Certified Reduced Basis Methods for Parametrized Distributed Optimal Control Problems*

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CERTIFIED REDUCED BASIS METHODS FOR PARAMETRIZED DISTRIBUTED OPTIMAL CONTROL PROBLEMS*

MARK KÄRCHER[†], MARTIN A. GREPL[‡], AND KAREN VEROY[§]

Abstract. In this paper, we consider the efficient and reliable solution of distributed optimal control problems governed by parametrized elliptic partial differential equations. The reduced basis method is used as a low-dimensional surrogate model to solve the optimal control problem. To this end, we introduce reduced basis spaces not only for the state and adjoint variable but also for the distributed control variable. We also propose two different error estimation procedures that provide rigorous bounds for the error in the optimal control and the associated cost functional. The reduced basis optimal control problem and associated *a posteriori* error bounds can be efficiently evaluated in an offline-online computational procedure, thus making our approach relevant in the many-query or real-time context. We compare our bounds with a previously proposed bound based on the Banach-Nečas-Babuška (BNB) theory and present numerical results for two model problems: a Graetz flow problem and a heat transfer problem.

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1. Introduction. Many problems in science and engineering can be modeled in terms of optimal control problems governed by parametrized partial differential equations (PDEs), see e.g. [19, 8, 18, 26] for theoretical results and applications. While the PDE describes the underlying system or component behavior, the parameters often serve to identify a particular configuration of the component — such as boundary and initial conditions, material properties, and geometry. In such cases — in addition to solving the optimal control problem itself — one is often interested in exploring many different parameter configurations and thus in speeding up the solution of the optimal control problem. However, using classical discretization techniques such as finite elements or finite volumes even a single solution is often computationally expensive and time-consuming, a parameter-space exploration thus prohibitive. One way to decrease the computational burden is the surrogate model approach, where the original high-dimensional model is replaced by a reduced order approximation. These ideas have received a lot of attention in the past and various model order reduction techniques have been used in this context: proper orthogonal decomposition (POD) e.g. in [16, 1, 17, 27], reduction based on inertial manifolds in [10], and reduced basis methods in [11, 4, 14, 15, 22]. However, the solution of the reduced order optimal control problem is generally suboptimal and reliable error estimation is thus crucial.

In this paper we employ the reduced basis method [23, 24] as a surrogate model for the solution of *distributed* optimal control problems governed by parametrized elliptic partial differential equations. We extend our previous work in [6, 14, 15] in several directions. First, we consider optimal control problems involving distributed controls. Distributed controls pose an additional challenge relative to scalar controls since the

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control space is also high-dimensional. To this end, we follow the approach originally proposed in [12] and introduce reduced basis spaces not only for the state and adjoint variable but also a separate reduced basis (control) space for the distributed control. We thus obtain a considerable dimension reduction of the first-order optimality system. Second, we propose two new *a posteriori* error bounds for the optimal control and associated cost functional. The first proposed bound is an extension of our work in [6, 14] to distributed controls, the second bound is derived directly from the error residual equations of the optimality system. Third, we compare our proposed bounds to the bound recently proposed in [22]. Finally, we show that the reduced order optimal control problem *and* error bounds can be efficiently evaluated in an offline-online computational procedure.

A posteriori error bounds for reduced order solutions of optimal control problems have been proposed for proper orthogonal decomposition (POD) and reduced basis surrogate models in [27] and [4, 22], respectively. In [27], the authors estimate the distance between the computed suboptimal control and the unknown optimal control using a perturbation argument proposed in [7, 20]. The approach allows one to use the POD approximation to efficiently solve the optimal control problem. The evaluation of the *a posteriori* error bounds, however, requires a "forward-backward" solution of the underlying high-dimensional state and adjoint equations and, as pointed out in [27], is thus computationally expensive. Furthermore, in the case of distributed controls there is no reduction of the possibly high-dimensional control space.

In [22], a reduced basis approach to distributed optimal control problems has been considered. The resulting *a posteriori* error bound follows directly from previous work on reduced basis methods for noncoercive problems [28]. However, the development in [28] only provides a combined bound for the error in the state, adjoint, and control variables. Furthermore, the approach requires the computation of (a lower bound to) the parameter-dependent Babuška inf-sup constant of the first-order optimality system, which is not only very expensive in terms of computational cost but also very involved in terms of implementation effort. We compare here the computational effort and performance, i.e., sharpness, of our proposed bounds with the bound from [22] when we discuss numerical results. We observe that our proposed bounds — in contrast to the bound from [22] — involve only constants (or their lower/upper bounds) that are straightforward and inexpensive to compute. Furthermore, numerical results show that the new bound derived from the error residual equations of the optimality system tends to be much sharper, especially in the case of optimal control problems involving small regularization parameters.

This paper is organized as follows. In Section 2 we introduce the optimal control problem: we start with a general (infinite-dimensional) problem statement, state the first order optimality conditions, and derive a finite element (truth) approximation. The reduced basis approximation of the optimal control problem is illustrated in Section 3, where we also explain the associated offline-online computational procedure and briefly summarize the greedy procedure to generate the reduced basis spaces. In Section 4, we discuss the *a posteriori* error estimation procedures. We briefly review the bound from [22] and then propose two new *a posteriori* error bounds for the optimal control and the associated cost functional. Finally, we present numerical results for a Graetz flow problem and a heat transfer problem in Section 5 and offer concluding remarks in Section 6.

2. General Problem Statement and Truth Discretization. In this section we introduce the parametrized linear-quadratic optimal control problem with elliptic PDE constraint and distributed control. We recall the first-order necessary (and in our case sufficient) optimality conditions and introduce a finite element truth discretization for the exact, i.e., continuous problem.

2.1. Preliminaries. Let Y_{e} with $H_0^1(\Omega) \subset Y_{\mathrm{e}} \subset H^1(\Omega)$ be a Hilbert space over the bounded Lipschitz domain $\Omega \subset \mathbb{R}^d, d = 1,2,3$, with boundary Γ.[1] The inner product and induced norm associated with Y_{e} are given by $(\cdot,\cdot)_{Y_{\mathrm{e}}}$ and $\|\cdot\|_{Y_{\mathrm{e}}} = \sqrt{(\cdot,\cdot)_{Y_{\mathrm{e}}}}$, respectively. We assume that the norm $\|\cdot\|_{Y_{\mathrm{e}}}$ is equivalent to the $H^1(\Omega)$-norm and denote the dual space of Y_{e} by Y_{e}'. We also introduce the control Hilbert space U_{e}, together with its reference inner product $(\cdot,\cdot)_{U_{\mathrm{e}}}$, induced reference norm $\|\cdot\|_{U_{\mathrm{e}}} = \sqrt{(\cdot,\cdot)_{U_{\mathrm{e}}}}$, and associated dual space U_{e}'. Furthermore, let $\mathcal{D} \subset \mathbb{R}^P$ be a prescribed P-dimensional compact parameter set in which our P-tuple (input) parameter $\mu = (\mu_1, \ldots, \mu_P)$ resides.

We next introduce the parameter-dependent bilinear form $a(\cdot,\cdot;\mu) : Y_{\mathrm{e}} \times Y_{\mathrm{e}} \to \mathbb{R}$, and shall assume that $a(\cdot,\cdot;\mu)$ is continuous,

$$0 < \gamma_a^{\mathrm{e}}(\mu) = \sup_{w \in Y_{\mathrm{e}} \setminus \{0\}} \sup_{v \in Y_{\mathrm{e}} \setminus \{0\}} \frac{a(w,v;\mu)}{\|w\|_{Y_{\mathrm{e}}} \|v\|_{Y_{\mathrm{e}}}} \leq \gamma_0^a < \infty, \quad \forall \mu \in \mathcal{D},$$

and coercive,

$$\alpha_a^{\mathrm{e}}(\mu) = \inf_{v \in Y_{\mathrm{e}} \setminus \{0\}} \frac{a(v,v;\mu)}{\|v\|_{Y_{\mathrm{e}}}^2} \geq \alpha_0^a > 0, \quad \forall \mu \in \mathcal{D}.$$

Furthermore we introduce the parameter-dependent continuous linear functional $f(\cdot;\mu) : Y_{\mathrm{e}} \to \mathbb{R}$ and the parameter-dependent bilinear form $d(\cdot,\cdot;\mu) : L^2(\Omega) \times L^2(\Omega) \to \mathbb{R}$, where $d(\cdot,\cdot;\mu)$ is continuous, symmetric, and positive semi-definite and hence induces an associated semi-norm $|\cdot|_{D(\mu)} = \sqrt{d(\cdot,\cdot;\mu)}$. Furthermore $c(\cdot,\cdot;\mu) : U_{\mathrm{e}} \times U_{\mathrm{e}} \to \mathbb{R}$ is a parameter-dependent energy inner product on U_{e}. The associated induced energy norm is denoted by $\|\cdot\|_{U_{\mathrm{e}}(\mu)} = \sqrt{c(\cdot,\cdot;\mu)}$ and we assume that it is equivalent to the reference norm $\|\cdot\|_{U_{\mathrm{e}}}$ on U_{e}. We also introduce the parameter-dependent bilinear form $b(\cdot,\cdot;\mu) : U_{\mathrm{e}} \times Y_{\mathrm{e}} \to \mathbb{R}$ and assume that $b(\cdot,\cdot;\mu)$ is continuous,

$$0 < \gamma_b^{\mathrm{e}}(\mu) = \sup_{w \in U_{\mathrm{e}} \setminus \{0\}} \sup_{v \in Y_{\mathrm{e}} \setminus \{0\}} \frac{b(w,v;\mu)}{\|w\|_{U_{\mathrm{e}}(\mu)} \|v\|_{Y_{\mathrm{e}}}} \leq \gamma_0^b < \infty, \quad \forall \mu \in \mathcal{D}.$$

Finally, in anticipation of the optimal control problem defined in Section 2.2, we introduce the parametrized desired state $y_{d,\mathrm{e}}(\mu) \in L^2(\Omega)$.

The involved bilinear and linear forms as well as the desired state are assumed to depend affinely on the parameter, i.e., for all $w, v \in Y_{\mathrm{e}}, u \in U_{\mathrm{e}}$ and all parameters $\mu \in \mathcal{D}$,

$$\begin{aligned}
a(w,v;\mu) &= \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, a^q(w,v), & b(w,v;\mu) &= \sum_{q=1}^{Q_b} \Theta_b^q(\mu)\, b^q(w,v), \\
d(w,v;\mu) &= \sum_{q=1}^{Q_d} \Theta_d^q(\mu)\, d^q(w,v), & c(w,v;\mu) &= \sum_{q=1}^{Q_c} \Theta_c^q(\mu)\, c^q(w,v), \\
f(v;\mu) &= \sum_{q=1}^{Q_f} \Theta_f^q(\mu)\, f^q(v), & y_{d,\mathrm{e}}(x;\mu) &= \sum_{q=1}^{Q_{yd}} \Theta_{yd}^q(\mu)\, y_{d,\mathrm{e}}^q(x),
\end{aligned} \tag{2.1}$$

[1]The subscripts and superscripts “e” denote “exact”.

for some (preferably) small integers Q_a, Q_b, Q_c, Q_d, Q_f, and Q_{yd}. Here, the coefficient functions $\Theta_*^q(\cdot) : \mathcal{D} \to \mathbb{R}$, are continuous and depend on μ, but the continuous bilinear forms $a^q(\cdot,\cdot) : Y_\mathrm{e} \times Y_\mathrm{e} \to \mathbb{R}$, $b^q(\cdot,\cdot) : U_\mathrm{e} \times Y_\mathrm{e} \to \mathbb{R}$, $d^q(\cdot,\cdot) : L^2(\Omega) \times L^2(\Omega) \to \mathbb{R}$, $c^q(\cdot,\cdot) : U_\mathrm{e} \times U_\mathrm{e} \to \mathbb{R}$, as well as the continuous linear forms $f^q : Y_\mathrm{e} \to \mathbb{R}$ and $y_{d,\mathrm{e}}^q \in L^2(\Omega)$ do *not* depend on μ.

2.2. General Problem Statement. We consider the parametrized optimal control problem[2]

$$(\mathrm{P_e}) \qquad \min_{y_\mathrm{e} \in Y_\mathrm{e}, u_\mathrm{e} \in U_\mathrm{e}} J_\mathrm{e}(y_\mathrm{e}, u_\mathrm{e}; \mu)$$
$$\text{s.t.} \quad (y_\mathrm{e}, u_\mathrm{e}) \in Y_\mathrm{e} \times U_\mathrm{e} \quad \text{solves} \quad a(y_\mathrm{e}, v; \mu) = b(u_\mathrm{e}, v; \mu) + f(v; \mu), \quad \forall v \in Y_\mathrm{e},$$

where the quadratic cost functional, $J_\mathrm{e}(\cdot,\cdot;\mu) : Y_\mathrm{e} \times U_\mathrm{e} \to \mathbb{R}$ is given by

$$J_\mathrm{e}(y, u; \mu) = \frac{1}{2} |y - y_{d,\mathrm{e}}(\mu)|^2_{D(\mu)} + \frac{\lambda}{2} \|u - u_{d,\mathrm{e}}\|^2_{U(\mu)}.$$

Here, $y_{d,\mathrm{e}}(\mu) \in L^2(\Omega), \forall \mu \in \mathcal{D}$ is the desired state and $u_{d,\mathrm{e}} \in U_\mathrm{e}$ is the desired control. The regularization parameter $\lambda > 0$ governs the trade-off between the cost associated with the deviation from the desired state and the desired control, respectively. For simplicity, we assume that the desired control $u_{d,\mathrm{e}}$ is parameter-independent; however, (affine) parameter dependence is readily admitted.

It follows from our assumptions that there exists a unique optimal solution $(y_\mathrm{e}^*, u_\mathrm{e}^*)$ to $(\mathrm{P_e})$ [19]. Employing a Lagrangian approach, we obtain the first-order optimality system consisting of the state equation, the adjoint equation, and the optimality equation: Given $\mu \in \mathcal{D}$, the optimal solution $(y_\mathrm{e}^*, p_\mathrm{e}^*, u_\mathrm{e}^*) \in Y_\mathrm{e} \times Y_\mathrm{e} \times U_\mathrm{e}$ satisfies[3]

$$a(y_\mathrm{e}^*, \phi; \mu) = b(u_\mathrm{e}^*, \phi; \mu) + f(\phi; \mu), \qquad \forall \phi \in Y_\mathrm{e}, \tag{2.2a}$$
$$a(\varphi, p_\mathrm{e}^*; \mu) = d(y_{d,\mathrm{e}}(\mu) - y_\mathrm{e}^*, \varphi; \mu), \qquad \forall \varphi \in Y_\mathrm{e}, \tag{2.2b}$$
$$\lambda\, c(u_\mathrm{e}^* - u_{d,\mathrm{e}}, \psi; \mu) - b(\psi, p_\mathrm{e}^*; \mu) = 0, \qquad \forall \psi \in U_\mathrm{e}. \tag{2.2c}$$

Here, p_e is the adjoint variable and the superscript * denotes optimality.

We note that for the linear-quadratic optimal control problem $(\mathrm{P_e})$ the first-order conditions (2.2) are necessary and sufficient for the optimality of $(y_\mathrm{e}^*, u_\mathrm{e}^*)$ [19].

Remark 2.1. In practice, the regularization parameter often serves as a design parameter which is tuned to achieve a desired performance of the optimal controller. From a reduced basis point of view, however, the regularization parameter may simply be considered an input parameter of the parametrized optimal control problem. This allows us to vary λ online and thus to efficiently design the optimal controller as discussed in the context of parabolic optimal control problems in [15].

2.3. Truth Approximation. In general, we of course cannot expect to find an analytic solution to (2.2). We thus replace the infinite-dimensional trial space Y_e and the control space U_e for the PDE constraint by "truth" finite element approximation spaces $Y \subset Y_\mathrm{e}$ and $U \subset U_\mathrm{e}$ of typically very large dimension $\mathcal{N} = \dim(Y)$ and $\mathcal{M} = \dim(U)$, respectively. Note that Y shall inherit the inner product and norm from Y_e: $(\cdot,\cdot)_Y = (\cdot,\cdot)_{Y_\mathrm{e}}$ and $\|\cdot\|_Y = \|\cdot\|_{Y_\mathrm{e}}$; analogously, $(\cdot,\cdot)_U = (\cdot,\cdot)_{U_\mathrm{e}}$ and $\|\cdot\|_U = \|\cdot\|_{U_\mathrm{e}}$.

[2] Here and in the following we often omit the dependence on μ to simplify notation.

[3] We again note that we omit the dependence on μ to simplify notation, i.e., we write $y_\mathrm{e} = y_\mathrm{e}(\mu)$, $p_\mathrm{e} = p_\mathrm{e}(\mu)$, and $u_\mathrm{e} = u_\mathrm{e}(\mu)$.

We shall assume that the truth spaces Y and U are sufficiently rich such that $y(\mu)$ and $y_{\mathrm{e}}(\mu)$ as well as $u(\mu)$ and $u_{\mathrm{e}}(\mu)$ are in practice indistinguishable. We further recall that the reduced basis approximation shall be built upon – and the reduced basis error thus evaluated with respect to – the truth solution $y(\mu) \in Y$ and $u(\mu) \in U$.

Clearly, the continuity and coercivity properties of the bilinear form a are inherited by the truth approximation, i.e.,

$$\gamma_a(\mu) = \sup_{w \in Y \setminus \{0\}} \sup_{v \in Y \setminus \{0\}} \frac{a(w, v; \mu)}{\|w\|_Y \|v\|_Y} \leq \gamma_a^{\mathrm{e}}(\mu) \leq \gamma_0^a < \infty, \quad \forall \mu \in \mathcal{D},$$

and

$$\alpha_a(\mu) = \inf_{v \in Y \setminus \{0\}} \frac{a(v, v; \mu)}{\|v\|_Y^2} \geq \alpha_a^{\mathrm{e}}(\mu) \geq \alpha_0^a > 0, \quad \forall \mu \in \mathcal{D}. \tag{2.3}$$

Similarly, it follows that

$$\gamma_b(\mu) = \sup_{w \in U \setminus \{0\}} \sup_{v \in Y \setminus \{0\}} \frac{b(w, v; \mu)}{\|w\|_{U(\mu)} \|v\|_Y} \leq \gamma_b^{\mathrm{e}}(\mu) \leq \gamma_0^b < \infty, \quad \forall \mu \in \mathcal{D}.$$

The discretized cost functional, $J(\cdot, \cdot; \mu) : Y \times U \to \mathbb{R}$ is given by

$$J(y, u; \mu) = \frac{1}{2} |y - y_d(\mu)|_{D(\mu)}^2 + \frac{\lambda}{2} \|u - u_d\|_{U(\mu)}^2.$$

Here, $y_d(\mu) = \sum_{q=1}^{Q_{yd}} \Theta_{yd}^q(\mu) y_d^q \in Y$ where $y_d^q \in Y,\ 1 \leq q \leq Q_{yd}$, and $u_d \in U$ are suitable approximations of $y_{d,\mathrm{e}}^q,\ 1 \leq q \leq Q_{yd}$, and $u_{d,\mathrm{e}}$, respectively. The corresponding truth optimal control problem is then given by

$$\text{(P)} \qquad \begin{aligned} &\min_{y \in Y, u \in U} J(y, u; \mu) \\ &\text{s.t.} \quad (y, u) \in Y \times U \quad \text{solves} \quad a(y, v; \mu) = b(u, v; \mu) + f(v; \mu), \quad \forall v \in Y. \end{aligned}$$

The associated first-order optimality system reads: Given $\mu \in \mathcal{D}$, the optimal solution $(y^*, p^*, u^*) \in Y \times Y \times U$ satisfies

$$a(y^*, \phi; \mu) = b(u^*, \phi; \mu) + f(\phi; \mu), \qquad \forall \phi \in Y, \tag{2.4a}$$

$$a(\varphi, p^*; \mu) = d(y_d(\mu) - y^*, \varphi; \mu), \qquad \forall \varphi \in Y, \tag{2.4b}$$

$$\lambda\, c(u^* - u_d, \psi; \mu) - b(\psi, p^*; \mu) = 0, \qquad \forall \psi \in U. \tag{2.4c}$$

We note that the trial and test spaces are identical for the state and adjoint equations. The "first-discretize-then-optimize" and "first-optimize-then-discretize" approach commute in this setting and hence lead to the same discretization of the optimality system (2.4), see for example [8].

The optimality system (2.4) constitutes a coupled set of equations of dimension $2\mathcal{N} + \mathcal{M}$ and is thus expensive to solve, especially if one is interested in various values of $\mu \in \mathcal{D}$. Our goal is therefore to significantly speed up the solution of (2.4) by employing the reduced basis approximation as a surrogate model for the PDE constraint in (P).

3. Reduced Basis Approximation. We will now employ the reduced basis method for the efficient solution of the truth optimal control problem (P). We first assume that we are given the greedily selected sample sets $S_M = \{\mu^1, \ldots, \mu^M\}, 1 \leq M \leq M_{\max}$, and associated integrated reduced basis spaces

$$
\begin{aligned}
Y_N &= \operatorname{span}\{\zeta_n^y,\ 1 \leq n \leq N = 2M\} \\
&= \operatorname{span}\{y^*(\mu^n), p^*(\mu^n),\ 1 \leq n \leq M\}, \quad 1 \leq M \leq M_{\max},
\end{aligned} \tag{3.1}
$$

where $y^*(\mu^n)$ and $p^*(\mu^n)$ are the solutions of (2.4) and $\zeta_n^y,\ 1 \leq n \leq N$, are mutually $(\cdot,\cdot)_Y$-orthogonal basis functions derived by a Gram-Schmidt orthogonalization procedure. Note that we integrate both state and adjoint snapshots in Y_N; thus the term "integrated." We refer to [14, 15, 22] for further details and discussion on the use of integrated spaces for the state and adjoint equations. Furthermore we assume that the reduced basis control spaces are given by

$$
U_M = \operatorname{span}\{\zeta_n^u,\ 1 \leq n \leq M\} = \operatorname{span}\{u^*(\mu^n),\ 1 \leq n \leq M\},\ 1 \leq M \leq M_{\max}. \tag{3.2}
$$

Here, the $\zeta_n^u,\ 1 \leq n \leq M$, are mutually $(\cdot,\cdot)_U$-orthogonal basis functions. We comment on the greedy sampling procedure to construct the spaces Y_N and U_M in Section 3.2.

We next replace the truth approximation of the PDE constraint in (P) by its reduced basis approximation. The reduced basis optimal control problem is thus given by

$$
(\mathrm{P_N}) \qquad \min_{y_N \in Y_N, u_M \in U_M} J(y_N, u_N; \mu)
$$

$$
\text{s.t.} \quad (y_N, u_M) \in Y_N \times U_M \quad \text{solves} \quad a(y_N, v; \mu) = b(u_M, v; \mu) + f(v; \mu), \quad \forall v \in Y_N.
$$

We can also directly state the associated first-order optimality system: Given $\mu \in \mathcal{D}$, find $(y_N^*, p_N^*, u_M^*) \in Y_N \times Y_N \times U_M$ such that

$$
a(y_N^*, \phi; \mu) = b(u_M^*, \phi; \mu) + f(\phi; \mu), \qquad \forall \phi \in Y_N, \tag{3.3a}
$$

$$
a(\varphi, p_N^*; \mu) = d(y_d(\mu) - y_N^*, \varphi; \mu), \qquad \forall \varphi \in Y_N, \tag{3.3b}
$$

$$
\lambda\, c(u_M^* - u_d, \psi; \mu) - b(\psi, p_N^*; \mu) = 0, \qquad \forall \psi \in U_M. \tag{3.3c}
$$

The reduced basis optimality system is only of dimension $2N + M$ and can be evaluated efficiently using an offline-online computational decomposition. The details are presented in the next subsection. We also note that — similar to the discussion in the last section — the "first-reduce-then-optimize" and "first-optimize-then-reduce" approach commute since the state and adjoint trial and test spaces are identical.

3.1. Computational Procedure. We now turn to the computational details of the reduced basis approximation of the optimality system. To this end, we express the reduced basis state, adjoint and control solutions as $y_N(\mu) = \sum_{i=1}^N y_{Ni}(\mu)\zeta_i^y$, $p_N(\mu) = \sum_{i=1}^N p_{Ni}(\mu)\zeta_i^y$ and $u_M(\mu) = \sum_{i=1}^M u_{Mi}(\mu)\zeta_i^u$, and denote the coefficient vectors by $\underline{y}_N(\mu) = [y_{N1}(\mu), \ldots, y_{NN}(\mu)]^T \in \mathbb{R}^N$, $\underline{p}_N(\mu) = [p_{N1}(\mu), \ldots, p_{NN}(\mu)]^T \in \mathbb{R}^N$ and $\underline{u}_M(\mu) = [u_{M1}(\mu), \ldots, u_{MM}(\mu)]^T \in \mathbb{R}^M$, respectively. If we choose as test functions $\phi = \zeta_i^y,\ 1 \leq i \leq N$, $\varphi = \zeta_i^y,\ 1 \leq i \leq N$, and $\psi = \zeta_i^u,\ 1 \leq i \leq M$, in (3.3), the reduced basis optimality system can be expressed in terms of the $(2N+M)\times(2N+M)$ linear system

$$
\begin{bmatrix} D_N(\mu) & 0 & A_N(\mu)^T \\ 0 & \lambda C_M(\mu) & -B_{N,M}(\mu)^T \\ A_N(\mu) & -B_{N,M}(\mu) & 0 \end{bmatrix}
\begin{bmatrix} \underline{y}_N \\ \underline{u}_M \\ \underline{p}_N \end{bmatrix}
=
\begin{bmatrix} Y_{d,N}(\mu) \\ \lambda U_{d,M}(\mu) \\ F_N(\mu) \end{bmatrix}. \tag{3.4}
$$

Here, we have reordered the variables and equations to exhibit the saddle point structure of the system. The matrices $A_N(\mu) \in \mathbb{R}^{N\times N}$, $B_{N,M}(\mu) \in \mathbb{R}^{N\times M}$, $D_N(\mu) \in \mathbb{R}^{N\times N}$, and $C_M(\mu) \in \mathbb{R}^{M\times M}$ are defined through the entries $(A_N(\mu))_{ij} = a(\zeta_j^y, \zeta_i^y; \mu)$, $1 \le i,j \le N$, $(B_{N,M}(\mu))_{ij} = b(\zeta_j^u, \zeta_i^y; \mu)$, $1 \le i \le N$, $1 \le j \le M$, $(D_N(\mu))_{ij} = d(\zeta_j^y, \zeta_i^y; \mu)$, $1 \le i,j \le N$, and $(C_M(\mu))_{ij} = c(\zeta_j^u, \zeta_i^u; \mu)$, $1 \le i,j \le M$, respectively. The vectors $F_N(\mu) \in \mathbb{R}^N$, $Y_{d,N}(\mu) \in \mathbb{R}^N$, and $U_{d,M}(\mu) \in \mathbb{R}^M$ are given by $(F_N(\mu))_i = f(\zeta_i^y; \mu)$, $1 \le i \le N$, $(Y_{d,N}(\mu))_i = d(y_d(\mu), \zeta_i^y; \mu)$, $1 \le i \le N$, and $(U_{d,M}(\mu))_i = c(u_d, \zeta_i^u; \mu)$, $1 \le i \le M$, respectively.

Invoking the affine parameter dependence (2.1) yields the expansion $A_N(\mu) = \sum_{q=1}^{Q_a} \Theta_a^q(\mu) A_N^q$, where the parameter-independent matrices $A_N^q \in \mathbb{R}^{N\times N}$ are given by $(A_N^q)_{ij} = a^q(\zeta_j^y, \zeta_i^y)$, $1 \le i,j \le N$, $1 \le q \le Q_a$. The matrices $B_{N,M}(\mu)$, $D_N(\mu)$, $C_M(\mu)$ and vectors $F_N(\mu)$, $Y_{d,N}(\mu)$, and $U_{d,M}(\mu)$ yield a similar expansion. Finally, to allow an efficient evaluation of the cost functional in the online stage, we also save the three-dimensional tensor $Y_{d,d}$ given by $(Y_{d,d})_{q,p,r} = d^q(y_d^p, y_d^r)$, $1 \le q \le Q_d$, $1 \le p \le Q_{yd}$, $1 \le r \le Q_{yd}$, as well as the vector $(U_{d,d})_q = c^q(u_d, u_d)$, $1 \le q \le Q_c$.

The offline-online decomposition is now clear. In the offline stage — performed only *once* — we first construct the reduced basis spaces Y_N and U_M. We then assemble the parameter-independent quantities A_N^q, $1 \le q \le Q_a$, $B_{N,M}^q$, $1 \le q \le Q_b$, D_N^q, $1 \le q \le Q_d$, C_M^q, $1 \le q \le Q_c$, F_N^q, $1 \le q \le Q_f$, $Y_{d,N}^q$, $1 \le q \le Q_d Q_{yd}$, $U_{d,M}^q$, $1 \le q \le Q_c$, $Y_{d,d}$ and $U_{d,d}$. The computational cost clearly depends on the truth finite element dimensions $\mathcal{N}$ and $\mathcal{M}$. In the online stage — for each new parameter value μ — we first assemble all parameter-dependent quantities in $\mathcal{O}((Q_a + Q_d)N^2 + Q_b NM + Q_c M^2 + (Q_f + Q_d Q_{yd})N + Q_c M + Q_d Q_{yd}^2 + Q_c)$ operations. We then solve the reduced basis optimality system (3.4) at cost $\mathcal{O}((2N+M)^3)$. Given the reduced basis optimal solution, the cost functional can then be evaluated efficiently from

$$
\begin{aligned}
J(y_N, u_M; \mu) =& \frac{1}{2}\left(\underline{y}_N^T D_N(\mu) \underline{y}_N - 2 Y_{d,N}(\mu)^T \underline{y}_N + Y_{d,d}(\mu)\right) \\
&+ \frac{\lambda}{2}\left(\underline{u}_M^T C_M(\mu) \underline{u}_M - 2 U_{d,M}(\mu)^T \underline{u}_M + U_{d,d}(\mu)\right),
\end{aligned}
$$

where we assemble $Y_{d,d}(\mu) = \sum_{q=1}^{Q_d} \sum_{p=1}^{Q_{yd}} \sum_{r=1}^{Q_{yd}} \Theta_d^q(\mu) \Theta_{yd}^p(\mu) \Theta_{yd}^r(\mu) (Y_{d,d})_{q,p,r}$ and $U_{d,d}(\mu) = \sum_{q=1}^{Q_c} \Theta_c^q(\mu) (U_{d,d})_q$. The computational cost for the cost functional evaluation (without assembly of the parameter-dependent quantities) is $\mathcal{O}(N^2)$ for the state misfit term plus $\mathcal{O}(M^2)$ for the control misfit term. Hence, the overall computational cost for the online stage is independent of $\mathcal{N}$ and $\mathcal{M}$, the dimensions of the underlying "truth" finite element approximation spaces. Since $N \ll \mathcal{N}$ and $M \ll \mathcal{M}$, we expect significant computational savings in the online stage relative to the solution of (2.4). However, we need to rigorously and efficiently assess the error introduced.

3.2. Greedy Algorithm. We generate the reduced basis space using the greedy sampling procedure [28] summarized in Algorithm 1. To this end, we presume the existence of an *a posteriori* error bound $\Delta_N(\mu)$ — to be introduced in the next section — for the optimal control or the associated cost functional. Furthermore, $\Xi_{\text{train}} \subset \mathcal{D}$ is a finite but suitably large parameter train sample; $\mu^1 \in \Xi_{\text{train}}$ is the initial parameter value; and $\epsilon_{\text{tol,min}} > 0$ is a prescribed desired error tolerance. Note that we expand the reduced basis spaces Y_N in step 6 with a snapshot of the corresponding truth state and adjoint equation, i.e., we use "integrated" spaces as discussed previously. Also note that we simultaneously reduce the control space, i.e., U_M is spanned by snapshots of the truth optimal control at the selected parameter values.

Algorithm 1 Greedy Sampling Procedure

1: Choose $\Xi_{\text{train}} \subset \mathcal{D}$, $\mu^1 \in \Xi_{\text{train}}$ (arbitrary), and $\epsilon_{\text{tol,min}} > 0$
2: Set $N \leftarrow 0, M \leftarrow 0$, $Y_N \leftarrow \{\}, U_M \leftarrow \{\}$
3: Set $\mu^* \leftarrow \mu^1$ and $\Delta_N(\mu^*) \leftarrow \infty$
4: **while** $\Delta_N(\mu^*) > \epsilon_{\text{tol,min}}$ **do**
5: $\quad N \leftarrow N+2, M \leftarrow M+1$
6: $\quad Y_N \leftarrow Y_{N-2} \oplus \text{span}\{\, y(\mu^*), p(\mu^*)\,\}$
7: $\quad U_M \leftarrow U_{M-1} \oplus \text{span}\{\, u(\mu^*)\,\}$
8: $\quad \mu^* \leftarrow \arg\max\limits_{\mu \in \Xi_{\text{train}}} \Delta_N(\mu)$
9: **end while**
10: $N_{\max} \leftarrow N, M_{\max} \leftarrow M$

4. A Posteriori Error Estimation. We next turn to the *a posteriori* error estimation procedure. We consider three different error bounds for the optimal control in Section 4.2 and subsequently derive associated cost functional error bounds in Section 4.3. The error bounds introduced are rigorous upper bounds for the errors and are online-efficient to compute; we summarize the computational procedure in Section 4.4.

4.1. Preliminaries. To begin, we assume that we are given a positive lower bound $\alpha_a^{\text{LB}}(\mu) : \mathcal{D} \to \mathbb{R}_+$ for the coercivity constant $\alpha_a(\mu)$ defined in (2.3) such that

$$0 < \alpha_0^a \leq \alpha_a^{\text{LB}}(\mu) \leq \alpha_a(\mu), \quad \forall \mu \in \mathcal{D}. \tag{4.1}$$

Furthermore, we assume that we have upper bounds available for the constant

$$C_D^{\text{UB}}(\mu) \geq C_D(\mu) \equiv \sup_{v \in Y \setminus \{0\}} \frac{|v|_{D(\mu)}}{\|v\|_Y} \geq 0, \quad \forall \mu \in \mathcal{D}, \tag{4.2}$$

and the continuity constant of the bilinear form $b(\cdot,\cdot;\mu)$

$$\gamma_b^{\text{UB}}(\mu) \geq \gamma_b(\mu), \quad \forall \mu \in \mathcal{D}. \tag{4.3}$$

It is possible to compute these constants (or their bounds) efficiently in terms of an offline-online procedure; see Section 4.4 for details. We also require

Definition 4.1. *The residuals of the state equation, the adjoint equation, and the optimality equation are defined by*

$$r_y(\phi;\mu) = f(\phi;\mu) + b(u_M^*, \phi;\mu) - a(y_N^*, \phi;\mu), \qquad \forall \phi \in Y, \quad \forall \mu \in \mathcal{D}, \tag{4.4}$$
$$r_p(\varphi;\mu) = d(y_d(\mu) - y_N^*, \varphi;\mu) - a(\varphi, p_N^*;\mu), \qquad \forall \varphi \in Y, \quad \forall \mu \in \mathcal{D}, \tag{4.5}$$
$$r_u(\psi;\mu) = b(\psi, p_N^*;\mu) - \lambda\, c(u_M^* - u_d, \psi;\mu), \qquad \forall \psi \in U, \quad \forall \mu \in \mathcal{D}. \tag{4.6}$$

4.2. Control Error Bounds. We now consider three different *a posteriori* error bounds for the optimal control. We start with a bound based on the Banach-Nečas-Babuška (BNB) theory [5] which was first used in [28] for reduced basis approximations to noncoercive problems and in [22] in the context of optimal control problems. We briefly recall the result here since we compare the BNB-bound with the two new error bounds introduced afterwards: the first is based on a perturbation approach proposed in [27], and the second is directly derived from the error residual equations of the optimality system.

4.2.1. Banach-Nečas-Babuška Approach (BNB). By rearranging the equations of the truth optimality system (2.4) we identify its saddle-point structure: Given $\mu \in \mathcal{D}$, find $x^* = (y^*, u^*, p^*) \in X = Y \times U \times Y$ such that

$$\begin{array}{llllllllll}
\text{(4.7a)} & d(y^*,\varphi;\mu) & + & 0 & + & a(\varphi,p^*;\mu) & = & d(y_d(\mu),\varphi;\mu), & \forall \varphi \in Y,\\
\text{(4.7b)} & 0 & + & \lambda\, c(u^*,\psi;\mu) & - & b(\psi,p^*;\mu) & = & \lambda\, c(u_d,\psi;\mu), & \forall \psi \in U,\\
\text{(4.7c)} & a(y^*,\phi;\mu) & - & b(u^*,\phi;\mu) & + & 0 & = & f(\phi;\mu), & \forall \phi \in Y.
\end{array}$$

For $x = (y, u, p) \in X$ and $\vartheta = (\varphi, \psi, \phi) \in X$, we introduce the bilinear form $K(\cdot,\cdot;\mu) : X \times X \to \mathbb{R}$ and the linear functional $F(\cdot;\mu) : X \to \mathbb{R}$ as

$$\begin{aligned}
K(x,\vartheta;\mu) &= d(y,\varphi;\mu) + a(\varphi,p;\mu) + \lambda\, c(u,\psi;\mu) - b(\psi,p;\mu) + a(y,\phi;\mu) - b(u,\phi;\mu),\\
F(\vartheta;\mu) &= d(y_d(\mu),\varphi;\mu) + \lambda\, c(u_d,\psi;\mu) + f(\phi;\mu).
\end{aligned}$$

We can then express (4.7) compactly via: find $x^* \in X$ such that

$$K(x^*,\vartheta;\mu) = F(\vartheta;\mu), \quad \forall \vartheta \in X.$$

For the optimal reduced basis solution $x_N^* = (y_N^*, u_M^*, p_N^*)$ of (3.3) the corresponding residual is given by

$$r_x(\vartheta;\mu) = F(\vartheta;\mu) - K(x_N^*,\vartheta;\mu) = r_y(\phi;\mu) + r_p(\varphi;\mu) + r_u(\psi;\mu), \quad \forall \vartheta \in X.$$

We now have all necessary ingredients and can state the standard BNB-bound (for a proof see [28, 25]).

PROPOSITION 4.2. *Let x^* and x_N^* be the optimal solutions to the truth and reduced basis optimal control problems, respectively. The error in the optimality triple satisfies*

$$\|x^* - x_N^*\|_X \le \Delta_N^{x,\mathrm{BNB}}(\mu) \equiv \frac{\|r_x(\cdot;\mu)\|_{X'}}{\beta_{\mathrm{Ba}}^{\mathrm{LB}}(\mu)}, \quad \forall \mu \in \mathcal{D}, \tag{4.8}$$

where $\beta_{\mathrm{Ba}}^{\mathrm{LB}}(\mu)$ is a lower bound of the inf-sup constant

$$\beta_{\mathrm{Ba}}(\mu) = \inf_{\vartheta \in X\setminus\{0\}} \sup_{x \in X\setminus\{0\}} \frac{K(x;\vartheta;\mu)}{\|x\|_X\, \|\vartheta\|_X},$$

and $\|\cdot\|_X$ is a given norm on X.

We make several remarks. First, we note that this is just the standard result for reduced basis approximations of noncoercive problems [28], which was used in [22] for reduced basis approximations of parametrized optimal control problems. Second, there is a certain freedom of choice on how to define the inner product and associated norm on X; we specify and compare two options when discussing numerical results in Section 5. Third, since $\|u^* - u_M^*\|_U \le C_{U,X} \|x^* - x_N^*\|_X$, the bound $\Delta_N^{x,\mathrm{BNB}}(\mu)$ can also be used to bound the error in the optimal control. We thus define $\Delta_N^{u,\mathrm{BNB}}(\mu) \equiv C_{U,X} \Delta_N^{x,\mathrm{BNB}}(\mu)$ for notational convenience. And finally, the computation of a lower bound of the inf-sup constant $\beta_{\mathrm{Ba}}(\mu)$ requires very large offline effort as discussed in the numerical results stated in [22].

4.2.2. Perturbation Approach (PER). The perturbation approach was originally proposed in [27] for POD approximations to optimal control problems. Based on this work, we developed rigorous *and* efficient reduced basis control error bounds in different contexts, i.e., for elliptic problems with scalar controls in [6, 14] and for parabolic problems in [15]. Here, we extend this work to problems involving distributed controls, also see [12]. The derivation is based on the following result from [27] (see Theorem 4.11 in [27] for the proof).

THEOREM 4.3. *Let u^* and u^*_M be the optimal solutions to the truth and reduced basis optimal control problems* (P) *and* ($\mathrm{P_N}$)*, respectively. The error in the optimal control then satisfies*

$$\|u^* - u^*_M\|_{U(\mu)} \le \Delta_N^{u,TV}(\mu) \equiv \frac{1}{\lambda}\|\lambda(u^*_M - u_d) - \mathcal{B}^\star p\,(y(u^*_M))\|_{U(\mu)}, \quad \forall \mu \in \mathcal{D}, \tag{4.9}$$

where $\mathcal{B}^\star : Y \to U$ is the adjoint operator defined by

$$b(\psi, \phi; \mu) = (\psi, \mathcal{B}^\star \phi)_{U(\mu)}, \quad \forall \psi \in U,\ \phi \in Y, \quad \forall \mu \in \mathcal{D}. \tag{4.10}$$

Note that the error bound measures the error in the energy control norm $\|\cdot\|_{U(\mu)}$, which is the more relevant norm for parametrized geometries, e.g. $U^{\mathrm{e}}(\mu) = L^2(\Omega(\mu))$. Furthermore for the sake of exposition we assume that the adjoint operator $\mathcal{B}^\star$ itself is parameter-independent, i.e. the parameter-dependence of $b(\cdot,\cdot;\mu)$ is caused only through the presence of the parameter-dependent inner product $(\cdot,\cdot)_{U(\mu)}$ in its definition. This assumption is satisfied by all numerical examples in this paper. However an extension to parameter-dependent $\mathcal{B}^\star$ is possible and straightforward. For the following error bound derivation we will need to compute the parameter-dependent constant (or an upper bound)

$$\|\mathcal{B}^\star\|_{Y\to U(\mu)} \equiv \sup_{\phi\in Y\setminus\{0\}} \frac{\|\mathcal{B}^\star\phi\|_{U(\mu)}}{\|\phi\|_Y},$$

such that $\|\mathcal{B}^\star\phi\|_{U(\mu)} \le \|\mathcal{B}^\star\|_{Y\to U(\mu)}\|\phi\|_Y$ holds for all $\phi \in Y$. Since

$$\|\mathcal{B}^\star\phi\|_{U(\mu)} = \sup_{\psi\in U\setminus\{0\}} \frac{(\mathcal{B}^\star\phi,\psi)_{U(\mu)}}{\|\psi\|_{U(\mu)}} = \sup_{\psi\in U\setminus\{0\}} \frac{b(\psi,\phi;\mu)}{\|\psi\|_{U(\mu)}},$$

by Cauchy-Schwarz and (4.10) it follows that $\|\mathcal{B}^\star\|_{Y\to U(\mu)} = \gamma_b(\mu)$.

We further note that $y(u^*_M)$ is the solution of the (truth) state equation (2.4a) with control u^*_M instead of u^*, and $p\,(y(u^*_M))$ is the solution of the (truth) adjoint equation (2.4b) with $y(u^*_M)$ instead of $y^*(u^*)$ on the right-hand side. Evaluation of the bound (4.9) thus requires a consecutive solution of both state and adjoint truth approximations and is computationally expensive. In contrast, the bound developed in the following is online-efficient, i.e, its evaluation is independent of $\mathcal{N}$ and $\mathcal{M}$. The underlying idea is to replace the truth approximation $p(y(u^*_M))$ in (4.9) with the reduced basis approximation $p^*_N(y^*_N(u^*_M))$ and to bound the error term $p(y(u^*_M)) - p^*_N(y^*_N(u^*_M))$.

Before we continue, let us make some notational remarks. Following the notation and terminology in [4], we refer to $\tilde{e}^y = y(u^*_M) - y^*_N(u^*_M)$ as the state predictability error and to $\tilde{e}^p = p(y(u^*_M)) - p^*_N(y^*_N(u^*_M))$ as the adjoint predictability error. They reflect the ability of the corresponding reduced basis solutions to approximate the truth state and adjoint solutions for a prescribed control. In contrast, we define the state, adjoint, and control optimality errors as $e^{y,*} = y^*(u^*) - y_N^*(u_M^*)$, $e^{p,*} = p^*(y^*(u^*)) - p_N^*(y_N^*(u_M^*))$, and $e^{u,*} = u^* - u_M^*$, respectively. Before turning to the bound for the optimal control we require two intermediate results for the state and adjoint predictability errors.

LEMMA 4.4. *The state predictability error, $\tilde{e}^y = y(u_M^*) - y_N^*(u_M^*)$, is bounded by*

$$\|\tilde{e}^y\|_Y \le \tilde{\Delta}_N^y(\mu) \equiv \frac{\|r_y(\cdot;\mu)\|_{Y'}}{\alpha_a^{\mathrm{LB}}(\mu)}, \quad \forall \mu \in \mathcal{D}, \tag{4.11}$$

where $y_N^*(u_M^*)$ is the solution of (3.3a) *and $y(u_M^*)$ is the solution of the truth state equation* (2.4a) *with control u_M^*.*

This is the standard *a posteriori* error bound for coercive elliptic PDEs [23].

LEMMA 4.5. *The adjoint predictability error, $\tilde{e}^p = p(y(u_M^*)) - p_N^*(y_N^*(u_M^*))$, is bounded by*

$$\|\tilde{e}^p\|_Y \le \tilde{\Delta}_N^p(\mu) \equiv \frac{1}{\alpha_a^{\mathrm{LB}}(\mu)} \Big(\|r_p(\cdot;\mu)\|_{Y'} + C_D^{\mathrm{UB}}(\mu)^2\, \tilde{\Delta}_N^y(\mu) \Big), \quad \forall \mu \in \mathcal{D}, \tag{4.12}$$

where $p_N^*(y_N^*(u_M^*))$ is the solution of (3.3b) *and $p(y(u_M^*))$ is the solution of the truth adjoint equation* (2.4b) *with $y(u_M^*)$ on the right-hand side.*

Proof. We note from (4.5) and (2.4b) that the error, $\tilde{e}^p$, satisfies

$$a(\varphi, \tilde{e}^p; \mu) = r_p(\varphi;\mu) + (y_N^*(u_M^*) - y(u_M^*), \varphi)_{D(\mu)}, \quad \forall \varphi \in Y.$$

We now choose $\varphi = \tilde{e}^p$, invoke (2.3), (4.1), the definition of the dual norm of the residual, and the Cauchy-Schwarz inequality to obtain

$$\alpha_a^{\mathrm{LB}}(\mu)\|\tilde{e}^p\|_Y^2 \le \|r_p(\cdot;\mu)\|_{Y'}\|\tilde{e}^p\|_Y + |y(u_M^*) - y_N^*(u_M^*)|_{D(\mu)}|\tilde{e}^p|_{D(\mu)}.$$

The desired result directly follows from the definition of $C_D(\mu)$ and Lemma 4.4. ∎

We note that this proof is in fact a simple extension of the proof of the standard error bound. The main difference is the additional error term due to the change in the right-hand sides of equations (2.4b) and (3.3b). This error in the right-hand side propagates and results in the additional term in the error bound (4.12). We are now ready to state the optimal control error bound in

PROPOSITION 4.6. *Let u^* and u_M^* be the optimal solutions of the truth and reduced basis optimal control problems, respectively. Given $\tilde{\Delta}_N^p(\mu)$ defined in* (4.12)*, the error in the optimal control satisfies*

$$\begin{aligned} \|u^* - u_M^*\|_{U(\mu)} \le \Delta_N^{u,\mathrm{PER}}(\mu) \equiv \frac{1}{\lambda}\|\lambda(u_M^* - u_d) - \mathcal{B}^\star p_N^*\|_{U(\mu)} \\ + \frac{1}{\lambda}\gamma_b^{\mathrm{UB}}(\mu)\,\tilde{\Delta}_N^p(\mu), \quad \forall \mu \in \mathcal{D}. \end{aligned} \tag{4.13}$$

Proof. We append $\pm\mathcal{B}^\star p_N^*(y_N^*(u_N^*))$ to the bound in (4.9) and invoke the triangle inequality to obtain for all $\mu \in \mathcal{D}$

$$\|u^* - u_M^*\|_{U(\mu)} \le \frac{1}{\lambda}\|\lambda(u_M^* - u_d) - \mathcal{B}^\star p_N^*\|_{U(\mu)} + \frac{1}{\lambda}\|\mathcal{B}^\star\big(p_N^* - p(y(u_M^*))\big)\|_{U(\mu)}.$$

The desired result directly follows from the definition of the constant $\|\mathcal{B}^\star\|_{Y\to U(\mu)} = \gamma_b(\mu)$ and Lemma 4.5. ∎

4.2.3. Alternative Approach (ALT). Here, we present a new approach to construct a control error bound which is based on a direct manipulation of the error residual equations of the optimality system. We will denote this bound — for lack of a better name — by ALT, for "alternative". As for the perturbation approach, the bound measures the error in the energy control norm $\|\cdot\|_{U(\mu)}$.

PROPOSITION 4.7. *Let u^* and u_M^* be the optimal solutions to the truth and reduced basis optimal control problems, respectively. The error in the optimal control satisfies for all parameters $\mu \in \mathcal{D}$*

$$\begin{aligned}\|u^* - u_M^*\|_{U(\mu)} \leq \Delta_N^{u,\mathrm{ALT}}(\mu) \equiv \frac{1}{2\lambda}\left(\|r_u(\cdot;\mu)\|_{U(\mu)'} + \frac{\gamma_b^{\mathrm{UB}}(\mu)}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_p(\cdot;\mu)\|_{Y'}\right) \\ + \frac{1}{2\lambda}\Bigg[\left(\|r_u(\cdot;\mu)\|_{U(\mu)'} + \frac{\gamma_b^{\mathrm{UB}}(\mu)}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_p(\cdot;\mu)\|_{Y'}\right)^2 \\ + \frac{8\lambda}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_y(\cdot;\mu)\|_{Y'}\|r_p(\cdot;\mu)\|_{Y'} + \frac{\lambda C_D^{\mathrm{UB}}(\mu)^2}{\alpha_a^{\mathrm{LB}}(\mu)^2}\|r_y(\cdot;\mu)\|_{Y'}^2\Bigg]^{\frac{1}{2}}.\end{aligned} \tag{4.14}$$

Although this error bound looks admittedly complicated, we note that it only contains the dual norms of the state, adjoint, and optimality equation residuals which also appear in the previous two bounds. Furthermore, it only depends on several constants resp. their lower/upper bounds which are straightforward to compute. We also note that, overall, terms involving the dual norm of the state residual, $\|r_y(\cdot;\mu)\|_{Y'}$, scale with $1/\sqrt{\lambda}$ whereas all other terms scale with $1/\lambda$. This is in contrast to the perturbation approach of the last section. Usually, small values of λ allow for a better fit of the optimal state y^* to the desired state $y_d(\mu)$. Since the difference $d(y_d(\mu) - y^*, \cdot;\mu))$ acts as a source term for the adjoint equation, a small misfit will typically result in a p^* of small norm compared to y^* and thus also $\|r_y(\cdot;\mu)\|_{Y'}$ will dominate $\|r_p(\cdot;\mu)\|_{Y'}$. As a result, we expect the bound (4.14) to perform better for small regularization parameters λ than (4.13). We will confirm this observation in the numerical results in Section 5. We turn to the proof of Proposition 4.7.

Proof. We start from the error residual equations

$$a(e^{y,*}, \phi;\mu) - b(e^{u,*}, \phi;\mu) = r_y(\phi;\mu), \qquad \forall \phi \in Y, \tag{4.15}$$

$$a(\varphi, e^{p,*};\mu) + (e^{y,*}, \varphi)_{D(\mu)} = r_p(\varphi;\mu), \qquad \forall \varphi \in Y, \tag{4.16}$$

$$(\lambda e^{u,*}, \psi)_{U(\mu)} - b(\psi, e^{p,*};\mu) = r_u(\psi;\mu), \qquad \forall \psi \in U. \tag{4.17}$$

From (4.15) with $\phi = e^{y,*}$ we obtain

$$\alpha_a^{\mathrm{LB}}(\mu)\|e^{y,*}\|_Y^2 \leq a(e^{y,*}, e^{y,*};\mu) = r_y(e^{y,*};\mu) + b(e^{u,*}, e^{y,*};\mu),$$

and therefore (as in Lemma 4.9)

$$\|e^{y,*}\|_Y \leq \frac{1}{\alpha_a^{\mathrm{LB}}(\mu)}\left(\|r_y(\cdot;\mu)\|_{Y'} + \gamma_b(\mu)\|e^{u,*}\|_{U(\mu)}\right). \tag{4.18}$$

Similarly, equation (4.16) with $\varphi = e^{p,*}$ yields

$$\alpha_a^{\mathrm{LB}}(\mu)\|e^{p,*}\|_Y^2 \leq a(e^{p,*}, e^{p,*};\mu) = r_p(e^{p,*};\mu) - (e^{y,*}, e^{p,*})_{D(\mu)},$$

and thus (almost as in Lemma 4.10)

$$\|e^{p,*}\|_Y \leq \frac{1}{\alpha_a^{\mathrm{LB}}(\mu)}\left(\|r_p(\cdot;\mu)\|_{Y'} + C_D(\mu)|e^{y,*}|_{D(\mu)}\right). \tag{4.19}$$

Choosing the test functions $\phi = e^{p,*}$, $\varphi = e^{y,*}$, and $\psi = e^{u,*}$ in equations (4.15) – (4.17), respectively, we obtain

$$a(e^{y,*}, e^{p,*}; \mu) - b(e^{u,*}, e^{p,*}; \mu) = r_y(e^{p,*}; \mu), \tag{4.20}$$

$$a(e^{y,*}, e^{p,*}; \mu) + (e^{y,*}, e^{y,*})_{D(\mu)} = r_p(e^{y,*}; \mu), \tag{4.21}$$

$$\lambda(e^{u,*}, e^{u,*})_{U(\mu)} - b(e^{u,*}, e^{p,*}; \mu) = r_u(e^{u,*}; \mu). \tag{4.22}$$

Adding (4.21) and (4.22) and subtracting (4.20) yields

$$\lambda(e^{u,*}, e^{u,*})_{U(\mu)} + (e^{y,*}, e^{y,*})_{D(\mu)} = -r_y(e^{p,*}; \mu) + r_p(e^{y,*}; \mu) + r_u(e^{u,*}; \mu)$$

and hence

$$\begin{aligned}\lambda\|e^{u,*}\|^2_{U(\mu)} + |e^{y,*}|^2_{D(\mu)} \le & \|r_y(\cdot;\mu)\|_{Y'}\|e^{p,*}\|_Y + \|r_p(\cdot;\mu)\|_{Y'}\|e^{y,*}\|_Y \\ & + \|r_u(\cdot;\mu)\|_{U(\mu)'}\|e^{u,*}\|_{U(\mu)}.\end{aligned} \tag{4.23}$$

We now plug (4.18) and (4.19) in (4.23) to obtain

$$\begin{aligned}\lambda\|e^{u,*}\|^2_{U(\mu)} + |e^{y,*}|^2_{D(\mu)} \le & \|r_u(\cdot;\mu)\|_{U(\mu)'}\|e^{u,*}\|_{U(\mu)} \\ & + \frac{1}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_p(\cdot;\mu)\|_{Y'}\left(\|r_y(\cdot;\mu)\|_{Y'} + \gamma_b(\mu)\|e^{u,*}\|_{U(\mu)}\right) \\ & + \frac{1}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_y(\cdot;\mu)\|_{Y'}\left(\|r_p(\cdot;\mu)\|_{Y'} + C_D(\mu)|e^{y,*}|_{D(\mu)}\right).\end{aligned}$$

Furthermore it follows from Young's inequality that

$$\frac{C_D(\mu)}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_y(\cdot;\mu)\|_{Y'}|e^{y,*}|_{D(\mu)} \le \frac{C_D(\mu)^2}{4\alpha_a^{\mathrm{LB}}(\mu)^2}\|r_y(\cdot;\mu)\|^2_{Y'} + |e^{y,*}|^2_{D(\mu)}.$$

Combining the last two inequalities, rearranging terms and employing the upper bounds for the constants in (4.2) and (4.3) results in

$$\begin{aligned}\lambda\|e^{u,*}\|^2_{U(\mu)} \le & \|r_u(\cdot;\mu)\|_{U(\mu)'}\|e^{u,*}\|_{U(\mu)} + \frac{2}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_y(\cdot;\mu)\|_{Y'}\|r_p(\cdot;\mu)\|_{Y'} \\ & + \frac{\gamma_b^{\mathrm{UB}}(\mu)}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_p(\cdot;\mu)\|_{Y'}\|e^{u,*}\|_{U(\mu)} + \frac{C_D^{\mathrm{UB}}(\mu)^2}{4\alpha_a^{\mathrm{LB}}(\mu)^2}\|r_y(\cdot;\mu)\|^2_{Y'}.\end{aligned}$$

This can be written in the form of a quadratic inequality for $\|e^{u,*}\|_{U(\mu)}$ by

$$A\|e^{u,*}\|^2_{U(\mu)} + B\|e^{u,*}\|_{U(\mu)} + C \le 0,$$

with

$$\begin{aligned} & A = \lambda, \qquad B = -\left(\|r_u(\cdot;\mu)\|_{U(\mu)'} + \frac{\gamma_b^{\mathrm{UB}}(\mu)}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_p(\cdot;\mu)\|_{Y'}\right), \\ & C = -\left(\frac{2}{\alpha_a^{\mathrm{LB}}(\mu)}\|r_y(\cdot;\mu)\|_{Y'}\|r_p(\cdot;\mu)\|_{Y'} + \frac{C_D^{\mathrm{UB}}(\mu)^2}{4\alpha_a^{\mathrm{LB}}(\mu)^2}\|r_y(\cdot;\mu)\|^2_{Y'}\right),\end{aligned}$$

which is satisfied iff

$$\Delta_N^- \le \|e^{u,*}\|_{U(\mu)} \le \Delta_N^+, \quad \text{where} \quad \Delta_N^{\pm} = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A}.$$

The results follows by setting $\Delta_N^{u,\mathrm{ALT}}(\mu) \equiv \Delta_N^+$. ∎

4.3. Cost Functional Error Bounds. Given the error bounds for the optimal triple $x^* \in X$ and the optimal control $u^* \in U$ we may readily derive a bound for the error in the cost functional. We again first review the BNB-result before presenting the results for the PER- and ALT-approach.

4.3.1. Banach-Nečas-Babuška Approach. The cost functional error bound is defined in

PROPOSITION 4.8. *Let $J^* = J(y^*, u^*; \mu)$ and $J_N^* = J(y_N^*, u_M^*; \mu)$ be the optimal values of the cost functionals of the truth and reduced basis optimal control problems, respectively. The error then satisfies*

$$|J^* - J_N^*| \leq \Delta_N^{J,\mathrm{BNB}}(\mu) \equiv \frac{1}{2} \frac{\|r_x(\cdot;\mu)\|_{X'}^2}{\beta_{\mathrm{Ba}}^{\mathrm{LB}}(\mu)}, \quad \forall \mu \in \mathcal{D}. \tag{4.24}$$

Proof. We use the standard result from [2] to estimate the error in the cost functional by

$$|J^* - J_N^*| = \frac{1}{2} r_x(e^{x,*};\mu) \leq \frac{1}{2} \|r_x(\cdot;\mu)\|_{X'} \|e^{x,*}\|_X, \quad \forall \mu \in \mathcal{D},$$

where $e^{x,*} = x^* - x_N^*$. The result then follows directly from Proposition 4.2. ◻

As pointed out previously, there is a freedom of choice on how to define the inner product and associated norm on X. In fact, one can choose the norm on X so as to minimize the effectivity of the error bound $\Delta_N^{J,\mathrm{BNB}}(\mu)$. We will comment on this issue in Section 5.

4.3.2. Perturbation and Alternative Approach. So far we only derived an *a posteriori* control error bound for the PER- and ALT-approach. For the cost functional error bound, however, we will also require associated *a posteriori* error bounds for the optimal state and adjoint. These are stated in the following two preparatory lemmata. We note that the proofs of these lemmata are similar to the proof of Lemma 4.5, i.e., the error in the optimal control — or, more precisely, the error bound of the optimal control — propagates and appears as an additional term in the state and adjoint optimality error bounds.

LEMMA 4.9. *The state optimality error, $e^{y,*} = y^*(u^*) - y_N^*(u_M^*)$, is bounded by*

$$\|e^{y,*}\|_Y \leq \Delta_N^{y,\bullet}(\mu) \equiv \frac{1}{\alpha_a^{\mathrm{LB}}(\mu)} \left(\|r_y(\cdot;\mu)\|_{Y'} + \gamma_b^{\mathrm{UB}}(\mu)\, \Delta_N^{u,\bullet}(\mu) \right), \quad \forall \mu \in \mathcal{D}, \tag{4.25}$$

where $\bullet \in \{\mathrm{PER}, \mathrm{ALT}\}$.

Proof. We note from (4.4) and (2.4a) that the error, $e^{y,*}$, satisfies

$$a(e^{y,*}, \phi; \mu) = r_y(\phi;\mu) + b(u^* - u_M^*, \phi; \mu), \quad \forall \phi \in Y.$$

We now choose $\phi = e^{y,*}$ and invoke (2.3), (4.1), and the definition of the dual norm of the residual to obtain

$$\alpha_a^{\mathrm{LB}}(\mu) \|e^{y,*}\|_Y^2 \leq \|r_y(\cdot;\mu)\|_{Y'} \|e^{y,*}\|_Y + b(u^* - u_M^*, e^{y,*}; \mu).$$

By the definition of $\gamma_b(\mu)$ and invoking Proposition 4.6 and Proposition 4.7, respectively, we obtain the desired result. ◻

LEMMA 4.10. *The adjoint optimality error, $e^{p,*} = p^*\left(y^*(u^*)\right) - p_N^*\left(y_N^*(u_M^*)\right)$, is bounded by*

$$\|e^{p,*}\|_Y \leq \Delta_N^{p,\bullet} \equiv \frac{1}{\alpha_a^{\mathrm{LB}}(\mu)} \left(\|r_p(\cdot;\mu)\|_{Y'} + C_D^{\mathrm{UB}}(\mu)^2\, \Delta_N^{y,\bullet} \right), \quad \forall \mu \in \mathcal{D}, \tag{4.26}$$

where $\bullet \in \{\mathrm{PER}, \mathrm{ALT}\}$.

The proof is analogous to the proof of Lemma 4.5 and therefore omitted. We can now state

PROPOSITION 4.11. *Let $J^* = J(y^*, u^*; \mu)$ and $J^*_N = J(y^*_N, u^*_M; \mu)$ be the optimal values of the cost functionals of the truth and reduced basis optimal control problems, respectively. The error then satisfies*

$$|J^* - J^*_N| \le \Delta_N^{J,\bullet} \equiv \frac{1}{2}\Big(\|r_y(\cdot;\mu)\|_{Y'}\, \Delta_N^{p,\bullet} + \|r_p(\cdot;\mu)\|_{Y'}\, \Delta_N^{y,\bullet} + \|r_u(\cdot;\mu)\|_{U(\mu)'}\, \Delta_N^{u,\bullet} \Big), \quad \forall \mu \in \mathcal{D}, \tag{4.27}$$

where $\bullet \in \{\mathrm{PER}, \mathrm{ALT}\}$.

Proof. We use the standard result from [2] to bound the cost functional error by

$$\begin{aligned} |J^* - J^*_N| =& \frac{1}{2} r_x(e^{x,*};\mu) = \frac{1}{2}\Big(r_y(e^{p,*};\mu) + r_p(e^{y,*};\mu) + r_u(e^{u,*};\mu) \Big) \\ \le& \frac{1}{2}\Big(\|r_y(\cdot;\mu)\|_{Y'}\, \|e^{p,*}\|_Y + \|r_p(\cdot;\mu)\|_{Y'}\, \|e^{y,*}\|_Y \\ & + \|r_u(\cdot;\mu)\|_{U(\mu)'}\, \|e^{u,*}\|_{U(\mu)} \Big), \quad \forall \mu \in \mathcal{D}. \end{aligned}$$

The result follows from Lemma 4.9 and 4.10 and Proposition 4.6 resp. 4.7. ∎

4.4. Computational Procedure. To evaluate the control and cost functional error bounds $\Delta_N^{u,\mathrm{PER}}(\mu)$, $\Delta_N^{u,\mathrm{ALT}}(\mu)$ and $\Delta_N^{J,\mathrm{PER}}(\mu)$, $\Delta_N^{J,\mathrm{ALT}}(\mu)$ described in Sections 4.2.2, 4.2.3 and 4.3.2, we need to compute

1. the dual norms of the state, adjoint, and optimality equation residuals, i.e. $\|r_y(\cdot;\mu)\|_{Y'}$, $\|r_p(\cdot;\mu)\|_{Y'}$, and $\|r_u(\cdot;\mu)\|_{U(\mu)'}$;
2. the lower and upper bounds $\alpha_a^{\mathrm{LB}}(\mu)$, $C_D^{\mathrm{UB}}(\mu)$ and $\gamma_b^{\mathrm{UB}}(\mu)$.

Since $\|r_y(\cdot;\mu)\|_{Y'}$ and $\|r_p(\cdot;\mu)\|_{Y'}$ can be evaluated using the standard offline-online decomposition [24], we only summarize the computational cost in the offline and online stage. For the computation of the dual norm of the state residual we have to solve $n_y = Q_a N + Q_b M + Q_f$ Poisson-type problems in the offline stage and can then evaluate $\|r_y(\cdot;\mu)\|_{Y'}$ in $\mathcal{O}(n_y^2)$ operations in the online stage for any given parameter $\mu \in \mathcal{D}$ and associated optimal solution x^*_N. Similarly, for the adjoint residual we require $n_p = Q_a N + Q_d N + Q_d Q_{yd}$ Poisson problem solves offline and $\mathcal{O}(n_p^2)$ operations online.

Since the evaluation of $\|r_u(\cdot;\mu)\|_{U(\mu)'}$ is not standard, we provide the necessary details here. From

$$r_u(\psi;\mu) = (\lambda(u^*_M - u_d) - \mathcal{B}^\star p^*_N, \psi)_{U(\mu)} = (\tilde{r}_u(\mu), \psi)_{U(\mu)},$$

it follows that $\tilde{r}_u(\mu) = \lambda(u^*_M - u_d) - \mathcal{B}^\star p^*_N$ is the Riesz-representation of $r_u(\cdot;\mu) \in U(\mu)'$ with respect to the $(\cdot,\cdot)_{U(\mu)}$ energy inner product. Since $\|r_u(\cdot;\mu)\|_{U(\mu)'} = \|\tilde{r}_u(\mu)\|_{U(\mu)}$, we can compute the dual norm of the optimality equation residual by

$$\begin{aligned} \|r_u(\cdot;\mu)\|^2_{U(\mu)'} &= \|\tilde{r}_u(\mu)\|^2_{U(\mu)} = \|\lambda(u^*_M - u_d) - \mathcal{B}^\star p^*_N\|^2_{U(\mu)} \\ &= \lambda^2 (u^*_M, u^*_M)_{U(\mu)} - 2\lambda (u^*_M, u_d)_{U(\mu)} + \lambda^2 (u_d, u_d)_{U(\mu)} \\ &\quad - 2\lambda (u^*_M, \mathcal{B}^\star p^*_N)_{U(\mu)} + 2\lambda (u_d, \mathcal{B}^\star p^*_N)_{U(\mu)} + (\mathcal{B}^\star p^*_N, \mathcal{B}^\star p^*_N)_{U(\mu)} \\ &= \lambda^2 (u^*_M)^T C_M(\mu) u^*_M - 2\lambda (u^*_M)^T U_{d,M}(\mu) + \lambda^2 U_{d,d}(\mu) \\ &\quad - 2\lambda (u^*_M)^T B^T_{M,N}(\mu) p^*_N + 2\lambda B_{d,N}(\mu)^T p^*_N + (p^*_N)^T B^\star_{N,N}(\mu) p^*_N. \end{aligned}$$

The matrix $B^\star_{N,N}(\mu) \in \mathbb{R}^{N\times N}$ and vector $B_{d,N}(\mu) \in \mathbb{R}^N$ have entries $(B^\star_{N,N}(\mu))_{ij} = c(\mathcal{B}^\star\zeta^y_j, \mathcal{B}^\star\zeta^y_i;\mu)$, $1 \le i,j \le N$, and $(B_{d,N}(\mu))_i = b(u_d, \zeta^y_i;\mu)$, $1 \le i \le N$. Exploiting the affine parameter dependence of $c(\cdot,\cdot;\mu)$ and $b(\cdot,\cdot;\mu)$, $B^\star_{N,N}(\mu)$ and $B_{d,N}(\mu)$ can be assembled online in $\mathcal{O}(Q_c N^2)$ and $\mathcal{O}(Q_b N)$ operations, respectively. The total online cost (to leading order) for computing $\|r_u(\cdot;\mu)\|_{U(\mu)'}$ is $\mathcal{O}(Q_c(M^2+N^2)+Q_b MN)$.

For the construction of the coercivity constant lower bound $\alpha_a^{\mathrm{LB}}(\mu)$ various recipes exist [9, 23, 29]. The specific choices for our numerical examples are stated in Section 5. Simple (yet for our examples effective) upper bounds $C_D^{\mathrm{UB}}(\mu)$ and $\gamma_b^{\mathrm{UB}}(\mu)$ can be computed by solving $Q_d + Q_u$ generalized eigenvalue problems in the offline stage and then assembled in $\mathcal{O}(Q_d + Q_u)$ operations online. In general (arbitrarily tight) upper bounds can be obtained by applying the successive constraint method.

In summary, the online evaluation of the error bounds $\Delta_N^{u,\mathrm{PER}}(\mu)$, $\Delta_N^{u,\mathrm{ALT}}(\mu)$, and $\Delta_N^{J,\mathrm{PER}}(\mu)$, $\Delta_N^{J,\mathrm{ALT}}(\mu)$ involves an operation count that is *independent* of the dimension of the finite element spaces $\mathcal{N}$ and $\mathcal{M}$.

For the evaluation of the error bounds $\Delta_N^{x,\mathrm{BNB}}(\mu) = \Delta_N^{u,\mathrm{BNB}}(\mu)$, and $\Delta_N^{J,\mathrm{BNB}}(\mu)$ described in Sections 4.2.1, and 4.3.1 we need to compute

1. the dual norm of the saddle point residual $\|r_x(\cdot;\mu)\|_{X'}$;
2. the constant $\beta_{\mathrm{Ba}}^{\mathrm{LB}}(\mu)$.

The computational procedure and effort to compute $\|r_x(\cdot;\mu)\|_{X'}$ are the same as for evaluating $\|r_y(\cdot;\mu)\|_{Y'}$, $\|r_p(\cdot;\mu)\|_{Y'}$, and $\|r_u(\cdot;\mu)\|_{U(\mu)'}$. However computing a lower bound $\beta_{\mathrm{Ba}}^{\mathrm{LB}}(\mu)$ for the stability constant is very involved and requires a very large computational effort in the offline stage [22].

5. Numerical Results. In this section we present two numerical examples: i) a Graetz flow and ii) a heat transfer problem motivated by hyperthermia cancer treatment. Both problems involve a distributed control over the whole domain. We stress that, throughout this section, we use the actual stability constant $\beta_{\mathrm{Ba}}(\mu)$ and *not* its lower bound $\beta_{\mathrm{Ba}}^{\mathrm{LB}}(\mu)$ for the evaluation of the BNB-bounds (4.8) and (4.24). The reason is the high computational cost and implementation effort required to obtain $\beta_{\mathrm{Ba}}^{\mathrm{LB}}(\mu)$ in combination with the fact that the BNB-bounds are just used for comparison here (and are not our original contribution). The computations were done in Matlab on a computer with a 2.6 GHz Intel Core i7 processor and 16 GB of RAM.

5.1. Graetz flow problem. We consider a linear-quadratic optimal control problem governed by a steady Graetz flow in a two-dimensional domain based on the numerical examples in [21, 22]. The spatial domain, an arbitrary point of which is $x = (x_1, x_2)$, is given by $\Omega = (0, 2.5) \times (0, 1)$ and is subdivided into the three subdomains $\Omega_1 = [0.2, 0.8] \times [0.3, 0.7]$, $\Omega_2 = [1.2, 2.5] \times [0.3, 0.7]$, and $\Omega_3 = \Omega \setminus \{\Omega_1 \cup \Omega_2\}$. A sketch of the domain is shown in Figure 5.1. We impose homogeneous Neumann and non-homogeneous Dirichlet boundary conditions on Γ_N and Γ_{D_1}, Γ_{D_2}, respectively. The amount of heat supply in the whole domain Ω is regulated by the distributed control function $u_{\mathrm{e}} \in U_{\mathrm{e}} \equiv L^2(\Omega)$. The parametrized optimal control problem is then

$$\begin{aligned}
&\min_{y_{\mathrm{e}} \in Y_{\mathrm{e}}^D, u_{\mathrm{e}} \in U_{\mathrm{e}}} J(y_{\mathrm{e}}, u_{\mathrm{e}};\mu) = \frac{1}{2}\|y_{\mathrm{e}} - y_{d,\mathrm{e}}(\mu)\|^2_{L^2(\Omega_1\cup\Omega_2)} + \frac{\lambda}{2}\|u_{\mathrm{e}} - u_{d,\mathrm{e}}\|^2_{L^2(\Omega)}\\
&\text{s.t.} \quad \frac{1}{\mu_1}\int_\Omega \nabla y_{\mathrm{e}} \cdot \nabla v \,\mathrm{d}x + \int_\Omega \beta(x)\cdot\nabla y_{\mathrm{e}}\, v\,\mathrm{d}x = \int_\Omega u_{\mathrm{e}}\, v\,\mathrm{d}x, \quad \forall v \in Y_{\mathrm{e}}^D,
\end{aligned}$$

for the given parabolic velocity field $\beta(x) = x_2(1-x_2)$ and $Y_{\mathrm{e}}^D = \{v \in H^1(\Omega) : v|_{\Gamma_{D_1}} \equiv 1, v|_{\Gamma_{D_2}} \equiv 2\}$. The parameter μ_1 describes the Péclet number of the flow and the parametrized desired state is given by $y_{d,\mathrm{e}}(\mu) = \mu_2$ on Ω_1 and $y_{d,\mathrm{e}}(\mu) = \mu_3$

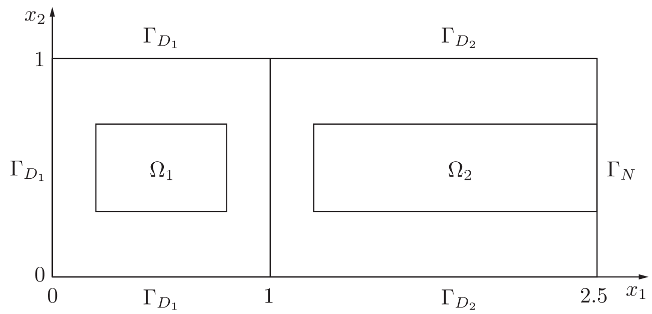


Fig. 5.1: Domain Ω for the Graetz flow problem with distributed control.

on Ω_2. The full parameter domain is $\mathcal{D} = [3, 20] \times [0.5, 1.5] \times [1.5, 2.5]$. For the cost functional we set $u_{d,\mathrm{e}} \equiv 0$. In Section 5.3 we consider different values for the regularization parameter λ. However, for the remainder of this subsection we will keep the regularization parameter $\lambda = 0.01$ fixed. We choose the inner product $(w, v)_{Y_\mathrm{e}} = \frac{1}{\mu_1^{\mathrm{ref}}} \int_\Omega \nabla w \cdot \nabla v \, \mathrm{d}x + \frac{1}{2}(\int_\Omega \beta(x) \cdot \nabla w \, v \, \mathrm{d}x + \int_\Omega \beta(x) \cdot \nabla v \, w \, \mathrm{d}x)$ for $\mu_1^{\mathrm{ref}} = 3$; we may hence choose $\alpha_a^{\mathrm{LB}}(\mu) = \min(\mu_1^{\mathrm{ref}}/\mu_1, 1)$ in (4.1). For the control space U_e we use the usual L^2-norm and inner product. After introducing suitable lifting functions that take into account the non-homogeneous Dirichlet boundary conditions, we can reformulate the problem in terms of the space $Y_\mathrm{e} = H_0^1(\Omega)$ and the considered problem satisfies the affine representation (2.1) of all involved quantities with $Q_a = 2$, $Q_b = Q_d = Q_c = 1$, $Q_f = 2$, and $Q_{yd} = 3$ (taking into account the affine terms required for the lifting functions). For details regarding the involved forms and functionals, cf. [21], [22], and [13].

For the truth discretization we consider linear finite element approximation spaces $Y \subset Y_\mathrm{e}$, $U \subset U_\mathrm{e}$ for the state, adjoint, and control variables. The number of degrees of freedom is $\dim(Y) = \mathcal{N} = 10,801$ and $\dim(U) = \mathcal{M} = 11,148$; hence the total dimension of the truth optimality system is $2\mathcal{N} + \mathcal{M} = 32,750$.

We construct the reduced basis spaces $Y_N \subset Y$ and $U_M \subset U$ according to the Greedy sampling procedure described in Section 3.2. To this end, we employ the train sample $\Xi_{\mathrm{train}} \subset \mathcal{D}$ consisting of $n_{\mathrm{train}} = 10 \cdot 7 \cdot 7 = 490$ equidistant parameter points over $\mathcal{D}$. We sample on the relative ALT control error bound $\Delta_N^{u,\mathrm{ALT}}(\mu)/\|u_M^*(\mu)\|_{U(\mu)}$. The desired error tolerance is $\epsilon_{\mathrm{tol,min}} = 10^{-4}$ and the initial parameter value is $\mu^1 = (3, 0.5, 1.5)^T$. We also introduce a parameter test sample $\Xi_{\mathrm{test}} \subset \mathcal{D}$ of size $n_{\mathrm{test}} = 20$ with a uniform-random distribution in $\mathcal{D}$.

On the product space $X = Y \times U \times Y$, we define for $\vartheta_1 = (\varphi_1, \psi_1, \phi_1) \in X$ and $\vartheta_2 = (\varphi_2, \psi_2, \phi_2) \in X$ the energy inner product as $(\vartheta_1, \vartheta_2)_{X(\mu)} = (\varphi_1, \varphi_2)_Y + (\psi_1, \psi_2)_{U(\mu)} + (\phi_1, \phi_2)_Y$, and associated energy norm as $\|\vartheta\|_{X(\mu)} = \sqrt{(\vartheta, \vartheta)_{X(\mu)}} = \sqrt{\|\varphi\|_Y^2 + \|\psi\|_{U(\mu)}^2 + \|\phi\|_Y^2}$. In Section 5.3 we will also consider a scaled energy inner product and norm given by $(\vartheta_1, \vartheta_2)_{X_\lambda(\mu)} = (\varphi_1, \varphi_2)_Y + \lambda(\psi_1, \psi_2)_{U(\mu)} + (\phi_1, \phi_2)_Y$ and $\|\vartheta\|_{X_\lambda(\mu)} = \sqrt{(\vartheta, \vartheta)_{X_\lambda(\mu)}} = \sqrt{\|\varphi\|_Y^2 + \lambda\|\psi\|_{U(\mu)}^2 + \|\phi\|_Y^2}$, respectively. This corresponds to $C_{U,X} = 1$ resp. $C_{U,X} = \sqrt{\lambda}$ in the remark after Proposition 4.2. We recall that the PER- and ALT-bounds measure the error in the energy control norm $\|\cdot\|_{U(\mu)}$, which is the more relevant norm for geometry parametrizations, e.g.

$U_{\rm e}(\mu) = L^2(\Omega(\mu))$. Note that for the Graetz flow problem we do not consider a geometrical parametrization and hence the reference and energy control norm coincide. Similarly, in the heat transfer problem involving a parametrized domain we observe no differences in the results between using the reference and energy norm (norm equivalence constants close to one), so we only present energy norm results.

M	$\epsilon^u_{N,\max,\mathrm{rel}}$	$\Delta^{u,\mathrm{BNB}}_{N,\max,\mathrm{rel}}$	$\bar\eta^{u,\mathrm{BNB}}_N$	$\Delta^{u,\mathrm{PER}}_{N,\max,\mathrm{rel}}$	$\bar\eta^{u,\mathrm{PER}}_N$	$\Delta^{u,\mathrm{ALT}}_{N,\max,\mathrm{rel}}$	$\bar\eta^{u,\mathrm{ALT}}_N$
2	1.12 E+00	1.76 E+02	1.35 E+02	1.12 E+02	4.68 E+01	4.01 E+01	1.49 E+01
4	4.96 E–01	9.18 E+01	9.58 E+01	7.84 E+00	2.66 E+01	1.72 E+00	4.34 E+00
8	3.07 E–02	3.82 E+00	7.82 E+01	4.58 E–01	2.25 E+01	1.43 E–01	6.27 E+00
12	1.66 E–03	1.36 E–01	6.89 E+01	4.03 E–02	1.51 E+01	7.74 E–03	4.49 E+00
16	9.67 E–05	8.19 E–03	9.20 E+01	1.95 E–03	2.33 E+01	3.43 E–04	4.95 E+00
19	1.26 E–05	8.13 E–04	7.82 E+01	2.46 E–04	1.49 E+01	4.86 E–05	3.64 E+00

Table 5.1: Control variable in Graetz flow example: error convergence, error bounds, and effectivities as a function of M.

In Table 5.1 we present, as a function of M, the maximum relative control error $\epsilon^u_{N,\max,\mathrm{rel}}$ and the maximum relative error bounds $\Delta^{u,\mathrm{BNB}}_{N,\max,\mathrm{rel}}$, $\Delta^{u,\mathrm{PER}}_{N,\max,\mathrm{rel}}$, $\Delta^{u,\mathrm{ALT}}_{N,\max,\mathrm{rel}}$ as well as the corresponding mean effectivities $\bar\eta^{u,\mathrm{BNB}}_N$,$\bar\eta^{u,\mathrm{PER}}_N$, $\bar\eta^{u,\mathrm{ALT}}_N$. Here, $\epsilon^u_{N,\max,\mathrm{rel}}$ is the maximum over Ξ_{test} of $\|e^{u,*}(\mu)\|_{U(\mu)}/\|u^*(\mu)\|_{U(\mu)}$, $\Delta^{u,\bullet}_{N,\max,\mathrm{rel}}$ is the maximum over Ξ_{test} of $\Delta^{u,\bullet}_N(\mu)/\|u^*(\mu)\|_{U(\mu)}$, and $\bar\eta^{u,\bullet}_N$ is the average over Ξ_{test} of $\Delta^{u,\bullet}_N(\mu)/\|e^{u,*}\|_{U(\mu)}$. We observe that the control error and all three error bounds are decreasing very rapidly with increasing reduced basis dimension M. The Greedy sampling procedure guarantees the prescribed sampling tolerance $\epsilon_{\mathrm{tol,min}} = 10^{-4}$ for the normalized error bound $\Delta^{u,\mathrm{ALT}}_N(\mu)/\|u^*_M(\mu)\|_{U(\mu)}$ over the training set Ξ_{train} after selecting only $M_{\max} = 19$ parameter snapshots. We note that the effectivities of the BNB-bound are slightly larger than the ones of the PER-bound, and that both are significantly larger than the ones of the ALT-bound. The ALT-bound clearly performs best with effectivities close to one for all values of M (except for $M = 2$). Again, the BNB-bound is computed with $\beta_{\mathrm{Ba}}(\mu)$ instead of $\beta^{\mathrm{LB}}_{\mathrm{Ba}}(\mu)$ and the effectivities may thus be considerably larger in actual practice. However, the BNB-bound is actually a bound for the combined error $\|e^{x,*}\|_{X(\mu)}$.

M	$\epsilon^x_{N,\max,\mathrm{rel}}$	$\Delta^{x,\mathrm{BNB}}_{N,\max,\mathrm{rel}}$	$\bar\eta^{x,\mathrm{BNB}}_N$	$\Delta^{x,\mathrm{PER}}_{N,\max,\mathrm{rel}}$	$\bar\eta^{x,\mathrm{PER}}_N$	$\Delta^{x,\mathrm{ALT}}_{N,\max,\mathrm{rel}}$	$\bar\eta^{x,\mathrm{ALT}}_N$
2	7.00 E–02	8.54 E+00	1.02 E+02	7.39 E+00	1.13 E+02	2.67 E+00	3.48 E+01
4	3.15 E–02	3.46 E+00	8.26 E+01	1.05 E+00	7.35 E+01	1.16 E–01	1.08 E+01
8	1.71 E–03	2.03 E–01	7.01 E+01	3.02 E–02	6.54 E+01	8.35 E–03	1.73 E+01
12	6.84 E–05	7.15 E–03	6.26 E+01	2.67 E–03	4.16 E+01	6.06 E–04	1.09 E+01
16	2.87 E–06	4.58 E–04	7.99 E+01	2.83 E–04	6.72 E+01	3.91 E–05	1.24 E+01
19	4.53 E–07	4.55 E–05	6.47 E+01	1.63 E–05	4.01 E+01	3.40 E–06	9.10 E+00

Table 5.2: Combined variable x in Graetz flow example: error convergence, error bounds, and effectivities as a function of M.

Motivated by this fact, we present results for the combined variable x in Table 5.2. We compare, as function of M, the maximum relative combined error $\epsilon^x_{N,\max,\mathrm{rel}}$ and the maximum relative error bounds $\Delta^{x,\mathrm{BNB}}_{N,\max,\mathrm{rel}}$, $\Delta^{x,\mathrm{PER}}_{N,\max,\mathrm{rel}}$, $\Delta^{x,\mathrm{ALT}}_{N,\max,\mathrm{rel}}$ as well as the corresponding mean effectivities $\bar{\eta}_N^{x,\mathrm{BNB}}$,$\bar{\eta}_N^{x,\mathrm{PER}}$, $\bar{\eta}_N^{x,\mathrm{ALT}}$. Here, $\epsilon^x_{N,\max,\mathrm{rel}}$ is the maximum over Ξ_{test} of $\|e^{x,*}(\mu)\|_{X(\mu)}/\|x^*(\mu)\|_{X(\mu)}$, $\Delta^{x,\bullet}_{N,\max,\mathrm{rel}}$ is the maximum over Ξ_{test} of $\Delta_N^{x,\bullet}(\mu)/\|x^*(\mu)\|_{X(\mu)}$, and $\bar{\eta}_N^{x,\bullet}$ is the average over Ξ_{test} of $\Delta_N^{x,\bullet}(\mu)/\|e^{x,*}\|_{X(\mu)}$. Note that we obtain this bound for the PER- and ALT-approach by simply combining the control error bound with the state and adjoint optimality error bounds defined in Lemma 4.9 and 4.10, respectively. Similar to the results for the control variable, the combined error and all three bounds are decreasing rapidly with increasing reduced basis dimension M. Although the BNB-bound is specifically designed to measure the combined error in the X-norm, its effectivities are comparable to the PER-bound and significantly (almost one order of magnitude) larger than for the ALT-bound.

M	$\epsilon^J_{N,\max,\mathrm{rel}}$	$\Delta^{J,\mathrm{BNB}}_{N,\max,\mathrm{rel}}$	$\bar{\eta}_N^{J,\mathrm{BNB}}$	$\Delta^{J,\mathrm{PER}}_{N,\max,\mathrm{rel}}$	$\bar{\eta}_N^{J,\mathrm{PER}}$	$\Delta^{J,\mathrm{ALT}}_{N,\max,\mathrm{rel}}$	$\bar{\eta}_N^{J,\mathrm{ALT}}$
2	1.10 E+01	3.38 E+03	2.29 E+03	9.30 E+03	7.12 E+02	3.37 E+03	1.81 E+02
4	1.31 E–01	9.23 E+02	4.51 E+03	4.78 E+01	1.18 E+03	6.25 E+00	1.74 E+02
8	4.90 E–04	1.98 E+00	5.49 E+03	1.42 E–01	5.94 E+02	4.60 E–02	1.72 E+02
12	2.53 E–06	2.59 E–03	3.40 E+03	1.21 E–03	3.60 E+02	2.29 E–04	1.16 E+02
16	1.54 E–09	8.86 E–06	9.32 E+03	2.91 E–06	1.25 E+04	3.91 E–07	1.91 E+03
19	1.21 E–10	8.72 E–08	4.61 E+03	4.53 E–08	5.04 E+02	9.08 E–09	1.08 E+02

Table 5.3: Cost functional J in Graetz flow example: error convergence, error bounds, and effectivities as a function of M.

Finally, we state in Table 5.3, as a function of M, the maximum relative cost functional error $\epsilon^J_{N,\max,\mathrm{rel}}$ and the maximum relative error bounds $\Delta^{J,\mathrm{BNB}}_{N,\max,\mathrm{rel}}$, $\Delta^{J,\mathrm{PER}}_{N,\max,\mathrm{rel}}$, $\Delta^{J,\mathrm{ALT}}_{N,\max,\mathrm{rel}}$ as well as the corresponding mean effectivities $\bar{\eta}_N^{J,\mathrm{BNB}}$,$\bar{\eta}_N^{J,\mathrm{PER}}$, $\bar{\eta}_N^{J,\mathrm{ALT}}$. Here, $\epsilon^J_{N,\max,\mathrm{rel}}$ is the maximum over Ξ_{test} of $|J^*(\mu) - J^*_N(\mu)|/J^*(\mu)$, $\Delta^{J,\bullet}_{N,\max,\mathrm{rel}}$ is the maximum over Ξ_{test} of $\Delta_N^{J,\bullet}(\mu)/J^*(\mu)$, and $\bar{\eta}_N^{J,\bullet}$ is the average over Ξ_{test} of $\Delta_N^{J,\bullet}(\mu)/|J^*(\mu) - J^*_N(\mu)|$. Again, a rapid decrease of the error and error bounds can be observed. The BNB- and PER-bound effectivities have the same order of magnitude whereas the ALT-bound again performances considerably better.

We finally consider the online computational cost for solving the reduced basis optimal control problem compared to the truth optimal control problem. On average (over Ξ_{test}) it takes 0.49 seconds to solve the truth optimal control problem based on our finite element discretization. Depending on the reduced basis dimension $1 \leq M \leq M_{\max} = 19$ it takes between 1.19 and 2.01 milliseconds to solve the reduced basis optimal control problem (without error bounds) resulting in speedups ranging from 244 to 412. Taking into account the computation of the error bounds (consisting mainly of the online residual calculation and evaluating $\alpha_a^{\mathrm{LB}}(\mu)$) the online cost for the reduced basis solution ranges from 1.61 to 2.11 milliseconds, which in turn corresponds to a speedup of 232 up to 304. Note that the computational time required for the error bound computation is only a small fraction of the reduced basis solution time.

5.2. Heat transfer problem. Next we consider a linear-quadratic optimal control problem governed by steady heat conduction in a parametrized two-dimensional domain. The spatial domain, a typical point of which is $x^o = (x_1^o, x_2^o)$, is given by $\Omega^o = (0,5) \times (0,5)$ and is subdivided into the three subdomains $\Omega_1^o(\mu) = \Omega^o \setminus \{\Omega_2^o \cup \Omega_3^o(\mu)\}$, $\Omega_2^o = \{(1,4) \times (1,2)\} \cup \{(1,2) \times (1,4)\}$, and $\Omega_3^o(\mu) = (\mu_1 - 0.5, \mu_1 + 0.5) \times (\mu_2 - 0.5, \mu_2 + 0.5)$. Here, the parameter $\mu = (\mu_1, \mu_2)^T \in \mathcal{D} = [3,4] \times [3,4]$ describes the horizontal and vertical translation of the square $\Omega_3^o(\mu)$ in the upper right corner of the domain Ω^o. A sketch of the domain is shown in Figure 5.2. The temperature satisfies

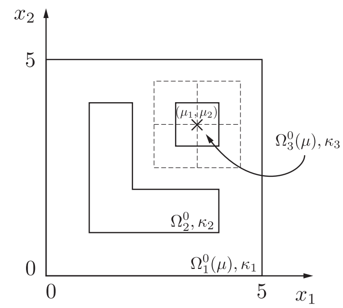


Fig. 5.2: Parametrized domain Ω^o for the heat transfer problem with distributed control.

Laplace's equation in Ω^o with continuity of temperature and heat flux across subdomain interfaces. The (reference) conductivity in the subdomain $\Omega_1^o(\mu)$ is set to unity, whereas the normalized conductivity is $\kappa_2 = 0.2$ in the subdomain Ω_2^o and $\kappa_3 = 5$ in the subdomain $\Omega_3^o(\mu)$. We impose zero Dirichlet conditions on the whole domain boundary $\partial\Omega^o$. The amount of heat supply in the whole domain Ω^o is regulated by the distributed control function $u_{\rm e}^o \in U_{\rm e}^o \equiv L^2(\Omega^o)$.

The parametrized optimal control problem then reads

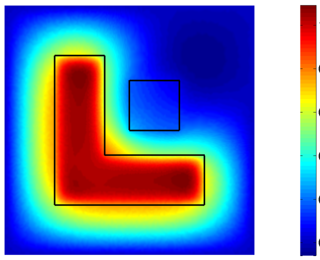
$$\begin{aligned}(5.1)\qquad &\min_{y_{\rm e}^o\in Y_{\rm e}^o, u_{\rm e}^o\in U_{\rm e}^o} J(y_{\rm e}^o, u_{\rm e}^o;\mu) = \frac{1}{2}\|y_{\rm e}^o - y_{d,{\rm e}}^o\|^2_{L^2(\Omega_2^o\cup\Omega_3^o(\mu))} + \frac{\lambda}{2}\|u_{\rm e}^o - u_{d,{\rm e}}^o\|^2_{L^2(\Omega^o)}\\ &\text{s.t.} \quad \sum_{i=1}^{3}\kappa_i\int_{\Omega_i^o(\mu)}\nabla y_{\rm e}^o\cdot\nabla v\;{\rm d}x = \int_{\Omega^o} u_{\rm e}^o\, v\;{\rm d}x, \quad \forall v\in Y_{\rm e}^o = H_0^1(\Omega^o).\end{aligned}$$

The desired state is given by $y_{d,{\rm e}}^o \equiv 1$ in Ω_2^o and $y_{d,{\rm e}}^o \equiv 0$ in $\Omega_3^o(\mu)$ and the desired control is $u_{d,{\rm e}}^0 \equiv 0$. As for the Graetz flow example we will keep the regularization parameter $\lambda = 0.01$ fixed for the remainder of this subsection. In Section 5.3 we consider different values for the regularization parameter λ. After recasting the problem to a reference domain Ω with corresponding subdomains $\Omega_{1,3} = \Omega_{1,3}^o(\mu^{\rm ref})$ for $\mu^{\rm ref} = (3.5, 3.5)^T$ [24], we obtain the affine representation (2.1) of all involved quantities with $Q_a = 17$, $Q_b = Q_c = 4$, $Q_d = 1$, $Q_f = 0$, and $Q_{yd} = 1$; see [13] for details.

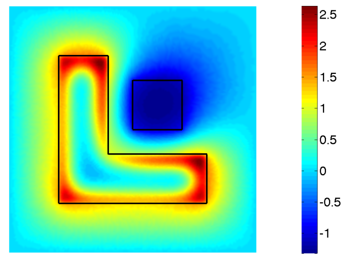
The problem is motivated by hyperthermia treatment of cancer, where the subdomain Ω_2^o could be interpreted as tumor tissue and the subdomain $\Omega_3^o(\mu)$ as so-called risk tissue. Hence, the goal is to heat up only the damaged part of the body ($y_{d,{\rm e}}^o \equiv 1$ in Ω_2^o) but not the regions at risk ($y_{d,{\rm e}}^o \equiv 0$ in $\Omega_3^o(\mu)$).

We further choose the inner product $(w,v)_{Y_{\rm e}} = \sum_{i=1}^3 \kappa_i \int_{\Omega_i} \nabla w\cdot\nabla v\;{\rm d}x$. To compute a lower bound $\alpha_a^{\rm LB}(\mu)$ for the coercivity constant in (4.1) we use the successive constraint method (SCM) [9, 3], where we chose the following parameters: $J^{\rm SCM} = 35\cdot 35 = 1225$ equidistant training points over $\mathcal{D}$, $M^{\rm SCM} = 2$ coercivity and $M_+^{\rm SCM} = 4$ positivity constraints. A required tolerance of $\epsilon^{\rm SCM} = 0.2$ then selects $K^{\rm SCM} = 53$ parameters in the SCM offline phase. The (reference) inner product for the control space $U_{\rm e}$ is given by $(\cdot,\cdot)_{U_{\rm e}} = c(\cdot,\cdot,\mu^{\rm ref})$.

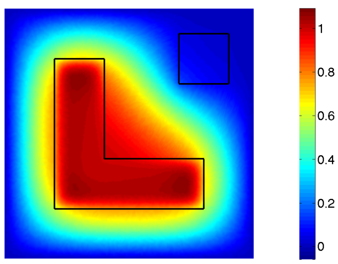
We next introduce linear truth finite element approximation spaces $Y \subset Y_{\rm e} = H_0^1(\Omega)$, $U \subset U_{\rm e} = L^2(\Omega)$ for the state, adjoint, and control variables. The number of degrees of freedom is $\dim(Y) = \mathcal{N} = 18,117$ and $\dim(U) = \mathcal{M} = 18,517$; hence the dimension of the truth optimality system is $2\mathcal{N} + \mathcal{M} = 54,751$.



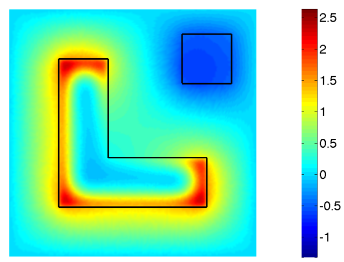
(a) Optimal state $y^*(\mu)$, $(\mu_1, \mu_2, \lambda) = (3, 3, 0.01)$, $J^*(\mu) = 0.13$



(b) Optimal control $u^*(\mu)$, $(\mu_1, \mu_2, \lambda) = (3, 3, 0.01)$, $J^*(\mu) = 0.13$



(c) Optimal state $y^*(\mu)$, $(\mu_1, \mu_2, \lambda) = (4, 4, 0.01)$, $J^*(\mu) = 0.08$



(d) Optimal control $u^*(\mu)$, $(\mu_1, \mu_2, \lambda) = (4, 4, 0.01)$, $J^*(\mu) = 0.08$

Fig. 5.3: Optimal state $y^*(\mu)$, optimal control $u^*(\mu)$, and optimal cost functional value $J^*(\mu)$ for different representative parameter values

We present results for the solution of the truth optimal control problem (5.1) for different parameter values in Figure 5.3. We plot the optimal temperature distribution and optimal control and report the associated cost functional value. We note that all parameters have a strong influence on the solution of the optimal control problem: the temperature, optimal control, and optimal cost functional value vary significantly.

Again, we construct the reduced basis spaces $Y_N \subset Y$ and $U_M \subset U$ according to the Greedy sampling procedure described in Section 3.2. The training set $\Xi_{\rm train} \subset \mathcal{D}$ consists of $n_{\rm train} = 15 \cdot 15 = 225$ equidistant parameter points over $\mathcal{D}$. We sample on the relative ALT control error bound $\Delta_N^{u,{\rm ALT}}(\mu)/\|u_M^*(\mu)\|_{U(\mu)}$, set the desired error tolerance to $\epsilon_{\rm tol,min} = 10^{-4}$, and choose as initial parameter value $\mu^1 = (3,3)^T$. We obtain $M_{\max} = 45$ to achieve the desired error tolerance. The test sample $\Xi_{\rm test} \subset \mathcal{D}$ consists of $n_{\rm test} = 20$ random parameter points distributed uniformly in $\mathcal{D}$.

Following the presentation of the numerical results for the Graetz flow example in the last section, we present the maximum relative errors and bounds as well as the average effectivities for the control, the combined variable x, and the cost functional in Tables 5.4–5.6. We first observe that the convergence is slower than in the Graetz flow examples due to the higher parametric complexity of this example. Also, the effectivities are consistently higher. For the control variable the effectivities of the BNB-bound and PER-bound are roughly the same, whereas for the combined variable and the cost functional the PER-bound effectivity is approximately one order of magnitude higher than the one of the BNB-bound. Taking into account the additional overestimation if $\beta_{\rm Ba}^{\rm LB}(\mu)$ is used instead of $\beta_{\rm Ba}(\mu)$, the performance of the BNB-bound and PER-bound would likely be equivalent in practice. For all three quantities, however, the ALT-bound again performs best: the overestimation is considerably lower than with the other two approaches.

M	$\epsilon^u_{N,\max,\rm rel}$	$\Delta^{u,\rm BNB}_{N,\max,\rm rel}$	$\bar\eta^{u,\rm BNB}_N$	$\Delta^{u,\rm PER}_{N,\max,\rm rel}$	$\bar\eta^{u,\rm PER}_N$	$\Delta^{u,\rm ALT}_{N,\max,\rm rel}$	$\bar\eta^{u,\rm ALT}_N$
2	1.01 E–01	1.28 E+02	6.19 E+02	1.66 E+02	7.30 E+02	3.71 E+00	2.16 E+01
8	7.16 E–03	3.54 E+00	4.25 E+02	3.86 E+00	4.71 E+02	1.18 E–01	1.56 E+01
16	1.21 E–03	3.09 E–01	4.65 E+02	3.04 E–01	5.33 E+02	1.32 E–02	1.86 E+01
24	8.40 E–05	4.77 E–02	4.89 E+02	5.37 E–02	5.56 E+02	1.71 E–03	2.09 E+01
32	2.22 E–05	1.02 E–02	5.49 E+02	1.72 E–02	6.37 E+02	4.72 E–04	2.39 E+01
40	1.09 E–05	4.38 E–03	6.08 E+02	4.43 E–03	6.91 E+02	1.93 E–04	2.54 E+01
45	1.52 E–06	1.44 E–03	7.52 E+02	1.52 E–03	8.55 E+02	4.21 E–05	2.96 E+01

Table 5.4: Control variable in heat transfer example: error convergence, error bounds, and effectivities as a function of M.

M	$\epsilon^x_{N,\max,\rm rel}$	$\Delta^{x,\rm BNB}_{N,\max,\rm rel}$	$\bar\eta^{x,\rm BNB}_N$	$\Delta^{x,\rm PER}_{N,\max,\rm rel}$	$\bar\eta^{x,\rm PER}_N$	$\Delta^{x,\rm ALT}_{N,\max,\rm rel}$	$\bar\eta^{x,\rm ALT}_N$
2	1.19 E–01	1.02 E+02	4.55 E+02	1.68 E+03	4.95 E+03	3.82 E+01	1.40 E+02
8	6.58 E–03	2.85 E+00	3.43 E+02	2.91 E+01	3.41 E+03	8.61 E–01	1.10 E+02
16	1.11 E–03	2.49 E–01	3.63 E+02	2.56 E+00	3.78 E+03	6.95 E–02	1.28 E+02
24	8.75 E–05	3.71 E–02	3.83 E+02	4.93 E–01	3.89 E+03	1.60 E–02	1.41 E+02
32	2.40 E–05	8.15 E–03	4.04 E+02	1.81 E–01	4.16 E+03	5.03 E–03	1.51 E+02
40	1.13 E–05	3.47 E–03	4.26 E+02	2.52 E–02	4.25 E+03	8.56 E–04	1.52 E+02
45	2.36 E–06	1.17 E–03	4.60 E+02	1.22 E–02	4.62 E+03	3.48 E–04	1.60 E+02

Table 5.5: Combined variable x in heat transfer example: error convergence, error bounds, and effectivities as a function of M.

M	$\epsilon^J_{N,\max,\rm rel}$	$\Delta^{J,\rm BNB}_{N,\max,\rm rel}$	$\bar\eta^{J,\rm BNB}_N$	$\Delta^{J,\rm PER}_{N,\max,\rm rel}$	$\bar\eta^{J,\rm PER}_N$	$\Delta^{J,\rm ALT}_{N,\max,\rm rel}$	$\bar\eta^{J,\rm ALT}_N$
2	3.48 E–02	1.12 E+03	1.59 E+04	1.77 E+04	1.71 E+05	4.04 E+02	4.69 E+03
8	6.67 E–05	1.09 E+00	2.68 E+04	9.46 E+00	3.18 E+05	2.85 E–01	8.22 E+03
16	1.09 E–06	1.30 E–02	3.01 E+04	5.79 E–02	3.79 E+05	2.60 E–03	1.24 E+04
24	1.07 E–08	2.04 E–04	2.39 E+04	1.95 E–03	3.29 E+05	6.34 E–05	1.05 E+04
32	1.83 E–09	1.26 E–05	1.75 E+04	1.91 E–04	2.07 E+05	5.32 E–06	7.02 E+03
40	3.17 E–10	2.54 E–06	1.41 E+04	1.23 E–05	1.56 E+05	4.98 E–07	5.33 E+03
45	1.40 E–11	2.27 E–07	2.44 E+04	1.43 E–06	3.96 E+05	4.11 E–08	1.29 E+04

Table 5.6: Cost functional J in heat transfer example: error convergence, error bounds, and effectivities as a function of M.

We finally consider the online computational cost for solving the reduced basis optimal control problem compared to the truth optimal control problem. On average (over Ξ_{test}) it takes 1.23 seconds to solve the truth optimal control problem based on our finite element discretization. Depending on the reduced basis dimension $1 \leq M \leq M_{\max} = 45$ it takes between 1.43 and 5.91 milliseconds to solve the reduced basis optimal control problem resulting in speedups ranging from 208 to 860. Taking into account the computation of the error bounds (consisting mainly of the online residual calculation and evaluating $\alpha_a^{\text{LB}}(\mu)$) the online cost for the reduced basis solution ranges from 2.21 to 9.02 milliseconds which in turn corresponds to a speedup of 136 up to 557. Note that the computational time required for the error bound computation is only a small fraction of the reduced basis solution time.

5.3. Performance of error bounds for varying regularization parameter. In this section we investigate the behavior of the parametrized optimal control problem and the performance of the error bounds for different choices of λ. We again consider the Graetz flow and heat transfer problem introduced in the last two sections and generate five different reduced basis spaces for $\lambda = 1$, 0.1, 0.01, 0.001, and 0.0001 using the greedy sampling procedure. In Table 5.7, we present the number of reduced basis functions $M_{\max}$ required to achieve the prescribed sampling tolerance $\epsilon_{\text{tol,min}} = 10^{-4}$ vs. the value of the regularization parameter λ (note that $\lambda = 0.01$ corresponds to the case discussed in the last two sections). As one can expect the reduced basis dimension $M_{\max}$ increases for decreasing λ. The main reason for this behavior is the increased parametric complexity for smaller values of λ, although we will next observe that the effectivities of the error bounds (in the greedy sampling we use the relative ALT control error bound) will also increase slightly for decreasing λ.

	λ	1	0.1	0.01	0.001	0.0001
Graetz flow	$M_{\max}$	13	16	19	22	24
Heat transfer	$M_{\max}$	35	39	45	50	61

Table 5.7: Size of Reduced Basis $M_{\max}$ to achieve desired accuracy of $\epsilon_{\text{tol,min}} = 10^{-4}$.

We will now turn to the influence of λ on the error bounds. In Figure 5.4, we present the average (over the test set Ξ_{test} and reduced basis dimension M) control error bound effectivities, $\Delta_N^{u,\bullet}(\mu)/\|e^{u,*}(\mu)\|_{U(\mu)}$, as a function of λ for the Graetz flow and heat transfer problem. Note that this corresponds to five separate evaluations each for a fixed $\lambda \in \{1, 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}\}$. In addition to the previous tables we also show two more bounds: the original perturbation bound as defined in (4.9) and the λ-scaled bound BNB-λ which measures the error in the $\|\cdot\|_{X_\lambda(\mu)}$-norm instead of the $\|\cdot\|_{X(\mu)}$-norm. Also recall that the original perturbation bound (4.9) is not online-efficient since it requires a state and adjoint truth solve. We first observe that the effectivities of all bounds increase with decreasing λ. Furthermore, they scale — except for the ALT-bound — with approximately $1/\lambda$ for $\lambda \leq 10^{-2}$, whereas the ALT-bound shows approximately a scaling with $1/\sqrt{\lambda}$. We recall our discussion after Proposition 4.7 explaining this effect. We also observe that the PER-bound performs slightly better than the BNB-λ and BNB-bounds (again, taking the additional overestimation due to $\beta_{\text{Ba}}^{\text{LB}}(\mu)$ into account); however, all three bounds become meaningless for small values of λ. In contrast, the ALT-bound effectivity remains acceptable even for $\lambda = 10^{-4}$ and is remarkably even smaller than the original (online-expensive) perturbation bound for small values of λ.

In Figure 5.5 and Figure 5.6, we present the corresponding results for the average

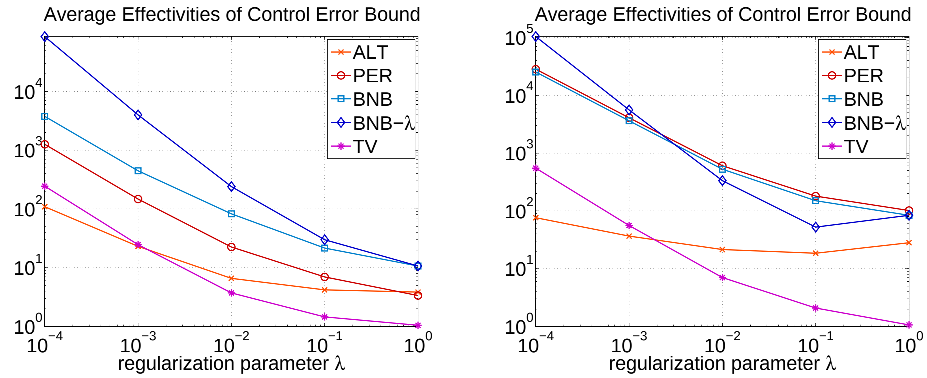


Fig. 5.4: Average control error bound effectivities (over M and Ξ_{test}) vs. regularization parameter λ for Graetz flow (left) and heat transfer problem (right)

combined error bound effectivities, $\Delta_N^{x,\bullet}(\mu)/\|e^{x,*}(\mu)\|_{X(\mu)}$, and average cost functional error bound effectivities, $\Delta_N^{J,\bullet}(\mu)/|J^*(\mu) - J_N^*(\mu)|$, respectively. Note that for the bound BNB-λ the error is measured in the $X_\lambda(\mu)$-norm. Overall, we observe a similar behavior as for the control variable. We do note, however, that the effectivity of the λ-scaled bound BNB-λ is in most cases approximately one order of magnitude smaller than for the non-scaled BNB-bound. The scaling thus allows to improve the effectivity especially for the cost functional error bound.

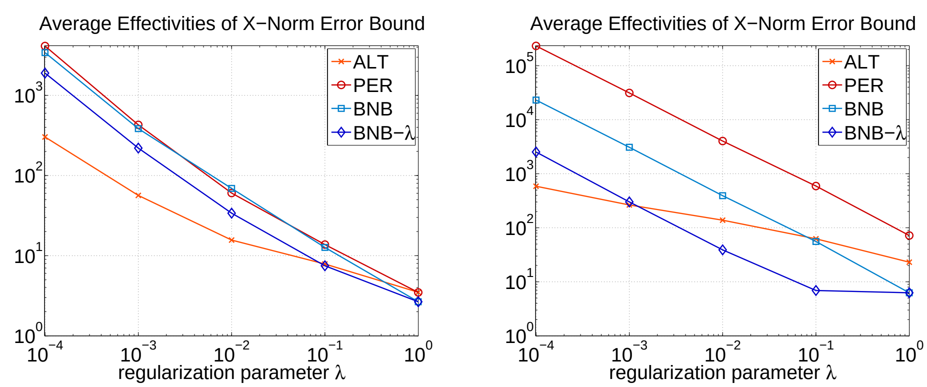


Fig. 5.5: Average X-norm error bound effectivities (over M and Ξ_{test}) vs. regularization parameter λ for Graetz flow (left) and heat transfer problem (right)

6. Conclusions. The solution of distributed optimal control problems governed by parametrized elliptic PDEs is a challenging and often time-consuming task, especially if one is interested in solutions at many different parameter values. We therefore employed the surrogate model approach and replaced the original high-dimensional PDE approximation by its reduced basis approximation. We also presented two new rigorous *a posteriori* error bounds for the optimal control and associated cost functional. The first one is based on a perturbation argument and is an extension of our previous work in [6, 14] to distributed optimal control problems. The second one is

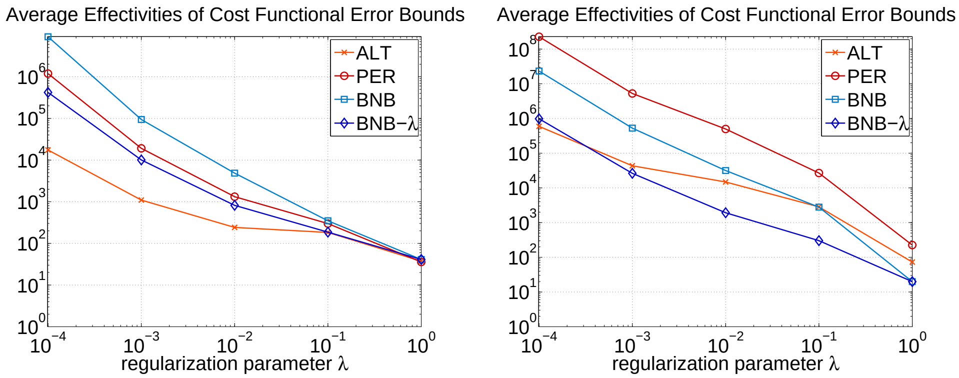


Fig. 5.6: Average cost functional error bound effectivities (over M and Ξ_{test}) vs. regularization parameter λ for Graetz flow (left) and heat transfer problem (right)

derived directly from the error residual equation of the optimality system and has — to the best of our knowledge — never been proposed before. We showed that the reduced basis optimal control problem and the *a posteriori* error bounds can be evaluated efficiently using the standard offline-online computational procedure, resulting in online computational savings of $\mathcal{O}(100)$.

We also compared the two proposed bounds to an *a posteriori* error bound based on the Banach-Nečas-Babuška (BNB) theory proposed in [22]. Concerning the computational cost and implementation effort, the proposed bounds present several advantages compared to the BNB-bound: we only require constants resp. their upper or lower bounds which are inexpensive and straightforward to evaluate, whereas evaluation of a lower bound of the Babuška inf-sup constant for the BNB-bound is (offline-)expensive and difficult to implement. Furthermore, although the performance of the PER-bound is overall similar to the BNB-bound, it has a much wider applicability, e.g., to parabolic problems involving control constraints [15]. The ALT-bound performed best overall, delivering the sharpest *a posteriori* error bounds and the best scaling with respect to the regularization parameter λ. The extension of this bound to parabolic optimal control problems is a topic of current research.

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