omega}^2 \\ \text{over } (y, u) \in H_0^1(\Omega) \times L^2(\Omega) \\ \text{subject to } -\Delta y = u + f, \\ \quad \quad \quad a \leq u \leq b \quad \text{a.e. in } \Omega, \end{cases}$$

Then the first order conditions involve a bilateral complementarity system.

$$\begin{aligned}
(49a) \quad & -\Delta y^* = u^* + f, \\
(49b) \quad & -\Delta p^* + y^* = z, \\
(49c) \quad & \alpha u^* + \lambda_b^* - \lambda_a^* - p^* = 0, \\
(49d) \quad & u^* \geq a, \lambda_a^* \geq 0, (u^* - a, \lambda_a^*)_{0,\Omega} = 0, \\
(49e) \quad & u^* \leq b, \lambda_b^* \geq 0, (u^* - b, \lambda_b^*)_{0,\Omega} = 0.
\end{aligned}$$

The analogous relations hold true for the discrete system. The same technique as before yields the bilateral version of Theorem 2.1.

Theorem 3.1. *Let $(x^*, \lambda^*) \in X \times L^2(\Omega)$ and $(x_h^*, \lambda_h^*) \in X_h \times L_h$ denote the solution of (49) and its finite dimensional counterpart. Then*

$$\begin{aligned}
J(y^*, u^*) - J_h(y_h^*, u_h^*) = & -\frac{1}{2} \nabla_{xx} \mathcal{L}(x_h^* - x^*, x_h^* - x^*) + (u_h^* - b, \lambda_b^*)_{0,\Omega} \\
& + (a - u_h^*, \lambda_a^*)_{0,\Omega} + \text{osc}_h(x_h^*).
\end{aligned}$$

Further we have the following representation; compare Theorem 2.2.

Theorem 3.2. *Let the assumptions of Theorem 3.1 be satisfied. Then*

$$\begin{aligned}
(50) \quad & J(y^*, u^*) - J_h(y_h^*, u_h^*) = \\
& = -\frac{1}{2} ((y_h^* - z_h, i_h^y y^* - y^*)_{0,\Omega} + (\nabla(i_h^y y^* - y^*), \nabla p_h^*)_{0,\Omega} \\
& + (\nabla(i_h^p p^* - p^*), \nabla y_h^*)_{0,\Omega} - (u_h^* + f_h, i_h^p p^* - p^*)_{0,\Omega}) \\
& + \frac{1}{2} [(b - u_h^*, \lambda_b^*)_{0,\Omega} + (b_h - u^*, \lambda_{b,h}^*)_{0,\Omega}] \\
& + \frac{1}{2} [(u_h^* - a, \lambda_a^*)_{0,\Omega} + (u^* - a_h, \lambda_{a,h}^*)_{0,\Omega}] + \frac{1}{2} (f - f_h, p_h^* - p^*)_{0,\Omega} \\
& + \frac{1}{2} (z - z_h, y_h^* - y^*)_{0,\Omega} + \text{osc}_h(x_h^*).
\end{aligned}$$

In the definition of $\hat{\nu}$ (see (39)) we use

$$\mu_1(\mathcal{C}_1^*) = \hat{C}^p(\mathcal{C}_1^*) + \hat{C}_5^p(\mathcal{C}_1^*) \|M_h p_h^* - p_h^*\|_{0,\mathcal{C}_1^*}^2 + \alpha \|u_h^* - c\|_{0,\mathcal{C}_1^*}^2.$$

where, in the definitions of \hat{C}^p , \hat{C}_0^p , $\hat{C}_4(\mathcal{C}_1^*)$ and $\hat{C}_4(\mathcal{C}_1^*)$, the bound b is replaced by

$$c(x) = \begin{cases} a(x) & \text{if } x \in \mathcal{I}_h^* \cap \mathcal{A}_a^*, \\ b(x) & \text{if } x \in \mathcal{I}_h^* \cap \mathcal{A}_b^*. \end{cases}$$

Here we use

$$\mathcal{A}_a^* = \{x \in \Omega : u^*(x) = a(x)\}, \mathcal{A}_b^* = \{x \in \Omega : u^*(x) = b(x)\}, \mathcal{A}^* = \mathcal{A}_a^* \cup \mathcal{A}_b^*.$$

An analogous modification is necessary for the estimator $\mu_2(\mathcal{C}_2^*)$.

3.2. Semilinear PDEs. Next we assume that the underlying PDE is semilinear:

$$(51) \quad A(y) = Bu + f,$$

where the operators A and B induce a semilinear form $a(\cdot)(\cdot)$ and a bilinear form $b(\cdot, \cdot)$, respectively. Hence, the weak form of (51) becomes

$$a(y)(v) = (f, v)_{0,\Omega} + b(u, v) \quad \forall v \in Y.$$

For our arguments to follow, we assume that A (resp. a) is sufficiently often differentiable. The corresponding Lagrange function has the structure

$$\mathcal{L}(x, \lambda_a, \lambda_b) = J(y, u) + a(y)(p) - (f, p)_{0,\Omega} - b(u, p) + (a - u, \lambda_a)_{0,\Omega} + (u - b, \lambda_b)_{0,\Omega}$$

The first order necessary optimality conditions are given by

$$(52a) \quad A(y^*) - Bu^* = f,$$

$$(52b) \quad A'(y^*)^* p^* + J_y(y^*, u^*) = 0,$$

$$(52c) \quad J_u(y^*, u^*) + \lambda_b^* - \lambda_a^* - B^* p^* = 0,$$

$$(52d) \quad u^* \geq a, \lambda_a^* \geq 0, (u^* - a, \lambda_a^*)_{0,\Omega} = 0,$$

$$(52e) \quad u^* \leq b, \lambda_b^* \geq 0, (u^* - b, \lambda_b^*)_{0,\Omega} = 0.$$

As the pointwise control constraints are affine, the error estimator for the nonlinear case is similar to the linear case. This parallels the situation in [2] where the unconstrained case was considered. Due to essentially the same proof arguments as in [2, Proposition 6.1], the following result holds true. In what follows we use

$$\mathcal{L}_0(x) = J(y, u) + a(y)(p) - (f, p)_{0,\Omega} - b(u, p)$$

and $\mathcal{L}_{0,h}(x)$ for its discrete counterpart.

Theorem 3.3. *For a Galerkin finite element discretization of the first order necessary optimality conditions (52) the following relation holds true:*

$$\begin{aligned} J(y^*, u^*) - J_h(y_h^*, u_h^*) &= \frac{1}{2} \nabla_x \mathcal{L}_{0,h}(x_h^*)(x^* - i_h x^*) \\ &+ \frac{1}{2} [(b - u_h^*, \lambda_b^*)_{0,\Omega} + (b_h - u^*, \lambda_{b,h}^*)_{0,\Omega}] \\ &+ \frac{1}{2} [(u_h^* - a, \lambda_a^*)_{0,\Omega} + (u^* - a_h, \lambda_{a,h}^*)_{0,\Omega}] \\ &+ \frac{1}{2} ((f - f_h, p_h^* - p^*)_{0,\Omega} + (z - z_h, y_h^* - y^*)_{0,\Omega}) + \text{osc}_h(x_h^*) \\ &+ r(x^*, x_h^*), \end{aligned}$$

where $r(x^*, x_h^*)$ denotes the remainder term of a Taylor expansion of \mathcal{L}_0 about x_h^* . It is bounded by

$$|r(x^*, x_h^*)| \leq \sup_{\bar{x} \in [x_h^*, x^*]} |\nabla_x^3 \mathcal{L}_0(\bar{x}) [x^* - x_h^*]^3|.$$

3.3. Alternative a posteriori estimate for $\hat{\nu}$. At the end of section 2 we derived an a posteriori estimate for $\hat{\nu}$; recall $\hat{\nu}^a$ in (48), where we replaced \mathcal{C}_1^* by \mathcal{I}_h^* and \mathcal{C}_2^* by \mathcal{A}_h^* , respectively. This may give rise to an overestimation of the error term pertinent to the complementarity system. In the following we provide an alternative approach based on set estimation.

Assuming, without loss of generality, $b_h = b$, we focus on the unilaterally constrained case and start by considering $\hat{\mu}_1(\mathcal{C}_1^*)$. For this purpose recall that $\mathcal{C}_1^* = \mathcal{I}_h^* \cap \mathcal{A}^*$. Similarly to [6, Section 3.3] we estimate the continuous active set \mathcal{A}^* by

$$\chi_h^{\mathcal{A}^*} = 1 - \frac{b - u_h^*}{\gamma h^r + b - u_h^*},$$

where γ denotes some (possibly small) positive constant, and $r > 0$ is fixed. Note that $\chi_h^{\mathcal{A}^*} = 1$ in \mathcal{A}_h^* . Further let $\chi(\mathcal{S})$ denote the characteristic function of a set $\mathcal{S} \subset \Omega$. We briefly argue that our approximation is useful. In fact, assume that $T \subset \mathcal{A}^*$. Then

$$\|\chi(\mathcal{A}^*) - \chi_h^{\mathcal{A}^*}\|_{0,T} = \left\| \frac{b - u_h^*}{\gamma h^r + b - u_h^*} \right\|_{0,T} \leq \min\{1, \gamma^{-1} h^{-r} \|u^* - u_h^*\|_{0,T}\}$$

which tends to zero whenever $\|u^* - u_h^*\|_{0,T} = \mathcal{O}(h^q)$ with $q > r$. If $T \in \mathcal{I}^*$, then we distinguish two cases:

(i) $T \subset \{b - u_h^* > \gamma h^{\epsilon r}\}$ for some $0 \leq \epsilon < 1$. Then

$$\|\chi(\mathcal{A}^*) - \chi_h^{\mathcal{A}^*}\|_{0,T} = \left\| \frac{\gamma h^r}{\gamma h^r + b - u_h^*} \right\|_{0,T} \leq h^{(1-\epsilon)r} \rightarrow 0 \text{ as } h \rightarrow 0.$$

(ii) Finally, in the case where $T \in \{b - u_h^* \leq \gamma h^{\epsilon r}\}$ we use $T \subset \mathcal{I}^*$ and $\|u^* - u_h^*\|_{0,\Omega} \rightarrow 0$ to conclude that the measure of this set tends to zero as $h \rightarrow 0$.

We therefore use the following approximation of $\chi(\mathcal{C}_1^*)$:

$$\chi(\mathcal{C}_1^*) \approx \chi(\mathcal{I}_h^*) \chi_h^{\mathcal{A}^*} =: \chi_h^{\mathcal{C}_1^*}.$$

In the definition of $\mu_1(\mathcal{C}_1^*)$ we then use

$$\|\chi_h^{\mathcal{C}_1^*}(u_h^* - b)\|_{0,\Omega} \quad \text{instead of} \quad \|u_h^* - b\|_{0,\mathcal{C}_1^*}$$

and analogously for $\|M_h p_h^* - p_h^*\|_{0,\mathcal{C}_1^*}$. Further, the measure of \mathcal{C}_1^* is approximated by

$$\text{meas}(\mathcal{C}_1^*) \approx \int_{\Omega} \chi_h^{\mathcal{C}_1^*} dx.$$

The definition of μ_2 involves the set $\mathcal{C}_2^* = \mathcal{A}_h^* \cap \mathcal{I}^*$. Here we employ the approximation

$$\chi_h^{\mathcal{C}_2^*} := \chi(\mathcal{A}_h^*) \chi_h^{\mathcal{I}^*}$$

with $\chi_h^{\mathcal{I}^*} = 1 - \chi_h^{\mathcal{A}^*}$. Then we replace $\|\lambda_h^*\|_{0,\mathcal{C}_2^*}$ by $\|\chi_h^{\mathcal{C}_2^*} \lambda_h^*\|_{0,\Omega}$, $\|b - \alpha p_h^*\|_{t,\mathcal{C}_2^*}$ by $\|\chi_h^{\mathcal{C}_2^*} (b - \alpha^{-1} p_h^*)\|_{t,\Omega}$, and

$$\text{meas}(\mathcal{C}_2^*) \approx \int_{\Omega} \chi_h^{\mathcal{C}_2^*} dx.$$

The extension of this concept to the bilaterally constrained case is straight forward.

APPENDIX A. A POSTERIORI ESTIMATES IN L^2 -NORM

In this section we derive a posteriori error estimates for $\|p^* - p_h^*\|_{0,\Omega}$ and $\|y^* - y_h^*\|_{0,\Omega}$. The subsequent proof technique is based on a combination of the approaches in [5] and [8].

In what follows we assume that Ω is convex, $b = b_h$ a.e. in Ω , and we use $a(y, w) = (\nabla y, \nabla w)_{0,\Omega}$. Given $u_h^* \in L_h$, by $y(u_h^*)$, $p(u_h^*) \in H_0^1(\Omega)$ we denote the solutions to

$$\begin{aligned} a(y(u_h^*), v) &= (f + u_h^*, v)_{0,\Omega}, \\ a(p(u_h^*), v) &= (z - y(u_h^*), v)_{0,\Omega} \end{aligned}$$

for all $v \in H_0^1(\Omega)$. The Poincaré-Friedrichs inequality yields

$$(53) \quad \|p(u_h^*) - p^*\|_{0,\Omega} \leq c(\Omega) \|y(u_h^*) - y^*\|_{0,\Omega},$$

$$(54) \quad \|y(u_h^*) - y^*\|_{0,\Omega} \leq c(\Omega) \|u_h^* - u^*\|_{0,\Omega},$$

where we assume that $y^* \in H_0^1(\Omega)$ satisfies $a(y^*, v) = (f + u^*, v)_{0,\Omega}$ for all $v \in H_0^1(\Omega)$ and $c(\Omega)$ is a constant depending on the domain Ω only. Hence, for $p^* \in H_0^1(\Omega)$ satisfying $a(p^*, v) = (z - y^*, v)_{0,\Omega}$ for all $v \in H_0^1(\Omega)$ we get

$$(55) \quad \|p^* - p_h^*\|_{0,\Omega} \leq \|p(u_h^*) - p_h^*\|_{0,\Omega} + c(\Omega)^2 \|u_h^* - u^*\|_{0,\Omega}.$$

Next let us assume that u^* respectively u_h^* satisfy the system

$$\alpha u^* - p^* + \lambda^* = 0 \quad \text{and} \quad \alpha u_h^* - M_h p_h^* + \lambda_h^* = 0.$$

Then we obtain

$$\begin{aligned} \alpha \|u^* - u_h^*\|_{0,\Omega}^2 &\leq (\lambda_h^* - \lambda^*, u^* - u_h^*)_{0,\Omega} + (p^* - p_h^*, u^* - u_h^*)_{0,\Omega} \\ &\quad + \frac{\alpha}{4} \|u^* - u_h^*\|_{0,\Omega}^2 + \frac{1}{\alpha} \|p_h^* - M_h p_h^*\|_{0,\Omega}^2 \\ (56) \quad &\leq (p^* - p_h^*, u^* - u_h^*)_{0,\Omega} + \frac{\alpha}{4} \|u^* - u_h^*\|_{0,\Omega}^2 \\ &\quad + \frac{1}{\alpha} \|p_h^* - M_h p_h^*\|_{0,\Omega}^2 \end{aligned}$$

since $(\lambda_h^* - \lambda^*, u^* - u_h^*)_{0,\Omega} \leq 0$. One also has

$$(p^* - p(u_h^*), u^* - u_h^*)_{0,\Omega} \leq 0.$$

Hence, we have

$$\begin{aligned} (p^* - p_h^*, u^* - u_h^*)_{0,\Omega} &\leq (p(u_h^*) - p_h^*, u^* - u_h^*)_{0,\Omega} \\ &\leq \frac{\alpha}{4} \|u^* - u_h^*\|_{0,\Omega}^2 + \frac{1}{\alpha} \|p_h^* - p(u_h^*)\|_{0,\Omega}^2. \end{aligned}$$

This allows us to continue (56):

$$(57) \quad \|u^* - u_h^*\|_{0,\Omega}^2 \leq \frac{2}{\alpha^2} \|p_h^* - p(u_h^*)\|_{0,\Omega}^2 + \frac{2}{\alpha^2} \|p_h^* - M_h p_h^*\|_{0,\Omega}^2$$

Combining the above estimates we result in

$$(58) \quad \|p^* - p_h^*\|_{0,\Omega} \leq \left(1 + \frac{\sqrt{2}}{\alpha} c(\Omega)^2\right) \|p_h^* - p(u_h^*)\|_{0,\Omega} \\ + \frac{\sqrt{2}}{\alpha} c(\Omega)^2 \|p_h^* - M_h p_h^*\|_{0,\Omega},$$

$$(59) \quad \|y^* - y_h^*\|_{0,\Omega} \leq \|y(u_h^*) - y_h^*\|_{0,\Omega} + \frac{\sqrt{2}}{\alpha} c(\Omega) (\|p_h^* - p(u_h^*)\|_{0,\Omega} \\ + \|p_h^* - M_h p_h^*\|_{0,\Omega}).$$

Utilizing standard L^2 -estimates (see, e.g., [8, Proposition 3.8]) we infer

$$(60) \quad \|y(u_h^*) - y_h^*\|_{0,\Omega}^2 \leq C \left(\sum_T h_T^2 \eta_{y,T}^2 + \sum_F h_F^2 \eta_{y,F}^2 \right) =: C \tilde{\eta}_{0,y}^2,$$

$$(61) \quad \|p(u_h^*) - p_h^*\|_{0,\Omega}^2 \leq C \left(\sum_T h_T^2 \tilde{\eta}_{p,T}^2 + \sum_F h_F^2 \eta_{p,F}^2 \right) =: C \tilde{\eta}_{0,p}^2,$$

where the element and edge residuals are given by

$$\begin{aligned} \eta_{y,T} &:= h_T \|f + u_h^*\|_{0,T}, \\ \eta_{y,F} &:= h_F^{1/2} \|n_F \cdot [\nabla y_h^*]\|_{0,F}, \\ \tilde{\eta}_{p,T} &:= h_T \|z - y(u_h^*)\|_{0,T}, \\ \eta_{p,F} &:= h_F^{1/2} \|n_F \cdot [\nabla p_h^*]\|_{0,F} \end{aligned}$$

with n_F denoting the exterior unit normal of T . The triangle inequality yields

$$\sum_T h_T^4 \|z - y(u_h^*)\|_{0,T}^2 \leq C h^2 \tilde{\eta}_{0,y}^2 + 2 \sum_T h_T^2 \eta_{p,T}^2$$

with the element residual

$$\eta_{p,T} := h_T^2 \|z - y_h^*\|_{0,T}.$$

Finally we derive the estimate

$$(62) \quad \|p^* - p_h^*\|_{0,\Omega} \leq C \left(h^2 \tilde{\eta}_{0,y}^2 + \sum_T h_T^2 \eta_{p,T}^2 + \sum_F h_F^2 \eta_{p,F}^2 \right)^{1/2} \\ + \frac{\sqrt{2}}{\alpha} c(\Omega)^2 \|p_h^* - M_h p_h^*\|_{0,\Omega} + \text{osc}_{0,h}(z) + \text{osc}_{0,h}(f) \\ =: C_0^p \eta_{0,p} + \text{osc}_{0,h}(z) + \text{osc}_{0,h}(f),$$

where the data oscillations are given by

$$\begin{aligned} \text{osc}_{0,h}(z) &= \left(\sum_T h_T^2 \text{osc}_T(z)^2 \right)^{1/2}, \\ \text{osc}_T(z) &= h_T \|z - z_h\|_{0,T} \end{aligned}$$

and analogously for $\text{osc}_{0,h}(f)$.

The error in the state is estimated a posteriori by

$$\begin{aligned}
 \|y^* - y_h^*\|_{0,\Omega} &\leq C\tilde{\eta}_{0,y} + \frac{\sqrt{2}}{\alpha}c(\Omega)(\tilde{\eta}_{0,p} + \|p_h^* - M_h p_h^*\|_{0,\Omega}) \\
 (63) \qquad &\quad + \text{osc}_{0,h}(f) + \text{osc}_{0,h}(z) \\
 &=: C_0^y \eta_{0,y} + \text{osc}_{0,h}(f) + \text{osc}_{0,h}(z).
 \end{aligned}$$

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