A Posteriori Error Estimation for Reduced Order Solutions of Parametrized Parabolic Optimal Control Problems*

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A POSTERIORI ERROR ESTIMATION FOR REDUCED ORDER SOLUTIONS OF PARAMETRIZED PARABOLIC OPTIMAL CONTROL PROBLEMS *

Mark Kärcher[1] and Martin A. Grepl[2]

Abstract. We consider the efficient and reliable solution of linear-quadratic optimal control problems governed by parametrized parabolic partial differential equations. To this end, we employ the reduced basis method as a low-dimensional surrogate model to solve the optimal control problem and develop a posteriori error estimation procedures that provide rigorous bounds for the error in the optimal control and the associated cost functional. We show that our approach can be applied to problems involving control constraints and that, even in the presence of control constraints, the reduced order optimal control problem and the proposed bounds can be efficiently evaluated in an offline-online computational procedure. We also propose two greedy sampling procedures to construct the reduced basis space. Numerical results are presented to confirm the validity of our approach.

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. [16,27,28,42] 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. The solution of these problems using classical discretization techniques such as finite elements or finite volumes is computationally expensive and time-consuming. 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 [4,25,26,41,43], reduction based on inertial manifolds in [19], and reduced basis methods in [8,9,20–22,31,34,41]; for a review of various model order reduction techniques we also refer to [2,6,40]. However, the solution of the reduced order optimal control problem is generally suboptimal and reliable error estimation is thus crucial.

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In this paper we employ the reduced basis method as a surrogate model for the solution of optimal control problems. The reduced basis method is a model order reduction technique which provides efficient yet reliable approximations to solutions of parametrized partial differential equations in the many-query or real-time context [29, 33]; also see [38] for a review of contributions to the methodology and further references. The methodology is thus ideally suited for the solution of parametrized PDE-constrained optimal control problems.

Here, we extend our previous work in [12, 24] in the following two directions: First, we consider optimal control problems governed by *time-dependent (parabolic)* PDEs. To this end, we allow for multiple controls which are scalar functions of time. Second, we consider problems involving box *constraints on the controls*, i.e., upper and lower bounds. We develop rigorous *a posteriori* error bounds for the optimal control *and* the associated cost functional and show that the reduced order optimal control problem *and* error bounds can be efficiently evaluated in an offline-online computational procedure. We note that the efficient, real-time solution of optimal control problems is essential in model predictive control of PDEs, see e.g. [1, 18, 36].

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 [43] and [8, 9, 31], respectively. In [43], the authors estimate the distance between the computed suboptimal control and the unknown optimal control using a perturbation argument proposed in [15, 30]. The approach allows 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 [43], is thus computationally expensive. In [8, 9], reduced basis approximations and associated *a posteriori* error estimation procedures have been derived to estimate the error in the optimal value of the cost functional. However, although the estimator is efficient to evaluate, it is not a rigorous upper bound for the error. Recently, a reduced basis approach to optimal control problems based on a saddle-point formulation has been considered in [31]. The resulting *a posteriori* error bound follows directly from previous work on reduced basis methods for saddle point problems [37, 39]. However, the saddle point theory only provides a combined bound for the error in the state, adjoint, and control variable. Furthermore, the approach is only applicable to optimal control problems without control constraints involving stationary (time-independent) PDEs. The former restriction is due to the fact that the results from [37, 39] do not apply to variational inequalities, the latter since calculating the stability constant of the space-time saddle point problem, i.e., (a lower bound to) the Babuška inf-sup constant, is computationally prohibitive.

This paper is organized as follows. In Section 1 we briefly review the reduced basis method for linear parabolic PDEs. The optimal control problem is discussed in Section 2: we start with the general problem statement, state the first order optimality conditions, and illustrate how the reduced basis approximation can be used as a surrogate model. In Section 3 we turn to the *a posteriori* error estimation and develop bounds for the optimal control and the associated cost functional. Finally we present numerical results for a model problem in Section 4.

1. The Reduced Basis Method

We start with the general problem formulation and a brief review of the reduced basis approximation and associated *a posteriori* error estimation for linear parabolic PDEs; we refer the reader to [13] for more details.

1.1. **Problem Formulation**

Let Y_e with $H_0^1(\Omega) \subset Y_e \subset H^1(\Omega)$ 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 $(\cdot, \cdot)_{Y_e}$ and $\|\cdot\|_{Y_e} = \sqrt{(\cdot, \cdot)_{Y_e}}$, respectively; we assume that the norm $\|\cdot\|_{Y_e}$ is equivalent to the $H^1(\Omega)$-norm. We also recall the Hilbert space $W(0, T) = \{v \in L^2(0, T; Y) : v_t \in L^2(0, T; Y')\}$ for a fixed final time T with its standard inner product, see for example [35]. In anticipation of the optimal control problem considered in Section 2 we also introduce the control space $\mathcal{U}_e = L^2(0, T; \mathbb{R}^m), m \in \mathbb{N}$, together with its inner product $(w, v)_{\mathcal{U}_e} = \int_0^T (w(t), v(t))_{\mathbb{R}^m} dt$ and

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[1]The subscript e denotes "exact".

induced norm $\|\cdot\|_{\mathcal{U}_e} = \sqrt{(\cdot,\cdot)_{\mathcal{U}_e}}$. We denote the associated dual spaces of Y_e and $\mathcal{U}_e$ by Y'_e and $\mathcal{U}'_e$, respectively. 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 (for the sake of simplicity) parameter-independent bilinear form $m(w,v) = (w,v)_{L^2(\Omega)}$, $\forall w, v \in L^2(\Omega)$, and the parameter-dependent bilinear form $a(\cdot,\cdot;\mu) : Y_e \times Y_e \to \mathbb{R}$. We shall assume that $a(\cdot,\cdot;\mu)$ is continuous,

$$\gamma_e(\mu) = \sup_{w \in Y_e \setminus \{0\}} \sup_{v \in Y_e \setminus \{0\}} \frac{a(w,v;\mu)}{\|w\|_{Y_e} \|v\|_{Y_e}} \leq \gamma_0 < \infty, \quad \forall \mu \in \mathcal{D}, \tag{1.1}$$

coercive,

$$\alpha_e(\mu) = \inf_{v \in Y_e \setminus \{0\}} \frac{a(v,v;\mu)}{\|v\|_{Y_e}^2} \geq \alpha_0 > 0, \quad \forall \mu \in \mathcal{D}, \tag{1.2}$$

and affinely parameter dependent,

$$a(w,v;\mu) = \sum_{q=1}^{Q_a} \Theta_a^q(\mu)\, a^q(w,v), \quad \forall w, v \in Y_e, \quad \forall \mu \in \mathcal{D}, \tag{1.3}$$

for some (preferably) small integer Q_a. Here, the coefficient functions $\Theta_a^q : \mathcal{D} \to \mathbb{R}$ are continuous and depend on μ, but the continuous bilinear forms a^q do *not* depend on μ. We also introduce the continuous and linear operator $\mathcal{B}_e : \mathcal{U}_e \to L^2(0,T;Y'_e)$, given by

$$\langle (\mathcal{B}_e u_e)(t), \cdot \rangle_{Y'_e, Y_e} = \sum_{i=1}^m b_i(\cdot) u_{e,i}(t), \tag{1.4}$$

where $\langle \cdot, \cdot \rangle_{Y'_e, Y_e}$ denotes the dual pairing between Y'_e and Y_e, $b_1, \ldots, b_m$ are given bounded linear functionals on $L^2(\Omega)$ and $u_e \in \mathcal{U}_e$ is the control with time-dependent control components $u_{e,i} \in L^2(0,T)$, $1 \leq i \leq m$. For simplicity, we assume that the functionals $b_1, \ldots, b_m$ do not depend on the parameter; however, (affine) parameter dependence of the b_i and thus of the operator $\mathcal{B}_e$ itself is readily admitted [13]. Finally, we require that all linear and bilinear forms are independent of time – the system is thus linear time-invariant (LTI). This is true for many physical problems governed by parabolic PDEs, including the classical heat equation.

We may now introduce the exact problem statement: For any parameter $\mu \in \mathcal{D}$ and fixed control $u_e \in \mathcal{U}_e$, find $y_e(t) \equiv y_e(t;\mu) \in W(0,T)^2$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t} m(y_e(t), v) + a(y_e(t), v; \mu) = \langle \mathcal{B}_e u_e(t), v \rangle_{Y'_e, Y_e}, \quad \forall v \in Y_e, \quad \text{f.a.a. } t \in (0,T], \tag{1.5}$$

with initial condition $y_e(0) = y_0 \equiv 0$. This equation constitutes the PDE constraint for the optimal control problem considered in Section 2. Note that the treatment of non-homogeneous and (affinely) parameter-dependent initial conditions is also possible [13].

1.2. **Truth Approximation**

For the time-discretization of the exact problem (1.5) we divide the time interval $[0,T]$ into K subintervals of equal length $\tau = \frac{T}{K}$ and define $t^k = k\tau, 0 \leq k \leq K$, and (for convenience) $\mathbb{K} = \{1, \ldots, K\}$. We shall employ the backward Euler method for the time integration; we note, however, that the treatment of higher-order schemes such as Crank-Nicolson (or a general Θ-scheme) is also possible. The discretized control space is given by $\mathcal{U} = (\mathbb{R}^m)^K$, the inner product by $(u,v)_{\mathcal{U}} = \tau \sum_{k=1}^K (u^k, v^k)_{\mathbb{R}^m}$, and the corresponding induced norm by $\|\cdot\|_{\mathcal{U}} = \sqrt{(\cdot,\cdot)_{\mathcal{U}}}$. Here, a control is denoted by $u = (u^1, \ldots, u^K), u^k \in \mathbb{R}^m$, such that $u_i^k \in \mathbb{R}$ corresponds to the i-th control input at time t^k, i.e., $u_i^k = u_i(t^k)$.

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

We next introduce a "truth" finite element approximation space $Y \subset Y_e$ of very large dimension $\mathcal{N}$. Note that Y shall inherit the inner product and norm from Y_e: $(\cdot, \cdot)_Y = (\cdot, \cdot)_{Y_e}$ and $\|\cdot\|_Y = \|\cdot\|_{Y_e}$. Clearly, the continuity and coercivity properties of the bilinear form a are inherited by the "truth" approximation, i.e.,

$$\gamma(\mu) = \sup_{w \in Y \backslash \{0\}} \sup_{v \in Y \backslash \{0\}} \frac{a(w, v; \mu)}{\|w\|_Y \|v\|_Y} \le \gamma_e(\mu) \le \gamma_0 < \infty, \quad \forall \mu \in \mathcal{D}, \tag{1.6}$$

and

$$\alpha(\mu) = \inf_{v \in Y \backslash \{0\}} \frac{a(v, v; \mu)}{\|v\|_Y^2} \ge \alpha_e(\mu) \ge \alpha_0 > 0, \quad \forall \mu \in \mathcal{D}. \tag{1.7}$$

We also define the operator $\mathcal{B} : \mathcal{U} = (\mathbb{R}^m)^K \to (Y')^K$ by

$$\langle (\mathcal{B}u)_k, \cdot \rangle_{Y', Y} = \sum_{i=1}^m b_i(\cdot) u_i^k, \quad k \in \mathbb{K}, \tag{1.8}$$

which is the discrete counterpart to the operator $\mathcal{B}_e$.

We can thus state the (fully discretized) truth approximation to the exact problem (1.5): Given a parameter $\mu \in \mathcal{D}$ and control $u \in \mathcal{U}$, find $y^k \equiv y(t^k; \mu) \in Y$, $\forall k \in \mathbb{K}$, such that

$$m(y^k, v) + \tau\, a(y^k, v; \mu) = m(y^{k-1}, v) + \tau \langle (\mathcal{B}u)_k, v \rangle_{Y', Y}, \quad \forall v \in Y, \quad \forall k \in \mathbb{K}, \tag{1.9}$$

with initial condition $y^0 = y_0 = 0$.

We shall assume that the truth space Y is sufficiently rich and the time-discretization is sufficiently fine such that $y^k(\mu)$ and $y_e(t^k; \mu)$ are indistinguishable. Finally, we recall that the reduced basis approximation shall be built upon – and the reduced basis error thus evaluated with respect to – the truth solution $y^k(\mu) \in Y, k \in \mathbb{K}$.

1.3. Reduced Basis Approximation

We suppose that we are given the nested Lagrangian reduced basis spaces $Y_N = \text{span}\{\zeta_n, 1 \le n \le N\}$, $1 \le N \le N_{\max}$, where the ζ_n, $1 \le n \le N$, are mutually $(\cdot, \cdot)_Y$-orthogonal basis functions. The basis functions are generally constructed using a POD/Greedy sampling procedure [14].

The reduced basis approximation is then obtained by a standard Galerkin projection onto the reduced basis space: Given $\mu \in \mathcal{D}$ and $u \in \mathcal{U}$, find $y_N^k \equiv y_N(t^k; \mu) \in Y_N$ such that

$$m(y_N^k, v) + \tau\, a(y_N^k, v; \mu) = m(y_N^{k-1}, v) + \tau \langle (\mathcal{B}u)_k, v \rangle_{Y', Y}, \quad \forall v \in Y_N, \quad \forall k \in \mathbb{K}, \tag{1.10}$$

with initial condition $y_N^0 = y_0 = 0$.

1.4. A Posteriori Error Estimation

A posteriori error estimation procedures play a decisive role in the reduced basis method. The error bounds help to (*i*) efficiently and rigorously assess the error introduced by the reduced basis approximation; and (*ii*) drive the POD/Greedy procedure for generating the reduced basis space Y_N.

To begin, we specify the inner product $(v, w)_Y = \frac{1}{2}\left(a(v, w; \mu^{\text{ref}}) + a(w, v; \mu^{\text{ref}})\right)$, where $\mu^{\text{ref}} \in \mathcal{D}$ is a reference parameter value. We next assume that we are given a positive lower bound $\alpha_{\text{LB}}(\mu) : \mathcal{D} \to \mathbb{R}_+$ for the coercivity constant $\alpha(\mu)$ such that

$$\alpha(\mu) \ge \alpha_{\text{LB}}(\mu) \ge \alpha_0 > 0, \quad \forall \mu \in \mathcal{D}; \tag{1.11}$$

various recipes exist to construct this lower bound [17, 33, 44]. We now state the standard "spatio-temporal" energy norm error bound in Theorem 1.1; for the proof we refer to [13].

Theorem 1.1. *Let y^k be the solution of the truth problem (1.9) and y_N^k be the corresponding reduced basis approximation satisfying (1.10). For the "spatio-temporal" energy norm*

$$|||v^k|||^y \equiv \left(m(v^k, v^k) + \sum_{k'=1}^{k} \tau\, a(v^{k'}, v^{k'}; \mu) \right)^{\frac{1}{2}}, \quad \forall k \in \mathbb{K}, \tag{1.12}$$

the error, $e^{y,k} = y^k - y_N^k$, satisfies

$$|||e^{y,k}|||^y \leq \Delta_N^k(\mu) \equiv \left(\frac{\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=1}^{k} \| r^{y,k'}(\cdot; \mu) \|_{Y'}^2 \right)^{\frac{1}{2}}, \quad \forall k \in \mathbb{K}, \tag{1.13}$$

where the residuals $r^{y,k}(\cdot; \mu) : Y \to \mathbb{R}$ are given by

$$r^{y,k}(v; \mu) = \langle (\mathcal{B}u)_k, v \rangle_{Y',Y} - a(y_N^k, v; \mu) - \frac{1}{\tau} m(y_N^k - y_N^{k-1}, v), \quad \forall v \in Y,\ \forall k \in \mathbb{K}, \tag{1.14}$$

and their dual norms by $\| r^{y,k}(\cdot; \mu) \|_{Y'} \equiv \sup_{v \in Y \setminus \{0\}} r^{y,k}(v; \mu) / \|v\|_Y$.

The proof for the energy norm bound can be slightly modified in order to obtain a bound for the error in the L^2-norm, i.e., one can show that [14]

$$\| e^{y,k} \|_{L^2(\Omega)} \leq \frac{1}{\sqrt{2}} \Delta_N^k(\mu), \quad \forall k \in \mathbb{K}. \tag{1.15}$$

We will use this bound on two occasions in Section 3.

1.5. Computational Procedure

The affine parameter dependence of the bilinear form a allows an efficient offline-online computational procedure to evaluate the reduced basis approximation y_N^k and associated *a posteriori* error bound $\Delta_N^k(\mu)$, $k \in \mathbb{K}$. We briefly recall the essential steps of the former and then summarize the online computational cost to evaluate y_N^k and $\Delta_N^k(\mu)$; see [13] for more details.

We write $y_N^k(\mu) = \sum_{i=1}^{N} y_{Ni}^k(\mu) \zeta_i$ and choose as test functions $v = \zeta_i$, $1 \leq i \leq N$, in (1.10). It then follows that $\underline{y}_N^k(\mu) = [y_{N1}^k(\mu), \ldots, y_{NN}^k(\mu)]^T \in \mathbb{R}^N$ satisfies

$$(M_N + \tau A_N(\mu))\, \underline{y}_N^k(\mu) = M_N \underline{y}_N^{k-1}(\mu) + \tau B_N u^k, \quad k \in \mathbb{K}, \tag{1.16}$$

with initial condition $y_{Ni}^0(\mu) = 0$, $1 \leq i \leq N$. Here, $u^k = (u_1^k, \ldots, u_m^k)^T \in \mathbb{R}^m$ are the control inputs at time t^k and $M_N \in \mathbb{R}^{N \times N}, A_N(\mu) \in \mathbb{R}^{N \times N}$, and $B_N(\mu) \in \mathbb{R}^{N \times m}$ are matrices with entries $(M_N)_{ij} = m(\zeta_j, \zeta_i)$, $1 \leq i,j \leq N$, $(A_N(\mu))_{ij} = a(\zeta_j, \zeta_i; \mu)$, $1 \leq i,j \leq N$, and $(B_N)_{ij} = b_j(\zeta_i)$, $1 \leq i \leq N$, $1 \leq j \leq m$, respectively. Invoking the affine parameter dependence (1.3) 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 $(A_N^q)_{ij} = a^q(\zeta_j, \zeta_i)$, $1 \leq i,j \leq N$, $1 \leq q \leq Q_a$.

The offline computational cost clearly depends on $\mathcal{N}$: we need to solve for the basis functions ζ_i, $1 \leq i \leq N$, and precompute the parameter-independent matrices M_N, B_N, and A_N^q, $1 \leq q \leq Q_a$; the offline cost associated to $\Delta_N^k(\mu)$ also depends on $\mathcal{N}$ [13]. However, in the online stage, for each new parameter value μ, we assemble the parameter-dependent matrix $A_N(\mu)$ at cost $\mathcal{O}(Q_a N^2)$ and then solve (1.16) at cost $\mathcal{O}(N^3 + K N^2)$ (based on LU factorization and our LTI assumption). We subsequently evaluate $\Delta_N^k(\mu)$, $k \in \mathbb{K}$, online at cost $\mathcal{O}(K(Q_a N + m)^2)$. The computational cost in the online stage is thus independent of the truth finite element dimension $\mathcal{N}$.

2. Optimal Control Problem

In this section we introduce the parametrized linear-quadratic optimal control problem with parabolic PDE constraint. We recall the first-order necessary (and in our case sufficient) optimality conditions and employ the reduced basis method for the efficient solution of the resulting optimality systems.

2.1. General Problem Statement

We consider the problem setting as stated in Section 1. We next introduce the quadratic cost functional $J_e(\cdot, \cdot; \mu) : W(0, T) \times \mathcal{U}_e \to \mathbb{R}$ given by

$$J_e(y_e, u_e; \mu) = \frac{\sigma_1}{2} \int_0^T \|y_e - y_{d,e}\|^2_{L^2(D)} dt + \frac{\sigma_2}{2} \|y_e(T) - y_{d,e}(T)\|^2_{L^2(D)} + \frac{\lambda}{2} \|u_e - u_{d,e}\|^2_{\mathcal{U}_e}, \qquad (2.1)$$

where $D \subset \Omega$ or $D \subset \Gamma$ is a measurable set; $y_{d,e} \in L^2(0, T; L^2(D))$ and $u_{d,e} \in \mathcal{U}_e$ are the desired state and control, respectively. For simplicity, we assume that the desired state $y_{d,e}$ and the desired control $u_{d,e}$ are parameter-independent; however, (affine) parameter dependence is readily admitted [24]. The given regularization parameters $\lambda > 0$ and $\sigma_1, \sigma_2 \geq 0$ govern the trade-off between the cost associated with the deviation from the desired control and the desired state (over the whole time trajectory and/or at the final time), respectively.

In practice, the regularization parameters often serve as design parameters which are tuned to achieve a desired performance of the optimal controller. From a reduced basis point of view, however, the regularization parameters may simply be considered input parameters of the parametrized optimal control problem. This allows us to vary (say) λ online and thus to efficiently design the optimal controller with the approach presented here. For our model problem in Section 4 we will in fact consider λ as an additional (reduced basis) input parameter.

Since we also consider box constraints on the control, we finally introduce the non-empty convex subset of admissible controls by

$$\mathcal{U}_{e,ad} = \{u_e \in \mathcal{U}_e : u_{a,e}(t) \leq u_e(t) \leq u_{b,e}(t)\} \subset \mathcal{U}_e. \qquad (2.2)$$

Here, $u_{a,e}, u_{b,e} \in L^2(0, T; \mathbb{R}^m)$, with $u_{a,e}(t) \leq u_{b,e}(t)$, f.a.a. $t \in [0, T]$, are given lower and upper bounds for the control components and the inequalities are interpreted component-wise in $\mathbb{R}^m$.

We can now state the parametrized optimal control problem as

$$\min J(y_e, u_e; \mu) \quad \text{s.t.} \quad (y_e, u_e) \in W(0, T) \times \mathcal{U}_{e,ad} \quad \text{solves}$$
$$\frac{d}{dt} m(y_e(t), v) + a(y_e(t), v; \mu) = \langle (\mathcal{B}_e u_e)(t), v \rangle_{Y'_e, Y_e}, \quad \forall v \in Y_e, \quad \text{f.a.a. } t \in (0, T], \qquad (\mathrm{P_e})$$

with initial condition $y_e(0) = y_0 \equiv 0$. It follows from our assumptions that there exists a unique optimal solution (y_e^*, u_e^*) to $(\mathrm{P_e})$ [28]. Employing a Lagrangian approach we obtain the first-order optimality system consisting of the state equation, the adjoint equation, and the optimality condition: Given $\mu \in \mathcal{D}$, the optimal solution $(y_e^*, p_e^*, u_e^*) \in W(0, T) \times W(0, T) \times \mathcal{U}_{e,ad}$ satisfies

$$\frac{d}{dt} m(y_e^*(t), \phi) + a(y_e^*(t), \phi; \mu) = \langle (\mathcal{B}_e u_e^*)(t), \phi \rangle_{Y'_e, Y_e}, \qquad \forall \phi \in Y_e, \quad \text{f.a.a. } t \in (0, T], \qquad (2.3a)$$

$$y_e^*(0) = y_0 \equiv 0 \qquad (2.3b)$$

$$-\frac{d}{dt} m(\varphi, p_e^*(t)) + a(\varphi, p_e^*(t); \mu) = \sigma_1(y_{d,e}(t) - y_e^*(t), \varphi)_{L^2(D)}, \qquad \forall \varphi \in Y_e, \quad \text{f.a.a. } t \in [0, T), \qquad (2.3c)$$

$$m(\varphi, p_e^*(T)) = \sigma_2(y_{d,e}(T) - y_e^*(T), \varphi)_{L^2(D)}, \qquad \forall \varphi \in Y_e, \qquad (2.3d)$$

$$(\lambda(u_e^* - u_{d,e}) - \mathcal{B}_e^\star p_e^*, \psi - u_e^*)_{\mathcal{U}_e} \geq 0, \qquad \forall \psi \in \mathcal{U}_{e,ad}. \qquad (2.3e)$$

Here, p_e is the adjoint variable and the superscript * denotes optimality. Furthermore, the linear and bounded dual operator of $\mathcal{B}_e$ in (2.3e) is given by $\mathcal{B}_e^\star : L^2(0,T;Y_e) \to \mathcal{U}_e$, where we identify $(L^2(0,T;Y_e'))'$ with $L^2(0,T;Y_e)$ and $\mathcal{U}_e'$ with $\mathcal{U}_e$. From the relationship

$$\langle \mathcal{B}_e u, \phi \rangle_{L^2(0,T;Y)',L^2(0,T;Y)} = \int_0^T \sum_{i=1}^m b_i(\phi(t)) u_i(t) \mathrm{d}t = \int_0^T \left(u(t), (\mathcal{B}_e^\star \phi)(t) \right)_{\mathbb{R}^m} \mathrm{d}t = (u, \mathcal{B}_e^\star \phi)_{\mathcal{U}_e} \qquad (2.4)$$

it follows that, for given $\phi \in L^2(0,T;Y_e)$, the dual operator $\mathcal{B}_e^\star \phi$ can be expressed as

$$(\mathcal{B}_e^\star \phi)_i(t) = b_i(\phi(t)), \quad 1 \leq i \leq m, \quad t \in [0,T]. \qquad (2.5)$$

We note that for the linear-quadratic optimal control problem (P$_e$) the first-order conditions (2.3) are necessary and sufficient for the optimality of (y_e^*, u_e^*) [28].

2.2. Truth Approximation

In general, we of course cannot expect to find an analytic solution to (2.3). We thus introduce a temporal and spatial discretization as discussed in Section 1.2: we divide $[0,T]$ into K subintervals of equal length $\tau = \frac{T}{K}$ and introduce a "truth" approximation space $Y \subset Y_e$ of very large dimension $\mathcal{N}$. The discretized cost functional $J(\cdot,\cdot;\mu) : Y^K \times \mathcal{U} \to \mathbb{R}$ is then given by

$$J(y,u;\mu) = \frac{\sigma_1}{2} \tau \sum_{k=1}^K \|y^k - y_d^k\|_{L^2(D)}^2 + \frac{\sigma_2}{2} \|y^K - y_d^K\|_{L^2(D)}^2 + \frac{\lambda}{2} \tau \sum_{k=1}^K \|u^k - u_d^k\|_{\mathbb{R}^m}^2, \qquad (2.6)$$

where $u_d^k = u_{d,e}(t^k) \in \mathbb{R}^m$ and $y_d^k \in Y$ is the L^2–projection of $y_{d,e}(t^k)$. The discretized admissible control set is

$$\mathcal{U}_{\mathrm{ad}} = \{ u \in \mathcal{U} : u_a^k \leq u^k \leq u_b^k, \ k \in \mathbb{K} \}, \qquad (2.7)$$

where $u_a^k = u_{a,e}(t^k) \in \mathbb{R}^m$ and $u_b^k = u_{b,e}(t^k) \in \mathbb{R}^m$. Consequently, the corresponding truth optimal control problem is then given by

$$\begin{aligned} &\min J(y,u;\mu) \quad \text{s.t.} \quad (y,u) \in Y^K \times \mathcal{U}_{\mathrm{ad}} \quad \text{solves} \\ &m(y^k, v) + \tau \, a(y^k, v; \mu) = m(y^{k-1}, v) + \tau \langle (\mathcal{B}u)_k, v \rangle_{Y',Y}, \quad \forall v \in Y, \quad \forall k \in \mathbb{K}, \end{aligned} \qquad \text{(P)}$$

with initial condition $y^0 = y_0 = 0$.

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

$$m(y^{*,k} - y^{*,k-1}, \phi) + \tau \, a(y^{*,k}, \phi; \mu) = \tau \, \langle (\mathcal{B}u^*)_k, \phi \rangle_{Y',Y}, \qquad \forall \phi \in Y, \quad \forall k \in \mathbb{K}, \qquad (2.8a)$$

$$y^{*,0} = y_0 \equiv 0, \qquad (2.8b)$$

$$m(\varphi, p^{*,k} - p^{*,k+1}) + \tau \, a(\varphi, p^{*,k}; \mu) = \tau \, \sigma_1 (y_d^k - y^{*,k}, \varphi)_{L^2(D)}, \qquad \forall \varphi \in Y, \quad \forall k \in \mathbb{K}, \qquad (2.8c)$$

$$m(\varphi, p^{*,K+1}) = \sigma_2 (y_d^K - y^{*,K}, \varphi)_{L^2(D)}, \qquad \forall \varphi \in Y, \qquad (2.8d)$$

$$(\lambda(u^* - u_d) - \mathcal{B}^\star p^*, \psi - u^*)_{\mathcal{U}} \geq 0, \qquad \forall \psi \in \mathcal{U}_{\mathrm{ad}}. \qquad (2.8e)$$

Here, the dual operator $\mathcal{B}^\star : Y^K \to \mathcal{U}$ is given for $\phi \in Y^K$ by

$$(\mathcal{B}^\star \phi)_i^k = b_i(\phi^k), \qquad (2.9)$$

which is the discrete counterpart to the dual operator $\mathcal{B}_e^\star$ defined in (2.5).

We further note that the Ansatz and test spaces are identical for the state and adjoint equations. This ensures that the solution of the optimality system (2.8) is indeed also an optimal solution of the truth optimal control problem (P).

The optimality system (2.8) constitutes a coupled set of equations (and variational inequalities) of dimension $2K\mathcal{N} + Km$ 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 (2.8) by employing the reduced basis approximation as a surrogate model for the PDE constraint in (P).

2.3. Reduced Basis Approximation

We first assume that we are given the reduced basis spaces

$$Y_N = \mathrm{span}\{\zeta_n, \ 1 \le n \le N\}, \quad 1 \le N \le N_{\max}, \tag{2.10}$$

where the $\zeta_n, \ 1 \le n \le N$, are mutually $(\cdot, \cdot)_Y$-orthogonal basis functions and $N, N_{\max}$ are even. We comment on the POD/Greedy sampling procedure to construct the spaces Y_N in Section 3.4.

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

$$\begin{aligned}
&\min J(y_N, u_N; \mu) \quad \text{s.t.} \quad (y_N, u_N) \in Y_N^K \times \mathcal{U}_{\mathrm{ad}} \quad \text{solves} \\
&m(y_N^k, v) + \tau\, a(y_N^k, v; \mu) = m(y_N^{k-1}, v) + \tau \langle (\mathcal{B}u_N)_k, v \rangle_{Y', Y}, \ \forall v \in Y_N, \quad \forall k \in \mathbb{K},
\end{aligned} \tag{$\mathrm{P_N}$}$$

with initial condition $y_N^0 = y_0 = 0$. Notice that the already low-dimensional truth control space $\mathcal{U}$ is not reduced, although this is possible for problems with high-dimensional control spaces, e.g., problems with distributed controls over parts of the domain or its boundary [23, 31].

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

$$m(y_N^{*,k} - y_N^{*,k-1}, \phi) + \tau\, a(y_N^{*,k}, \phi; \mu) = \tau \langle (\mathcal{B}u_N^*)_k, \phi \rangle_{Y', Y}, \qquad \forall \phi \in Y_N, \quad \forall k \in \mathbb{K}, \tag{2.11a}$$

$$y_N^{*,0} = y_0 \equiv 0, \tag{2.11b}$$

$$m(\varphi, p_N^{*,k} - p_N^{*,k+1}) + \tau\, a(\varphi, p_N^{*,k}; \mu) = \tau\, \sigma_1 (y_d^k - y_N^{*,k}, \varphi)_{L^2(D)}, \qquad \forall \varphi \in Y_N, \quad \forall k \in \mathbb{K}, \tag{2.11c}$$

$$m(\varphi, p_N^{*,K+1}) = \sigma_2 (y_d^K - y_N^{*,K}, \varphi)_{L^2(D)}, \qquad \forall \varphi \in Y_N, \tag{2.11d}$$

$$(\lambda(u_N^* - u_d) - \mathcal{B}^\star p_N^*, \psi - u_N^*)_{\mathcal{U}} \ge 0, \qquad \forall \psi \in \mathcal{U}_{\mathrm{ad}}. \tag{2.11e}$$

The reduced basis optimality system is only of dimension $2KN + Km$ and can be evaluated efficiently using an offline-online computational decomposition. Before presenting the details in the next section we make several remarks.

We note that we use a single "integrated" reduced basis Ansatz and test space for the state and adjoint equations. The reason is twofold: first, the reduced basis optimality system (2.11) reflects the reduced basis optimal control problem ($\mathrm{P_N}$) only if the spaces of the state and adjoint equations are identical; and second, using different spaces may result in an unstable system (2.11). This issue is closely related to the stability of reduced basis formulations for saddle point problems, see [11] for details. If we use the same space Y_N for the state *and* the adjoint equation, on the other hand, the system (2.11) is provably stable. Finally, since the state and adjoint solutions need to be well-approximated using the single space Y_N, we choose "integrated" spaces, i.e., we integrate both snapshots of the state and adjoint equations into the space Y_N defined in (2.10).

2.4. **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 and adjoint solutions as $y_N^k(\mu) = \sum_{i=1}^N y_{Ni}^k(\mu)\zeta_i$ and $p_N^k(\mu) = \sum_{i=1}^N p_{Ni}^k(\mu)\zeta_i$ and denote the coefficient vectors by $\underline{y}_N^k(\mu) = [y_{N1}^k(\mu), \ldots, y_{NN}^k(\mu)]^T \in \mathbb{R}^N$ and $\underline{p}_N^k(\mu) = [p_{N1}^k(\mu), \ldots, p_{NN}^k(\mu)]^T \in \mathbb{R}^N$, respectively. If we choose as test functions $\phi = \zeta_i$, $1 \leq i \leq N$, and $\varphi = \zeta_i$, $1 \leq i \leq N$, in (2.11), the reduced basis optimality system can be written as

$$(M_N + \tau A_N(\mu))\, \underline{y}_N^k(\mu) = M_N\, \underline{y}_N^{k-1}(\mu) + \tau B_N u_N^k, \qquad\qquad k \in \mathbb{K}, \qquad\qquad (2.12\text{a})$$

$$\underline{y}_N^0(\mu) = 0, \qquad\qquad (2.12\text{b})$$

$$(M_N + \tau A_N(\mu))\, \underline{p}_N^k(\mu) = M_N\, \underline{p}_N^{k+1}(\mu) + \tau\sigma_1\, (Y_{d,N}^k - D_N\, \underline{y}_N^k(\mu)), \qquad k \in \mathbb{K}, \qquad (2.12\text{c})$$

$$M_N\, \underline{p}_N^{K+1}(\mu) = \sigma_2\, (Y_{d,N}^K - D_N\, \underline{y}_N^K(\mu)), \qquad\qquad (2.12\text{d})$$

$$(\lambda(u_N^k - u_d^k) - B_N^T \underline{p}_N^k(\mu), \psi^k - u_N^k)_{\mathcal{U}} \geq 0, \qquad\qquad \forall \psi^k \in \mathcal{U}_{\text{ad}}^k, \quad k \in \mathbb{K}. \qquad (2.12\text{e})$$

Here, $A_N(\mu) \in \mathbb{R}^{N \times N}$, $M_N \in \mathbb{R}^{N \times N}$ and $B_N \in \mathbb{R}^{N \times m}$ are the matrices defined in Section 1.5; $D_N \in \mathbb{R}^{N \times N}$ is a matrix with the entries $(D_N)_{ij} = (\zeta_j, \zeta_i)_{L^2(D)}$, $1 \leq i, j \leq N$; and $Y_{d,N}^k \in \mathbb{R}^N, k \in \mathbb{K}$, are vectors with entries $(Y_{d,N})_i^k = (y_d^k, \zeta_i)_{L^2(D)}$, $1 \leq i \leq N$. Invoking the affine parameter dependence (1.3) yields the expansion $A_N(\mu) = \sum_{q=1}^{Q_a} \Theta_a^q(\mu) A_N^q$ as discussed in Section 1.5. Finally, to allow an efficient evaluation of the cost functional in the online stage, we also compute and store the scalars $\tilde{Y}_d^k \in \mathbb{R}, k \in \mathbb{K}$, given by $\tilde{Y}_d^k = (y_d^k, y_d^k)_{L^2(D)}$.

The offline-online decomposition is now clear. In the offline stage — performed only *once* — we first construct the reduced basis space Y_N. We then assemble the parameter-independent quantities A_N^q, $1 \leq q \leq Q_a$, M_N, D_N, B_N, $Y_{d,N}^k$, and $\tilde{Y}_d^k$. The computational cost clearly depends on the truth finite element dimension $\mathcal{N}$. In the online stage — for each new parameter value μ — we first assemble the parameter-dependent quantity $A_N(\mu)$ in $\mathcal{O}(Q_a N^2)$ operations. We then solve the reduced basis optimality system (2.12) iteratively with a BFGS Quasi-Newton method. The cost for one BFGS-iteration on the "reduced" cost functional $j_N(u_N; \mu) := J(y_N(u_N), u_N; \mu)$ is to leading order $\mathcal{O}(N^3 + KN^2 + KNm + (Km)^2)$. In the control constrained case we use the primal dual active set method (PDAS) resulting in an outer loop around the BFGS iteration. In our numerical tests we needed at most 4 PDAS iterations.

Given a reduced basis approximation, the cost functional can be evaluated efficiently from

$$J(y_N, u_N; \mu) = \frac{\sigma_1}{2}\tau \sum_{k=1}^K \left((\underline{y}_N^k)^T D_N \underline{y}_N^k - 2(Y_{d,N}^k)^T \underline{y}_N^k + \tilde{Y}_d^k \right)$$

$$+ \frac{\sigma_2}{2} \left((\underline{y}_N^K)^T D_N \underline{y}_N^K - 2(Y_{d,N}^K)^T \underline{y}_N^K + \tilde{Y}_d^K \right) + \frac{\lambda}{2}\tau \sum_{k=1}^K \|u_N^k - u_d^k\|_{\mathbb{R}^m}^2 \qquad (2.13)$$

in (to leading order) $\mathcal{O}(KN^2 + Km)$ operations.

Hence, the computational cost for the online stage is independent of $\mathcal{N}$, the dimension of the underlying "truth" finite element approximation space. Since $N \ll \mathcal{N}$, we expect significant computational savings in the online stage relative to the solution of (2.8). However, we need to rigorously and efficiently assess the error introduced.

3. A Posteriori Error Estimation

We will now develop *a posteriori* error bounds for the error in the optimal control and the error in the associated cost functional. The derivation is an extension of our previous results for elliptic and control unconstrained problems in [12, 24]. We note that *a posteriori* error bounds are not only crucial to confirm the fidelity of the

reduced basis optimal control solution, but are also an essential ingredient in the Greedy procedure to generate the reduced basis space Y_N.

We discuss the control and cost functional bounds in Sections 3.1 and Section 3.2, respectively. The error bounds introduced are rigorous upper bounds for the true errors and are efficient to compute; we summarize the computational procedure in Section 3.3. Finally, we present the Greedy procedure to generate Y_N in Section 3.4.

3.1. **Error Bound for the Optimal Control**

The point of departure for our bound is a result from [43], where the authors estimate the distance between the computed POD suboptimal control and the unknown truth optimal control using a perturbation argument proposed in [15,30]. This approach has also been applied to optimal control problems governed by elliptic PDEs in [3,7]. The idea is to introduce a perturbation function $\zeta \in \mathcal{U}$ such that the RB optimal control u_N^*, i.e., the perturbed control, satisfies the optimality condition

$$(\lambda(u_N^* - u_d) - \mathcal{B}^\star \tilde{p} + \zeta, \psi - u_N^*)_{\mathcal{U}} \geq 0, \quad \forall \psi \in \mathcal{U}_{\mathrm{ad}}, \tag{3.1}$$

of a perturbed optimal control problem. Here, $\tilde{p} = p(y(u_N^*))$ is the solution of the (truth) adjoint equation (2.8c) with $y(u_N^*)$ instead of $y^*(u^*)$ on the right-hand side, and $\tilde{y} = y(u_N^*)$ is the solution of the (truth) state equation (2.8a) with control u_N^* instead of u^*. It is then possible to explicitly construct ζ in terms of u_N^*, $\tilde{y}$, and $\tilde{p}$ such that (3.1) holds and to bound the error in the optimal control, $u^* - u_N^*$, in terms of ζ. More specifically, for notational convenience we define

$$\xi = \lambda(u_N^* - u_d) - \mathcal{B}^\star \tilde{p} \tag{3.2}$$

with components ξ_i^k, $i = 1, \ldots, m$, $k \in \mathbb{K}$. We then distinguish for every component ζ_i^k, $i = 1, \ldots, m$, $k \in \mathbb{K}$, the following three cases to construct ζ (see [43] for a more detailed discussion):

(1) If $u_{N,i}^{*,k} = u_{a,i}^k$, then $\psi_i^k - u_{N,i}^{*,k} \geq 0$ for all $\psi_i^k \in \mathcal{U}_{\mathrm{ad},i}^k$ and hence $\xi_i^k + \zeta_i^k \geq 0$ has to hold: we set $\zeta_i^k = \left[\xi_i^k\right]_-$.

(2) If $u_{N,i}^{*,k} = u_{b,i}^k$, then $\psi_i^k - u_{N,i}^{*,k} \leq 0$ for all $\psi_i^k \in \mathcal{U}_{\mathrm{ad},i}^k$ and hence $\xi_i^k + \zeta_i^k \leq 0$ has to hold: we set $\zeta_i^k = -\left[\xi_i^k\right]_+$.

(3) If $u_{N,i}^{*,k} \in \left(u_{a,i}^k, u_{b,i}^k\right)$, then $\psi_i^k - u_{N,i}^{*,k}$ can attain positive and negative values for $\psi_i^k \in \mathcal{U}_{\mathrm{ad},i}^k$ and hence $\xi_i^k + \zeta_i^k = 0$ has to hold: we set $\zeta_i^k = -\xi_i^k$.

Here, $[\cdot]_+$ and $[\cdot]_-$ denote the positive and negative part functions, respectively. To summarize, $\zeta \in \mathcal{U}$ is given component-wise by

$$\zeta_i^k = \begin{cases} \left[\xi_i^k\right]_- & \text{if } u_{N,i}^{*,k} = u_{a,i}^k; \\ -\left[\xi_i^k\right]_+ & \text{if } u_{N,i}^{*,k} = u_{b,i}^k; \\ -\xi_i^k & \text{if } u_{N,i}^{*,k} \in \left(u_{a,i}^k, u_{b,i}^k\right). \end{cases} \tag{3.3}$$

We can now state the main result (see Theorem 4.11 in [43]).

Theorem 3.1. *Let u^* and u_N^* be the optimal solutions of the truth and reduced basis optimal control problems* (P) *and* (P_N), *respectively. The error in the optimal control then satisfies*

$$\|u^* - u_N^*\|_{\mathcal{U}} \leq \frac{1}{\lambda}\|\zeta\|_{\mathcal{U}}, \quad \forall \mu \in \mathcal{D}. \tag{3.4}$$

To prove the error bound for the optimal control in our fully-discrete setting we require an intermediate result which we state in the following lemma. We refer the reader to Appendix A.1 for its proof.

Lemma 3.2. *Let $u_N^* \in \mathcal{U}_{\mathrm{ad}}$ be a perturbed control input and denote the associated solution of the truth state equation by $\tilde{y}^k \in Y, 1 \leq k \leq K$, and the associated solution of the truth adjoint equation by $\tilde{p}^k \in Y, 1 \leq k \leq K$. We then have*

$$\tau \sum_{k=1}^K \sum_{i=1}^m b_i(p^{*,k} - \tilde{p}^k)(u_{N,i}^{*,k} - u_i^{*,k}) \geq 0, \tag{3.5}$$

or equivalently

$$(\mathcal{B}^\star(p^* - \tilde{p}), u_N^* - u^*)_{\mathcal{U}} \geq 0. \tag{3.6}$$

We are now ready to prove Theorem 3.1.

Proof. We recall the truth optimality condition

$$(\lambda(u^* - u_d) - \mathcal{B}^\star p^*, \psi - u^*)_{\mathcal{U}} \geq 0, \quad \forall \psi \in \mathcal{U}_{\mathrm{ad}}, \tag{3.7}$$

and the perturbed optimality condition

$$(\lambda(u_N^* - u_d) - \mathcal{B}^\star \tilde{p} + \zeta, \psi - u_N^*)_{\mathcal{U}} \geq 0, \quad \forall \psi \in \mathcal{U}_{\mathrm{ad}}. \tag{3.8}$$

We set $\psi = u_N^*$ in (3.7), $\psi = u^*$ in (3.8), and add both equations to obtain

$$\begin{aligned}
0 &\leq (\lambda(u_N^* - u_d) - \lambda(u^* - u_d) + \mathcal{B}^\star p^* - \mathcal{B}^\star \tilde{p} + \zeta, u^* - u_N^*)_{\mathcal{U}} \\
&= -\lambda \|u^* - u_N^*\|_{\mathcal{U}}^2 - (\mathcal{B}^\star(p^* - \tilde{p}), u_N^* - u^*)_{\mathcal{U}} + (\zeta, u^* - u_N^*)_{\mathcal{U}} \\
&\leq -\lambda \|u^* - u_N^*\|_{\mathcal{U}}^2 + \|\zeta\|_{\mathcal{U}} \|u^* - u_N^*\|_{\mathcal{U}},
\end{aligned} \tag{3.9}$$

where we used Lemma 3.2 and the Cauchy-Schwarz inequality. The desired result directly follows. $\square$

We note that evaluation of ζ and thus the bound in (3.4) is computationally expensive since it requires a forward-backward solve of the truth state and adjoint equations. Our goal is to develop a bound which can be computed using an offline-online decomposition such that the computational cost for the online-evaluation is independent of $\mathcal{N}$. The main idea is to replace the truth approximation $p(y(u_N^*))$ in (3.4) with the reduced basis approximation $p_N^*(y_N^*(u_N^*))$ and to bound the error term $p(y(u_N^*)) - p_N^*(y_N^*(u_N^*))$.

Before we continue, let us make some notational remarks. Following the notation and terminology in [8], we refer to $\tilde{e}^{y,k} = y^k(u_N^*) - y_N^{*,k}(u_N^*)$ as the state predictability error and to $\tilde{e}^{p,k} = p^k(y(u_N^*)) - p_N^{*,k}(y_N^*(u_N^*))$ 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 $e^{y,*,k} = y^{*,k}(u^*) - y_N^{*,k}(u_N^*)$, $e^{p,*,k} = p^{*,k}(y^*(u^*)) - p_N^{*,k}(y_N^*(u_N^*))$, and $e^{u,*} = u^* - u_N^*$, respectively. We start with the following definition.

Definition 3.3. The residuals for the state equation, the adjoint equation, and the optimality condition are defined by

$$r^{y,k}(\phi; \mu) = \langle(\mathcal{B}u_N^*)_k, \phi\rangle_{Y',Y} - a(y_N^{*,k}, \phi; \mu) - \frac{1}{\tau}m(y_N^{*,k} - y_N^{*,k-1}, \phi), \quad \forall \phi \in Y, \quad \forall k \in \mathbb{K}, \tag{3.10}$$

$$r^{p,k}(\varphi; \mu) = \sigma_1(y_d^k - y_N^{*,k}, \varphi)_{L^2(D)} - a(\varphi, p_N^{*,k}; \mu) - \frac{1}{\tau}m(\varphi, p_N^{*,k} - p_N^{*,k+1}), \quad \forall \varphi \in Y, \quad k \in \mathbb{K} \setminus \{K\}, \tag{3.11}$$

$$r^{p,K}(\varphi; \mu) = \sigma_1(y_d^K - y_N^{*,K}, \varphi)_{L^2(D)} + \frac{\sigma_2}{\tau}(y_d^K - y_N^{*,K}, \varphi)_{L^2(D)} - a(\varphi, p_N^{*,K}; \mu) - \frac{1}{\tau}m(\varphi, p_N^{*,K}), \quad \forall \varphi \in Y, \tag{3.12}$$

$$r_i^{u,k}(\psi; \mu) = (\lambda(u_{N,i}^{*,k} - u_{d,i}^k) - b_i(p_N^{*,k}), \psi_i^k), \quad \forall \psi_i^k \in \mathcal{U}_{\mathrm{ad},i}^k, \quad \forall k \in \mathbb{K}, \quad i = 1, \ldots, m. \tag{3.13}$$

Before turning to the bound for the optimal control we require the following two intermediate results for the state and adjoint predictability errors.

Lemma 3.4. *The state predictability error $\tilde{e}^{y,k} = y^k(u_N^*) - y_N^{*,k}(u_N^*)$ satisfies*

$$|||\tilde{e}^{y,k}|||^y \leq \tilde{\Delta}_N^{y,k}(\mu), \qquad \forall \mu \in \mathcal{D}, \ \forall k \in \mathbb{K}, \tag{3.14}$$

where the error bound $\tilde{\Delta}_N^{y,k}(\mu)$ is defined as

$$\tilde{\Delta}_N^{y,k}(\mu) \equiv \left(\frac{\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=1}^{k} \|r^{y,k'}(\cdot;\mu)\|_{Y'}^2 \right)^{\frac{1}{2}}. \tag{3.15}$$

This is the standard *a posteriori* error bound for parabolic PDEs, cf. Theorem 1.1; for a proof see [13]. We state the corresponding result for the adjoint in the following lemma; see Appendix A.2 for the proof.

Lemma 3.5. *Let $\tilde{e}^{p,k} = \tilde{p}^k - p_N^{*,k}$ be the adjoint predictability error and define*

$$|||v^k|||^p \equiv \left(m(v^k, v^k) + \sum_{k'=k}^{K} \tau\, a(v^{k'}, v^{k'}; \mu) \right)^{\frac{1}{2}}. \tag{3.16}$$

The adjoint predictability error satisfies

$$|||\tilde{e}^{p,k}|||^p \leq \tilde{\Delta}_N^{p,k}(\mu), \qquad \forall \mu \in \mathcal{D},\ \forall k \in \mathbb{K}, \tag{3.17}$$

where the error bound $\tilde{\Delta}_N^{p,k}(\mu)$ is defined as

$$\tilde{\Delta}_N^{p,k}(\mu) \equiv \left(\frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=k}^{K} \|r^{p,k'}(\cdot;\mu)\|_{Y'}^2 + \left(\frac{2C_D^4 \sigma_1^2}{\alpha_{\mathrm{LB}}(\mu)^2} + \frac{\sigma_2^2}{2} \right) (\tilde{\Delta}_N^{y,K}(\mu))^2 \right)^{\frac{1}{2}}. \tag{3.18}$$

and $C_D \equiv \sup_{v \in Y \setminus \{0\}} \frac{\|v\|_{L^2(D)}}{\|v\|_Y}$.

For simplicity of exposition we first derive the control error bound for the unconstrained case in the following section and then turn to the constrained case in Section 3.1.2.

3.1.1. *Problems without Control Constraints*

We obtain the following result for the error in the optimal control.

Proposition 3.6. *Let u^* and u_N^* be the optimal solutions of the truth and reduced basis optimal control problems* (P) *and* (P$_N$), *respectively. Given $\tilde{\Delta}_N^{p,k}(\mu)$ defined in* (3.18), *the error in the optimal control satisfies*

$$\|u^* - u_N^*\|_{\mathcal{U}} \leq \Delta_N^{u,*}(\mu) \equiv \frac{1}{\lambda\sqrt{\alpha_{\mathrm{LB}}}} \left(\sum_{i=1}^{m} \|b_i\|_{Y'}^2 \right)^{\frac{1}{2}} \tilde{\Delta}_N^{p,1}(\mu), \quad \forall \mu \in \mathcal{D}. \tag{3.19}$$

Proof. In the unconstrained case $\zeta \in \mathcal{U}$ is given by

$$\zeta = -\left(\lambda(u_N^* - u_d) - \mathcal{B}^{\star}\tilde{p} \right). \tag{3.20}$$

We add $\pm \mathcal{B}^{\star} p_N^*$ and note that $\lambda(u_N^* - u_d) - \mathcal{B}^{\star} p_N^* = 0$ to obtain

$$\zeta = \mathcal{B}^{\star}(\tilde{p} - p_N^*), \tag{3.21}$$

or component-wise

$$\zeta_i^k = b_i(\tilde{p}^k - p_N^{*,k}), \quad \forall i = 1, \ldots, m,\ \forall k \in \mathbb{K}. \tag{3.22}$$

We can then bound

$$|\zeta_i^k| \leq \|b_i\|_{Y'} \|\tilde{p}^k - p_N^{*,k}\|_Y, \quad \forall i = 1, \ldots, m,\ \forall k \in \mathbb{K}, \tag{3.23}$$

and thus arrive at

$$\|u^* - u_N^*\|_{\mathcal{U}} \le \frac{1}{\lambda}\|\zeta\|_{\mathcal{U}} \le \frac{1}{\lambda}\left(\tau\sum_{k=1}^{K}\sum_{i=1}^{m}\|b_i\|_{Y'}^2\|\tilde{p}^k - p_N^{*,k}\|_Y^2\right)^{\frac{1}{2}} = \frac{1}{\lambda}\left(\sum_{i=1}^{m}\|b_i\|_{Y'}^2\right)^{\frac{1}{2}}\left(\tau\sum_{k=1}^{K}\|\tilde{p}^k - p_N^{*,k}\|_Y^2\right)^{\frac{1}{2}}. \quad (3.24)$$

Finally, it follows from Lemma 3.5 that

$$\left(\tau\sum_{k=1}^{K}\|\tilde{p}^k - p_N^{*,k}\|_Y^2\right)^{\frac{1}{2}} \le \frac{1}{\sqrt{\alpha_{\mathrm{LB}}}}\left(\tau\sum_{k=1}^{K}a(\tilde{e}^{p,k}, \tilde{e}^{p,k}; \mu)\right)^{\frac{1}{2}} \le \frac{1}{\sqrt{\alpha_{\mathrm{LB}}}}\left(m(\tilde{e}^{p,1}, \tilde{e}^{p,1}) + \tau\sum_{k=1}^{K}a(\tilde{e}^{p,k}, \tilde{e}^{p,k}; \mu)\right)^{\frac{1}{2}}$$
$$\le \frac{1}{\sqrt{\alpha_{\mathrm{LB}}}}\tilde{\Delta}^{p,1}(\mu). \quad (3.25)$$

The desired result directly follows from (3.24) and (3.25). □

3.1.2. *Problems with Control Constraints*

The construction of ζ from (3.3) in the control constrained case requires evaluation of the positive and negative part functions of ξ defined in (3.2). Again, we want to avoid an explicit evaluation of ξ since this would require a forward-backward truth solve. The idea here is to construct an efficiently evaluable upper and lower bound for ξ and to conservatively replace the positivity resp. negativity condition by the lower resp. upper bound in order to obtain an approximation of ζ. To this end, we first define

$$\xi_N = \lambda(u_N^* - u_d) - \mathcal{B}^\star p_N^* \quad (3.26)$$

and realize that

$$\xi_i^k = \xi_{N,i}^k - b_i(\tilde{p}^k - p_N^{*,k}), \quad \forall i = 1, \dots, m. \quad \forall k \in \mathbb{K}. \quad (3.27)$$

We can then prove the following lemma.

Lemma 3.7. *The function ξ defined in (3.2) satisfies*

$$\xi_{N,i,\mathrm{LB}}^k(\mu) \le \xi_i^k \le \xi_{N,i,\mathrm{UB}}^k(\mu), \quad \forall i = 1, \dots, m. \quad \forall k \in \mathbb{K}, \quad (3.28)$$

where the upper and lower bound are given by

$$\xi_{N,i,\mathrm{LB}}^k(\mu) \equiv \xi_{N,i}^k - \Delta_{N,i}^{\xi,k}(\mu), \qquad \xi_{N.i,\mathrm{UB}}^k(\mu) \equiv \xi_{N,i}^k + \Delta_{N,i}^{\xi,k}(\mu), \quad \forall i = 1, \dots, m. \quad \forall k \in \mathbb{K}, \quad (3.29)$$

the error bound, $\Delta_{N,i}^{\xi,k}(\mu)$, is defined as

$$\Delta_{N,i}^{\xi,k}(\mu) \equiv \frac{1}{\sqrt{2}}\|\tilde{b}_i\|_{L^2(\Omega)}\tilde{\Delta}_N^{p,k}(\mu), \quad \forall i = 1, \dots, m. \quad \forall k \in \mathbb{K}, \quad (3.30)$$

and $\tilde{b}_i$ is the $L^2(\Omega)$ Riesz representation of $b_i \in Y'$.

Proof. We note that

$$|b_i(\tilde{p}^k - p_N^{*,k})| \le \|\tilde{b}_i\|_{L^2(\Omega)}\|\tilde{p}^k - p_N^{*,k}\|_{L^2(\Omega)} \le \|\tilde{b}_i\|_{L^2(\Omega)}\frac{1}{\sqrt{2}}\tilde{\Delta}_N^{p,k}(\mu) = \Delta_{N,i}^{\xi,k}(\mu), \quad (3.31)$$

where we used the L^2-norm bound (1.15) and Lemma 3.5 for the last inequality. The desired result directly follows from (3.27) □

To clarify the next steps we sketch the various quantities involved in constructing the control error bound in Figure 1. For simplicity, we only consider a single control component. On top we show the (unknown) truth optimal control, $u^*(t)$, and reduced basis optimal control, $u_N^*(t)$, over time. The function $\xi(t)$ and its approximation $\xi_N(t)$ as well as the upper and lower bounds $\xi_{N,\mathrm{UB}}(t)$ $\xi_{N,\mathrm{LB}}(t)$ are shown in the middle. We note that $\xi_N(t)$ is identically zero if the constraints for $u_N^*(t)$ are inactive and that $\xi(t)$ is bounded from below and above by $\xi_{N,\mathrm{LB}}(t)$ and $\xi_{N,\mathrm{UB}}(t)$, respectively. Given $u_N^*(t)$ and $\xi(t)$ we may now evaluate ζ from (3.3); we plot the absolute value of ζ on the bottom of Figure 1.

To construct an upper bound for $|\zeta(t)|$, we first note from Lemma 3.7 that

$$|\xi_i^k| \leq |\xi_{N,i}^k| + \Delta_{N,i}^{\xi,k}(\mu) = \max\left(|\xi_{N,i,\mathrm{LB}}^k(\mu)|, |\xi_{N,i,\mathrm{LB}}^k(\mu)|\right), \ \forall i = 1,\ldots,m, \ \forall k \in \mathbb{K}. \tag{3.32}$$

Furthermore, we can conservatively replace the positive and negative part function of $\xi(t)$ in (3.3) by the lower and upper bound of $\xi(t)$: For example, assume that for some index (i,k) we have $u_{N,i}^{*,k} = u_{a,i}^k$. If additionally $\xi_{N,i,\mathrm{LB}}^k(\mu) > 0$ we know that $\xi_i^k > 0$ and thus $\left[\xi_i^k\right]_- = 0$, i.e., there is no contribution to the error bound. This corresponds to the index set I_1 defined next. To distinguish the relevant different cases we define the index sets

$$
\begin{aligned}
I_1 &= \{(i,k) \in \{1,\ldots,m\} \times \mathbb{K} : u_{N,i}^{*,k} = u_{a,i}^k \text{ and } \xi_{\mathrm{LB}}^{i,k}(\mu) \geq 0\} \\
&\quad \cup \{(i,k) \in \{1,\ldots,m\} \times \mathbb{K} : u_{N,i}^{*,k} = u_{b,i}^k \text{ and } \xi_{\mathrm{UB}}^{i,k}(\mu) \leq 0\}; \\
I_2 &= \{(i,k) \in \{1,\ldots,m\} \times \mathbb{K} : u_{N,i}^{*,k} = u_{a,i}^k \text{ and } \xi_{\mathrm{LB}}^{i,k}(\mu) < 0\} \\
&\quad \cup \{(i,k) \in \{1,\ldots,m\} \times \mathbb{K} : u_{N,i}^{*,k} = u_{b,i}^k \text{ and } \xi_{\mathrm{UB}}^{i,k}(\mu) > 0\}; \\
I_3 &= \{(i,k) \in \{1,\ldots,m\} \times \mathbb{K} : u_{N,i}^{*,k} \in ((u_a)_i, (u_b)_i)\}.
\end{aligned}
\tag{3.33}
$$

We note that I_1 corresponds to the indices where the constraint is active *and* we can guarantee the positivity or negativity of ξ_i^k, I_2 corresponds to the indices where the constraint is active *but we do not know* if ξ_i^k is positive or negative, and I_3 corresponds to the indices where the constraint is inactive. Note that we can evaluate the index sets $I_{1,2,3}$ efficiently online. We may thus define

$$\zeta_{N,i}^k = \begin{cases} 0 & \text{if } (i,k) \in I_1 \\ |\xi_{N,i}^k| + \Delta_N^{i,k}(\mu) & \text{if } (i,k) \in I_2 \cup I_3. \end{cases} \tag{3.34}$$

It follows by construction that $|\zeta_i^k| \leq |\zeta_{N,i}^k|$, $\forall i = 1,\ldots,m$, $\forall k \in K$. We sketch $|\zeta_{N,i}^k|$ and mark the index sets $I_{1,2,3}$ in the bottom coordinate system of Figure 1. To summarize, we obtain the following result for the error in the optimal control.

Proposition 3.8. *Let u^* and u_N^* be the optimal solutions of the truth and reduced basis optimal control problems* (P) *and* (P$_N$), *respectively. The error in the optimal control satisfies*

$$\|u^* - u_N^*\|_{\mathcal{U}} \leq \Delta_N^{u,*}(\mu) \equiv \frac{1}{\lambda}\|\zeta_N\|_{\mathcal{U}}, \quad \forall \mu \in \mathcal{D}, \tag{3.35}$$

where ζ_N is defined in (3.34).

Proof. The result directly follows from Theorem 3.1, (3.3), (3.32), and the definition of the index sets (3.33). $\square$

We again note that we overestimate the error bound (3.4) for two reasons: first, we replace $|\xi(t)|$ by the upper bound (3.32) which we can efficiently evaluate using the standard offline-online decomposition; and second, we incur additional contributions to the bound by including the time-intervals where we cannot guarantee the required sign of ξ. In Figure 1 we denote these additional intervals by Δ_I. However, since the error bound $\Delta_{N,i}^{\xi,k}(\mu)$ defined in (3.30) converges to zero as N increases, we can expect Δ_I to decrease. We will confirm this numerically in Section 4.
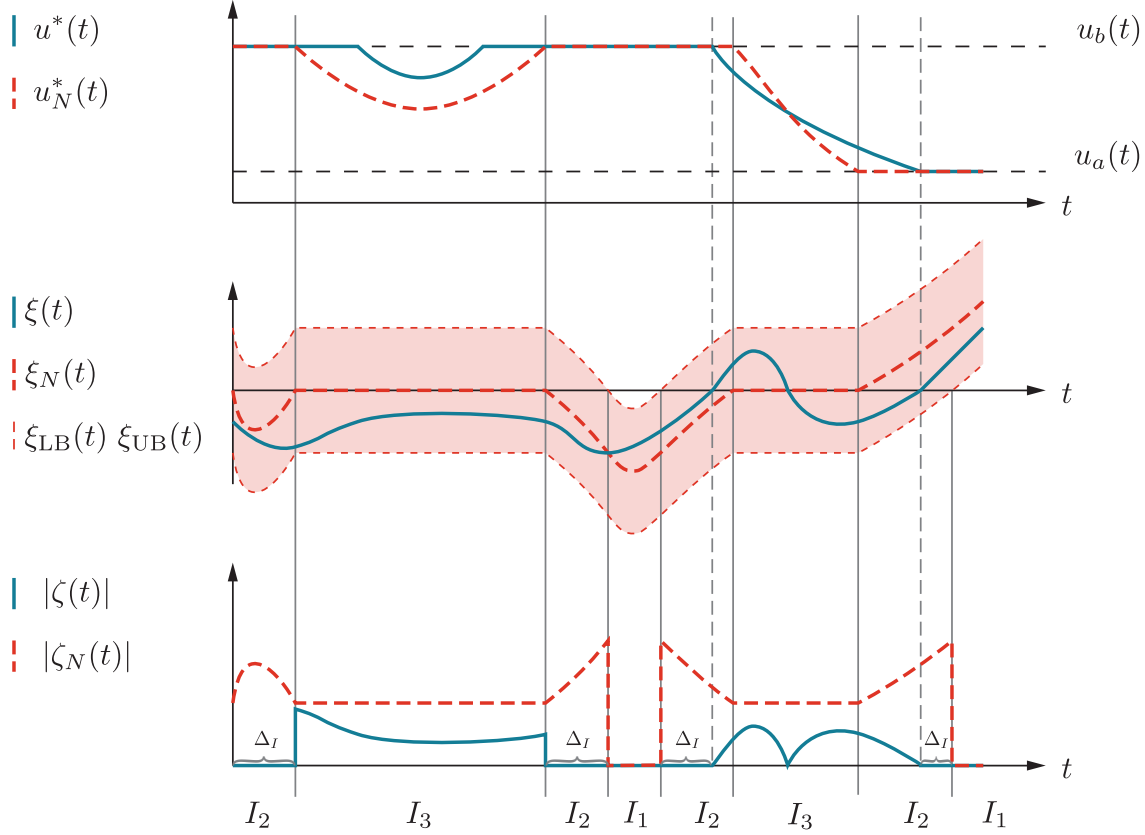
FIGURE 1. Sketch of the error bound construction for control constraints.

Finally, we stress that Δ_I is not identical to the index set I_2: consider some index (i, k) where $u_{N,i}^{*,k} = u_{a,i}^k$ and $\xi_i^k < 0$, then $\left[\xi_i^k\right]_-$ in (3.3) is nonzero and we need to rightfully account for its contribution to the error bound (see the rightmost interval I_2 in Figure 1). We do this by replacing ξ_i^k with the upper bound (3.32) and by including all contributions in I_2 in (3.34). Also note that we cannot determine Δ_I online, since this would require the evaluation of ξ_i^k. In fact, we introduce Δ_I solely for the presentation of the numerical results, i.e., to show the convergence of Δ_I to zero as N increases.

3.2. Error Bound for the Cost Functional

Given the error bound $\Delta_N^{u,*}(\mu)$ for the optimal control we may readily derive a bound for the error in the cost functional. We again distinguish between the control constrained and control unconstrained case in Sections 3.2.1 and 3.2.2, respectively. However, we first require the following two preparatory lemmata stating the *a posteriori* error bounds for the state and adjoint optimality errors. We note that the proofs of these lemmata are similar to the proof of Lemma 3.5, 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 bound.

Lemma 3.9. *The state optimality error* $e^{y,*,k} = y^{*,k}(u) - y_N^{*,k}(u_N^*)$ *satisfies*

$$|||e^{y,*,k}|||^y \leq \Delta_N^{y,*,k}(\mu), \qquad \forall \mu \in \mathcal{D}, \ \forall k \in \mathbb{K}, \tag{3.36}$$

where the error bound $\Delta_N^{y,*,k}(\mu)$ is defined as

$$\Delta_N^{y,*,k}(\mu) \equiv \left(\frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=1}^{k} \|r^{y,k'}(\cdot;\mu)\|_{Y'}^2 + \frac{2}{\alpha_{\mathrm{LB}}(\mu)} \left(\sum_{i=1}^{m} \|b_i\|_{Y'}^2 \right) \left(\Delta_N^{u,*}(\mu) \right)^2 \right)^{\frac{1}{2}}. \tag{3.37}$$

We refer the reader to Appendix A.3 for the proof of Lemma 3.9.

Lemma 3.10. *The adjoint optimality error $e^{p,*,k} = p^{*,k} - p_N^{*,k}$ satisfies*

$$|||e^{p,*,k}|||^p \le \Delta_N^{p,*,k}(\mu), \qquad \forall \mu \in \mathcal{D}, \ \forall k \in \mathbb{K}, \tag{3.38}$$

where the error bound $\Delta_N^{p,*,k}(\mu)$ is defined as

$$\Delta_N^{p,*,k}(\mu) \equiv \left(\frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=k}^{K} \|r^{p,k'}(\cdot;\mu)\|_{Y'}^2 + \left(\frac{2C_D^4 \sigma_1^2}{\alpha_{\mathrm{LB}}(\mu)^2} + \frac{\sigma_2^2}{2} \right) \left(\Delta_N^{y,*,K}(\mu) \right)^2 \right)^{\frac{1}{2}}. \tag{3.39}$$

Proof. The desired result follows directly from the proof of Lemma 3.5 by replacing $\tilde{e}^{y,k}$ with $e^{y,*,k}$, $\tilde{e}^{p,k}$ with $e^{p,*,k}$, and finally invoking Lemma 3.9. We therefore omit the detailed proof. $\square$

3.2.1. Problems without Control Constraints

We can now state

Proposition 3.11. *Let $J^* = J(y^*, u^*; \mu)$ and $J_N^* = J(y_N^*, u_N^*; \mu)$ be the optimal values of the cost functionals of the truth and reduced basis optimal control problems, respectively. The error then satisfies*

$$|J^* - J_N^*| \le \Delta_N^{J,*}(\mu) \equiv \frac{1}{2} \left(\Delta_N^{y,K}(\mu) \Delta_N^{p,*,1}(\mu) + \Delta_N^{p,1}(\mu) \Delta_N^{y,*,K}(\mu) \right), \quad \forall \mu \in \mathcal{D}, \tag{3.40}$$

where the standard "spatio-temporal" energy norm error bounds $\Delta_N^{y,k}(\mu)$ and $\Delta_N^{p,k}(\mu)$ for the state and adjoint equations are given by

$$\Delta_N^{y,k}(\mu) \equiv \left(\frac{\tau}{\alpha_{\mathrm{LB}}} \sum_{k'=1}^{k} \|r^{y,k'}(\cdot;\mu)\|_{Y'}^2 \right)^{\frac{1}{2}} \tag{3.41}$$

and

$$\Delta_N^{p,k}(\mu) \equiv \left(\frac{\tau}{\alpha_{\mathrm{LB}}} \sum_{k'=k}^{K} \|r^{p,k'}(\cdot;\mu)\|_{Y'}^2 \right)^{\frac{1}{2}}, \tag{3.42}$$

respectively.

Proof. We again use the standard result from [5] to estimate the error in the cost functional by

$$J^* - J_N^* = \frac{1}{2}\tau \sum_{k=1}^{K} r^{y,k}(e^{p,*,k};\mu) + \frac{1}{2}\tau \sum_{k=1}^{K} r^{p,k}(e^{y,*,k};\mu), \quad \forall \mu \in \mathcal{D}. \tag{3.43}$$

We note that (see (3.25))

$$\left(\tau \sum_{k=1}^{K} \|e^{y,*,k}\|_Y^2 \right)^{\frac{1}{2}} \le \frac{1}{\sqrt{\alpha_{\mathrm{LB}}}} |||e^{y,*,K}|||^y \tag{3.44}$$

and

$$\left(\tau\sum_{k=1}^{K}\|e^{p,*,k}\|_Y^2\right)^{\frac{1}{2}} \leq \frac{1}{\sqrt{\alpha_{\mathrm{LB}}}}|||e^{p,*,1}|||^p. \tag{3.45}$$

Together with the Cauchy-Schwarz inequality we obtain

$$|J^* - J_N^*| \leq \frac{1}{2}\left(\tau\sum_{k=1}^{K}\|r^{y,k}(\cdot;\mu)\|_{Y'}^2\right)^{\frac{1}{2}}\left(\tau\sum_{k=1}^{K}\|e^{p,*,k}\|_Y^2\right)^{\frac{1}{2}} + \frac{1}{2}\left(\tau\sum_{k=1}^{K}\|r^{p,k}(\cdot;\mu)\|_{Y'}^2\right)^{\frac{1}{2}}\left(\tau\sum_{k=1}^{K}\|e^{y,*,k}\|_Y^2\right)^{\frac{1}{2}}$$

$$\leq \frac{1}{2}\left(\Delta_N^{y,K}(\mu)\,|||e^{p,*,1}|||^p + \Delta_N^{p,1}(\mu)\,|||e^{y,*,K}|||^y\right). \tag{3.46}$$

The result then follows from Lemma 3.9 and 3.10. □

3.2.2. *Problems with Control Constraints*

There are two main differences between the cost functional error bound for the constrained case compared to the unconstrained case. First, we cannot bound the absolute value of the error, $J^* - J_N^*$, and thus only obtain an upper bound for the value of J^*; and second, we need to account for the non-vanishing residual of the optimality condition in the formulation of the bound. We thus obtain the following result.

Proposition 3.12. *Let $J^* = J(y^*, u^*; \mu)$ and $J_N^* = J(y_N^*, u_N^*; \mu)$ be the optimal values of the cost functionals of the truth and reduced basis optimal control problems, respectively. The error then satisfies*

$$J^* - J_N^* \leq \Delta_N^{J,*}(\mu) \equiv \frac{1}{2}\left(\Delta_N^{y,K}(\mu)\,\Delta_N^{p,*,1}(\mu) + \Delta_N^{p,1}(\mu)\,\Delta_N^{y,*,K}(\mu) + \left(\tau\sum_{i=1}^{m}\sum_{k=1}^{K}|\tilde{r}_i^{u,k}|^2\right)^{\frac{1}{2}}\Delta_N^{u,*}(\mu)\right), \quad \forall\mu\in\mathcal{D}, \tag{3.47}$$

where $\tilde{r}_i^{u,k} = \lambda(u_{N,i}^{*,k} - u_{d,i}^k) - b_i(p_N^{*,k})$.

Proof. We use the standard result from [5] to estimate the error in the cost functional by

$$J^* - J_N^* \leq \frac{1}{2}\tau\sum_{k=1}^{K}r^{y,k}(e^{p,*,k};\mu) + \frac{1}{2}\tau\sum_{k=1}^{K}r^{p,k}(e^{y,*,k};\mu) + \frac{1}{2}\tau\sum_{i=1}^{m}\sum_{k=1}^{K}r_i^{u,k}(e_i^{u,*,k};\mu), \quad \forall\mu\in\mathcal{D}, \tag{3.48}$$

where $e_i^{u,*,k} = (u_{N,i}^{*,k} - u_i^{*,k})$, $i = 1,\dots,m$, $k\in\mathbb{K}$. We can bound the first two terms in (3.48) following the proof of Proposition 3.11. For the last term we obtain

$$\frac{1}{2}\tau\sum_{i=1}^{m}\sum_{k=1}^{K}r_i^{u,k}(e_i^{u,*,k};\mu) \leq \frac{1}{2}\tau\sum_{i=1}^{m}\sum_{k=1}^{K}|\tilde{r}_i^{u,k}||e_i^{u,*,k}|$$

$$\leq \frac{1}{2}\left(\tau\sum_{i=1}^{m}\sum_{k=1}^{K}|\tilde{r}_i^{u,k}|^2\right)^{\frac{1}{2}}\left(\tau\sum_{i=1}^{m}\sum_{k=1}^{K}|e_i^{u,*,k}|^2\right)^{\frac{1}{2}}$$

$$= \frac{1}{2}\left(\tau\sum_{i=1}^{m}\sum_{k=1}^{K}|\tilde{r}_i^{u,k}|^2\right)^{\frac{1}{2}}\|e^{u,*}\|_{\mathcal{U}}. \tag{3.49}$$

The result then follows directly by invoking Proposition 3.8. □

We remark that the cost functional bound for the unconstrained case defined in (3.40) converges superlinearly with respect to the state and adjoint optimality errors. The bound for the constrained case defined in (3.47) on the other hand loses this property if the optimal control has active sets, i.e., one of the control constraints

is active. The reason is that the last term in (3.47) contains the sum of the residuals $|\tilde{r}_i^{u,k}|$ which does not converge to zero as N increases but tends to a (positive) constant if the optimal control has active sets. We may thus expect the bound (3.47) to perform considerably worse than the bound (3.40); we will confirm this behavior when discussing numerical results in Section 4.

3.3. **Computational Procedure**

For the evaluation of the control and cost functional error bounds described in Section 3.1 and 3.2 the following quantities need to be computed: the dual norms of the state and adjoint equation residuals $\|r^{y,k}(\cdot;\mu)\|_{Y'}$ and $\|r^{p,k}(\cdot;\mu)\|_{Y'}$, respectively; the constant C_D; the dual norms of the linear functionals $\|b_i\|_{Y'}$, $1 \leq i \leq m$; and the coercivity lower bound $\alpha_{\mathrm{LB}}(\mu)$. Since all of these quantities can be evaluated using the standard offline-online decomposition [13], we only summarize the computational cost in the online stage. Given a new parameter $\mu \in \mathcal{D}$ and associated optimal solution (y_N^*, p_N^*, u_N^*), evaluation of $\Delta_N^{u,*}(\mu)$ and $\Delta_N^{J,*}(\mu)$ requires (to leading order) $\mathcal{O}(K(Q_a N + m)^2)$ operations, and is thus *independent* of $\mathcal{N}$.

3.4. **Greedy Algorithm**

We propose two alternatives for generating the reduced basis space Y_N. The optimal sampling approach discussed in Section 3.4.1 is more expensive during the offline stage — it requires the solution of the truth optimal control problem (P) at selected parameter values — but is more efficient online due to a smaller reduced basis dimension N. The impulse sampling proposed in Section 3.4.2, on the other hand, is more efficient during the offline stage — we generate a reduced basis space for the impulse response and *do not* solve the truth optimal control problem — but results in a higher reduced basis dimension N and thus higher online cost. The two alternatives thus present a trade-off between offline and online efficiency. However, we can in fact combine both ideas following the idea presented in [10]; we briefly comment on this option at the end of this section.

3.4.1. *Optimal Sampling*

The optimal sampling approach is a straightforward extension of the POD/Greedy sampling procedure introduced in [14]. The method is briefly summarized in Algorithm 1. Here, $\Xi_{\mathrm{train}} \subset \mathcal{D}$ is a finite but suitably large parameter train sample; $\mu^1 \in \Xi_{\mathrm{train}}$ is the initial parameter value; and $\epsilon_{\mathrm{tol,min}} > 0$ is a prescribed desired error tolerance. Furthermore, for a given time history $v_k \in Y$, $k \in \mathbb{K}$, the operator $\mathrm{POD}_Y(\{v_k : k \in \mathbb{K}\})$ returns the largest POD mode with respect to the $(\cdot,\cdot)_Y$ inner product (and normalized with respect to the Y-norm), and $v_{\mathrm{proj},N}^k(\mu)$ denotes the Y-orthogonal projection of $v^k(\mu)$ onto the reduced basis space Y_N. We apply the POD in steps 6 and 7 of Algorithm 1 to the time history of the optimal state and adjoint projection errors, i.e., $\{e_{\mathrm{proj},N}^{y,k}(\mu) = y^{*,k}(\mu) - y_{\mathrm{proj},N}^{*,k}(\mu) : k \in \mathbb{K}\}$ and $\{e_{\mathrm{proj},N}^{p,k}(\mu) = p^{*,k}(\mu) - p_{\mathrm{proj},N}^{*,k}(\mu) : k \in \mathbb{K}\}$, and not to the optimal solutions $\{y^{*,k}(\mu) : k \in \mathbb{K}\}$ and $\{p^{*,k}(\mu) : k \in \mathbb{K}\}$ themselves.

Note that we expand the reduced basis space with the largest POD mode of the state and the adjoint equation, i.e., we use "integrated" spaces as discussed previously. Also, we may use different metrics, $\Delta_N(\mu)$, during the greedy parameter search. In fact, for the sampling procedure in the unconstrained case we propose to use the (relative) cost functional error bound, $\Delta_N^{J,*}(\mu)/J_N^*(\mu)$, whereas in the control constrained case we use the (relative) control error bound $\Delta_N^{u,*}(\mu)/\|u_N^*(\mu)\|_{\mathcal{U}}$. The reason is that in the presence of control constraints the cost functional error estimator is not a provable upper bound for the error in the cost functional as discussed in Section 3.2.2. This choice is also used in Section 4 for the numerical results.

3.4.2. *Impulse Sampling*

Algorithm 1 requires the solution of $N/2$ truth optimal control problems (P). Although this operation is performed during the offline stage, the cost can be considerable. We therefore propose an alternative sampling procedure which is purely based on the impulse response of the state and adjoint equations. To this end, we follow the procedure described in [13] to generate an integrated reduced basis space. More precisely, we

---

Algorithm 1 Optimal POD/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 $N \leftarrow 1$, $\zeta_1 = \text{POD}_Y(\{y^{*,k}(\mu^1) : k \in \mathbb{K}\})$, $Y_1 \leftarrow \text{span}\{\zeta_1\}$

3: Set $N \leftarrow 2$, $\zeta_2 = \text{POD}_Y(\{e^{p,k}_{\text{proj},N-1}(\mu^1) : k \in \mathbb{K}\})$, $Y_2 \leftarrow Y_1 \oplus \text{span}\{\zeta_2\}$

4: $\mu^* \leftarrow \underset{\mu \in \Xi_{\text{train}}}{\arg\max} \ \Delta_N(\mu)$

5: **while** $\Delta_N(\mu^*) > \epsilon_{\text{tol,min}}$ **do**

6: $\quad N \leftarrow N + 1$, $\zeta_N = \text{POD}_Y(\{e^{y,k}_{\text{proj},N-1}(\mu^*) : k \in \mathbb{K}\})$, $Y_N \leftarrow Y_{N-1} \oplus \text{span}\{\zeta_N\}$

7: $\quad N \leftarrow N + 1$, $\zeta_N = \text{POD}_Y(\{e^{p,k}_{\text{proj},N-1}(\mu^*) : k \in \mathbb{K}\})$, $Y_N \leftarrow Y_{N-1} \oplus \text{span}\{\zeta_N\}$

8: $\quad \mu^* \leftarrow \underset{\mu \in \Xi_{\text{train}}}{\arg\max} \ \Delta_N(\mu)$

9: **end while**

10: $N_{\text{max}} \leftarrow N$

---

apply the standard POD/Greedy sampling procedure but alternate between the following equations after each POD/Greedy step:

(1) the state equation (2.8a) with an impulse consecutively applied at each input;

(2) the adjoint equation (2.8c) with $\tau\,(y^k_d, \varphi)_{L^2(D)}$ on the right-hand side;

(3) the adjoint equation (2.8c) with $\tau\,(\hat{y}^k_m, \varphi)_{L^2(D)}$ on the right-hand side, where $\hat{y}^k_m$ is the step response for the m-th input (note that we again apply these different right-hand sides consecutively).

Note that we sample on the standard energy-norm error bound and consecutively expand the basis until the desired error tolerance is reached. We are aware that the linear time-invariance (LTI) property — which justifies the impulse approach — does not hold for the adjoint equation (2.8c). However, we still expect the reduced basis to well-approximate the adjoint solution by applying the step response $\hat{y}^k_m$ on the right-hand side of the adjoint in the POD/Greedy procedure. Furthermore, we can always confirm the fidelity of the optimal control solution online thanks to our *a posteriori* error bounds. We will present numerical results in in Section 4.

The appealing feature of the impulse sampling is that we can provide an *a posteriori* error bound for the optimal control problem *without ever* solving the truth optimal control problem. The disadvantage is that we end up with a higher-dimensional basis than with the optimal sampling approach. This is due to the fact that the impulse basis can approximate all possible control inputs, whereas the basis using the optimal sampling is tailored towards — and can thus only well-approximate — the optimal control.

Finally, we note that we can combine both sampling procedures following the approach presented in [10]. The idea is as follows: We first generate a reduced basis space Y_N using the impulse sampling. Then, given Y_N, we run the optimal sampling in Algorithm 1 but instead of solving the truth optimal control problem (P) to generate the snapshots we solve the reduced optimal control problem (P_N) with the given Y_N. The second step allows us to condense the basis Y_N and obtain an optimal "derived" basis Y_M of smaller dimension $M \leq N$. This approach combines the advantages of both sampling procedures: a small reduced basis dimension without having to solve the truth optimal control problem.

4. Numerical Results

We consider a linear-quadratic optimal control problem governed by unsteady heat conduction in a two-dimensional domain [32]. The spatial domain, a typical point of which is $x = (x_1, x_2)^T$, is given by $\Omega = (0,7) \times (0,3)$ and is subdivided into the four subdomains $\Omega_1 = ((1,2) \times (0,1)) \cup ((5,6) \times (0,1))$, $\Omega_2 = (3,4) \times (0,1)$, $\Omega_3 = (1,6) \times (2.5,3)$, and $\Omega_4 = \Omega \setminus \{\Omega_1 \cup \Omega_2 \cup \Omega_3\}$. A sketch of the domain is shown in Figure 2. We impose zero Dirichlet conditions on the left and right boundaries and zero Neumann conditions on the bottom and top

boundaries. The amount of heat supply in the heater domains Ω_1 and Ω_2 is regulated by the first and second component of the (time–dependent) control $\{u^k = (u_1^k, u_2^k)^T\}_{k \in \mathbb{K}} \in \mathcal{U} \equiv (\mathbb{R}^2)^K$, respectively. The (reference) conductivity in the subdomain $\Omega_1 \cup \Omega_2$ is set to unity. We consider the normalized conductivity κ in the subdomain $\Omega_3 \cup \Omega_4$ as our first parameter $\mu_1 \in [0.5, 5]$.
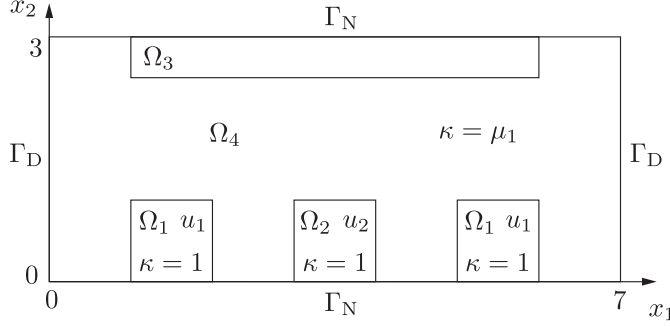

FIGURE 2. Domain Ω for the model problem.

The underlying partial differential equation is the heat (diffusion) equation and we shall directly consider the truth approximation of the problem. The temperature $y^k(\mu) \in Y$ thus satisfies (1.9), where $Y \subset Y^e \equiv \{v \in \mathrm{H}^1(\Omega) : v|_{\Gamma_D} = 0\}$ is a linear finite element truth approximation subspace of dimension $\mathcal{N} = 8479$ over a triangulation of Ω. We shall consider the time interval $[0, T] = [0, 6]$ and a time step $\tau = 0.06$; we thus have $K = 100$. The initial condition is set to zero. The bilinear and linear forms are given by $a(w, v; \mu) = \mu_1 \int_{\Omega_3 \cup \Omega_4} \nabla w \nabla v \, \mathrm{d}x + \int_{\Omega_1 \cup \Omega_2} \nabla w \nabla v \, \mathrm{d}x$ and $b_i(v) = \int_{\Omega_i} v \, \mathrm{d}x$ for $i = 1, 2$, respectively. The bilinear form $a(\cdot, \cdot; \mu)$ admits the affine representation (1.3) with $\Theta_a^1(\mu) = \mu_1, \Theta_a^2(\mu) = 1$ and $Q_a = 2$. We also define the inner product $(w, v)_Y = \mu_1^{\mathrm{ref}} \int_{\Omega_3 \cup \Omega_4} \nabla w \nabla v \, \mathrm{d}x + \int_{\Omega_1 \cup \Omega_2} \nabla w \nabla v \, \mathrm{d}x$ for $\mu_1^{\mathrm{ref}} = \sqrt{2.5}$; we may hence choose $\alpha_{\mathrm{LB}}(\mu) = \min(\mu_1/\mu_1^{\mathrm{ref}}, 1)$ in (1.11).

We consider the quadratic cost functional $J(y, u; \mu) = \frac{1}{2} \sum_{k=1}^{K} \|y^k - y_d^k\|_{L^2(D)}^2 + \frac{\lambda}{2}\|u - u_d\|_{\mathcal{U}}^2$, corresponding to (2.6) with fixed regularization parameters $\sigma_1 = 1, \sigma_2 = 0$. We further choose $u_d \equiv 0$ and $D = \Omega_3$; the desired state $y_d \in Y^K$ is given as the discretization of $y_{d,e}(x, t) = (1.2 + \sin(\pi t))\chi_D(x)$, where $\chi_D(x)$ is the characteristic function on D. In the presence of control constraints we choose $u_{a,1}^k = u_{a,2}^k = 0.2$ and $u_{b,1}^k = u_{b,2}^k = 1, k \in \mathbb{K}$. Finally, we assume that the regularization parameter λ is allowed to vary in the range from 0.1 to 1. The full parametrization of our problem is thus given by $\mu = (\mu_1, \mu_2 = \lambda) \in \mathcal{D} \equiv [0.5, 5] \times [0.1; 1]$; we have $P = 2$ parameters.

We first present results for the solution of the truth optimal control problem (P) for different parameter combinations. In Figure 3 we plot the optimal control $u^*(t)$ for the two "corners" of the parameter domain for the unconstrained and constrained case on the top and bottom, respectively. We note that the parameters have a strong influence on the solution of the optimal control problem and that the lower and upper bound on the control become active depending on the parameter.

We construct the reduced basis space Y_N according to both sampling procedures described in Section 3.4. To this end, we employ the train sample $\Xi_{\mathrm{train}} \subset \mathcal{D}$ consisting of $n_{\mathrm{train}} = 200$ parameter points over $\mathcal{D}$ and choose $\mu^1 = (0.5, 0.1)$ as the initial parameter value. We also introduce a parameter test sample Ξ_{test} of size $n_{\mathrm{test}} = 40$ with a log-random distribution in μ_1 and λ. Throughout this section, we present maximum relative errors and bounds as well as average effectivities. We normalize the state (resp. adjoint) predictability error and bound by $|||y^K(u_N^*)|||^y$ (resp. $|||p^1(y(u_N^*))|||^p$), the state (resp. adjoint) optimality error and bound by $|||y^{*,K}|||^y$ (resp. $|||p^{*,1}|||^p$), the control error and bound by $\|u^*\|_{\mathcal{U}}$, and the cost functional error and bound by J^*. The
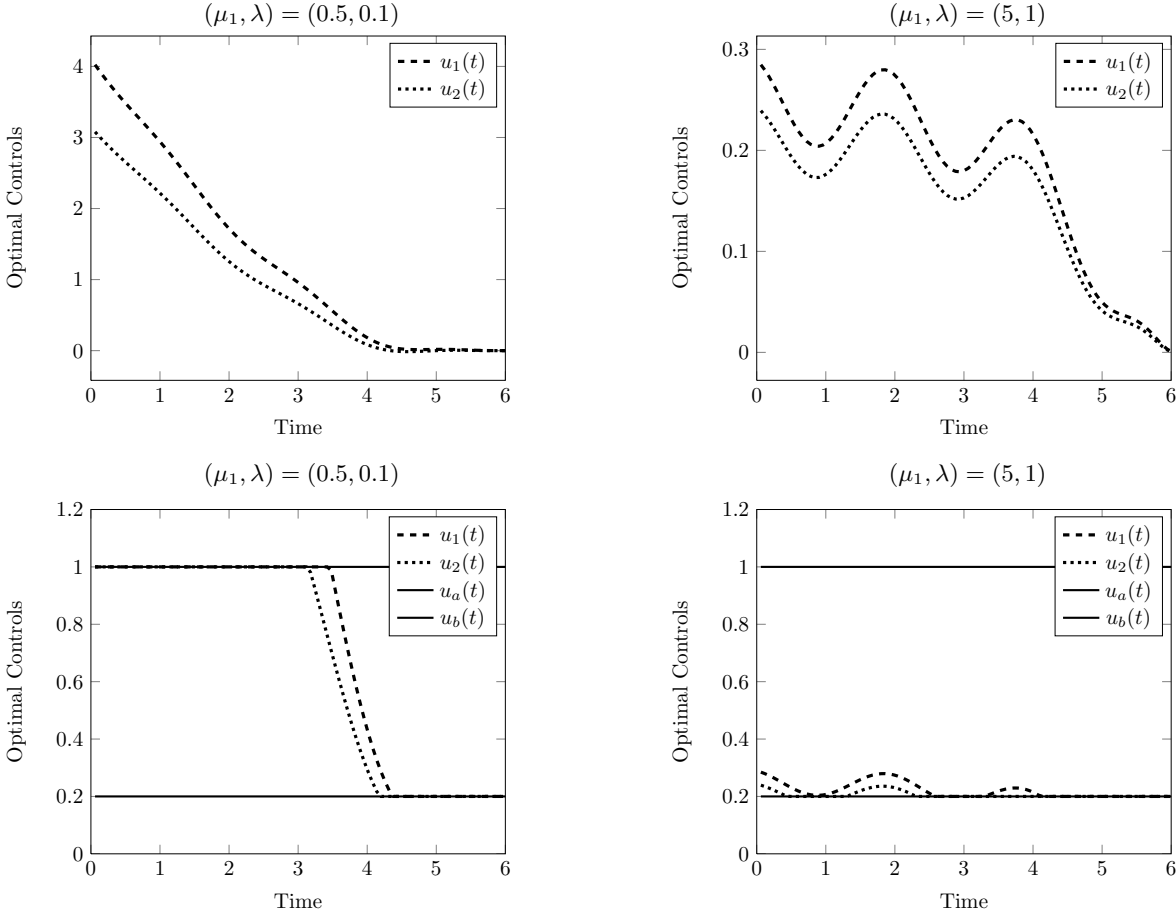
FIGURE 3. Optimal control $u^*(\mu)$ for different representative parameter values

effectivities are given by the ratios of the error bound to the actual error. The maxima and average values are taken over Ξ_{test}.

We first employ the optimal sampling described in Section 3.4.1 and present results for the unconstrained and constrained case in Sections 4.1 and 4.2, respectively. In the unconstrained case we choose the metric $\Delta_N(\mu) = \Delta_N^{J,*}(\mu)/J_N^*(\mu)$ and a desired error tolerance of $\epsilon_{\text{tol,min}} = 1\,\text{E}{-}8$, in the constrained case we sample on the relative control error bound $\Delta_N^{u,*}(\mu)/\|u_N\|_{\mathcal{U}}$ and set the desired error tolerance to $\epsilon_{\text{tol,min}} = 1\,\text{E}{-}4$. In Section 4.3 we present results for the impulse sampling described in Section 3.4.2, where we use a desired error tolerance $\epsilon_{\text{tol,min}} = 1\,\text{E}{-}5$ for the POD/Greedy procedure.

4.1. Optimal sampling without control constraints

In Table 1 we present, as a function of N, the maximum relative predictability errors $\epsilon_{N,\text{max,rel}}^y$ and $\epsilon_{N,\text{max,rel}}^p$, the maximum relative error bounds $\tilde{\Delta}_{N,\text{max,rel}}^y$ and $\tilde{\Delta}_{N,\text{max,rel}}^p$, and the average effectivities $\bar{\eta}_N^y$ and $\bar{\eta}_N^p$ for the state and adjoint equation, respectively. We also present the maximum relative control error $\epsilon_{N,\text{max,rel}}^{u,*}$, error bound $\Delta_{N,\text{max,rel}}^{u,*}$, and average effectivity $\bar{\eta}_N^{u,*}$. We observe that the state and adjoint predictability errors and bounds are decreasing very rapidly with increasing dimension of the reduced basis space and that the error bounds are very sharp for all values of N. The slightly larger effectivities of the adjoint error bound are due to the error contribution of the state predictability error bound in (3.18). We also observe that the error in the

optimal control exhibits a superlinear convergence with respect to the state and adjoint predictability errors. Since the control error bound (3.19) is proportional to the adjoint predictability error bound it cannot quite capture the error decay. The mean effectivities thus deteriorate slightly as N increases, but are still acceptable for all values of N.

	State			Adjoint			Control		
N	$\epsilon^{y}_{N,\max,\mathrm{rel}}$	$\tilde{\Delta}^{y}_{N,\max,\mathrm{rel}}$	$\bar{\eta}^{y}_{N}$	$\epsilon^{p}_{N,\max,\mathrm{rel}}$	$\tilde{\Delta}^{p}_{N,\max,\mathrm{rel}}$	$\bar{\eta}^{p}_{N}$	$\epsilon^{u,*}_{N,\max,\mathrm{rel}}$	$\Delta^{u,*}_{N,\max,\mathrm{rel}}$	$\bar{\eta}^{u,*}_{N}$
8	$2.10E{-}1$	$2.99E{-}1$	$1.29E{+}0$	$1.67E{-}1$	$4.47E{-}1$	$3.03E{+}0$	$6.26E{-}2$	$1.89E{+}0$	$5.01E{+}1$
16	$1.32E{-}2$	$1.69E{-}2$	$1.24E{+}0$	$9.07E{-}3$	$3.02E{-}2$	$4.01E{+}0$	$5.07E{-}3$	$1.28E{-}1$	$1.10E{+}2$
24	$3.37E{-}3$	$4.39E{-}3$	$1.26E{+}0$	$1.78E{-}3$	$7.90E{-}3$	$4.59E{+}0$	$5.58E{-}4$	$3.49E{-}2$	$2.47E{+}2$
32	$5.94E{-}4$	$8.09E{-}4$	$1.23E{+}0$	$3.56E{-}4$	$1.33E{-}3$	$3.83E{+}0$	$1.99E{-}5$	$8.67E{-}3$	$5.43E{+}2$
40	$3.81E{-}4$	$5.22E{-}4$	$1.28E{+}0$	$1.59E{-}4$	$8.47E{-}4$	$4.08E{+}0$	$6.04E{-}6$	$3.58E{-}3$	$2.49E{+}3$
48	$7.40E{-}5$	$1.10E{-}4$	$1.26E{+}0$	$3.33E{-}5$	$1.72E{-}4$	$3.87E{+}0$	$2.55E{-}7$	$1.06E{-}3$	$5.60E{+}3$
56	$4.72E{-}5$	$7.24E{-}5$	$1.27E{+}0$	$1.67E{-}5$	$9.24E{-}5$	$3.80E{+}0$	$1.52E{-}7$	$4.91E{-}4$	$4.86E{+}3$

TABLE 1. Unconstrained case with optimal sampling: state predictability, adjoint predictability, and control errors, error bounds, and effectivities as a function of N.

We next turn to the optimality errors and the cost functional. In Table 2 we present, as a function of N, the maximum relative optimality errors $\epsilon^{y,*}_{N,\max,\mathrm{rel}}$ and $\epsilon^{p,*}_{N,\max,\mathrm{rel}}$, the maximum relative error bounds $\Delta^{y,*}_{N,\max,\mathrm{rel}}$ and $\Delta^{p,*}_{N,\max,\mathrm{rel}}$, and the average effectivities $\bar{\eta}^{y,*}_{N}$ and $\bar{\eta}^{p,*}_{N}$ for the state and adjoint variable, respectively. We also present the maximum relative cost functional error $\epsilon^{J,*}_{N,\max,\mathrm{rel}}$, the maximum relative error bound $\Delta^{J,*}_{N,\max,\mathrm{rel}}$, and the average effectivities $\bar{\eta}^{J,*}_{N}$. Again, we observe a rapid decay of both the state and adjoint optimality errors with increasing N. However, the effectivities of the optimality error bounds are larger than the predictability ones because of the contribution of the control error bound in (3.37) and subsequently in (3.39). We note that — as opposed to the control — the error in the cost functional *and* the error bound converge superlinearly with respect to the predictability and optimality errors and the effectivities thus do not deteriorate with increasing N. Unfortunately, the effectivities are $\mathcal{O}(10^{3})$ for all values of N, i.e., we consistently overestimate the error in the cost functional. However, given the superlinear convergence, the additional online computational cost due to the overestimation is still acceptable.

We finally consider the online computational cost for solving the reduced basis optimal control problem compared to the truth optimal control problem. For $N = 32$ — corresponding to a relative error bound for the control of less than 1% — we obtain a speed-up of approximately 580 for the solution of the optimal control problem; furthermore, we obtain a speed-up of approximately 200 for the solution of the optimal control problem *and* evaluation of the error bound for the control and cost functional.

	State			Adjoint			Cost Functional		
N	$\epsilon^{y,*}_{N,\max,\mathrm{rel}}$	$\Delta^{y,*}_{N,\max,\mathrm{rel}}$	$\bar{\eta}^{y,*}_{N}$	$\epsilon^{p,*}_{N,\max,\mathrm{rel}}$	$\Delta^{p,*}_{N,\max,\mathrm{rel}}$	$\bar{\eta}^{p,*}_{N}$	$\epsilon^{J,*}_{N,\max,\mathrm{rel}}$	$\Delta^{J,*}_{N,\max,\mathrm{rel}}$	$\bar{\eta}^{J,*}_{N}$
8	$2.11E{-}1$	$4.72E{+}0$	$4.09E{+}1$	$1.67E{-}1$	$8.11E{+}0$	$9.58E{+}1$	$1.41E{-}3$	$8.26E{-}1$	$2.60E{+}3$
16	$1.32E{-}2$	$3.30E{-}1$	$3.48E{+}1$	$9.07E{-}3$	$9.58E{-}1$	$1.57E{+}2$	$1.07E{-}5$	$3.75E{-}3$	$1.68E{+}3$
24	$3.35E{-}3$	$1.07E{-}1$	$3.42E{+}1$	$1.78E{-}3$	$3.16E{-}1$	$1.73E{+}2$	$2.47E{-}7$	$2.46E{-}4$	$1.52E{+}4$
32	$5.94E{-}4$	$2.57E{-}2$	$3.34E{+}1$	$3.56E{-}4$	$7.62E{-}2$	$1.27E{+}2$	$2.28E{-}8$	$1.53E{-}5$	$2.61E{+}3$
40	$3.81E{-}4$	$8.88E{-}3$	$3.58E{+}1$	$1.59E{-}4$	$1.85E{-}2$	$1.34E{+}2$	$3.24E{-}9$	$2.80E{-}6$	$4.47E{+}3$
48	$7.40E{-}5$	$3.24E{-}3$	$3.42E{+}1$	$3.33E{-}5$	$9.60E{-}3$	$1.13E{+}2$	$1.70E{-}10$	$2.10E{-}7$	$4.71E{+}3$
56	$4.72E{-}5$	$1.47E{-}3$	$4.79E{+}1$	$1.67E{-}5$	$3.43E{-}3$	$1.10E{+}2$	$5.25E{-}11$	$3.39E{-}8$	$3.03E{+}3$

TABLE 2. Unconstrained case with optimal sampling: state optimality, adjoint optimality, and cost functional errors, error bounds, and effectivities as a function of N.

4.2. **Optimal sampling with control constraints**

We next turn to the problem involving constraints on the control. We again present analogous results as in the previous section. The predictability and control errors, bounds, and effectivities are shown in Table 3, the optimality and cost functional errors, bounds, and effectivities are presented in Table 4.

We observe that the results for the state and adjoint predictability and optimality errors, bounds, and hence effectivities very much resemble the unconstrained case. However, the error in the optimal control converges even faster than in the unconstrained case and the effectivities thus deteriorate faster. Although we overestimate the error by another order of magnitude, we still require $N = 32$ for a 1% relative accuracy of the control error bound. We also observe that the convergence of the cost functional error bound is close to linear with respect to the state and adjoint optimality errors and thus much slower than before. The reason — as discussed in Section 3.2.2 — is the additional term in the cost functional error bound (3.47). As a result, the effectivities deteriorate considerably.

Comparing the online computational times in the constrained case for $N = 32$, we again obtain a speed-up of approximately 500 for solving the optimal control problem; furthermore, we obtain a speed-up of approximately 270 for solving the optimal control problem *and* evaluating the control and cost functional error bounds.

	State			Adjoint			Control		
N	$\epsilon^{y}_{N,\max,\text{rel}}$	$\tilde{\Delta}^{y}_{N,\max,\text{rel}}$	$\bar{\eta}^{y}_{N}$	$\epsilon^{p}_{N,\max,\text{rel}}$	$\tilde{\Delta}^{p}_{N,\max,\text{rel}}$	$\bar{\eta}^{p}_{N}$	$\epsilon^{u,*}_{N,\max,\text{rel}}$	$\Delta^{u,*}_{N,\max,\text{rel}}$	$\bar{\eta}^{u,*}_{N}$
8	$6.77E{-}2$	$7.43E{-}2$	$1.24E{+}0$	$2.74E{-}2$	$7.50E{-}2$	$2.78E{+}0$	$2.58E{-}1$	$2.43E{+}1$	$1.25E{+}2$
16	$2.51E{-}2$	$2.76E{-}2$	$1.18E{+}0$	$1.07E{-}2$	$1.82E{-}2$	$3.16E{+}0$	$1.34E{-}1$	$1.26E{+}1$	$1.99E{+}2$
24	$3.74E{-}3$	$4.09E{-}3$	$1.20E{+}0$	$1.67E{-}3$	$3.43E{-}3$	$3.25E{+}0$	$2.24E{-}2$	$3.94E{+}0$	$1.06E{+}2$
32	$1.39E{-}3$	$1.46E{-}3$	$1.21E{+}0$	$2.74E{-}4$	$9.06E{-}4$	$4.89E{+}0$	$1.51E{-}2$	$2.02E{+}0$	$1.11E{+}2$
40	$3.95E{-}4$	$4.62E{-}4$	$1.30E{+}0$	$1.39E{-}4$	$4.12E{-}4$	$4.52E{+}0$	$6.45E{-}3$	$1.01E{+}0$	$2.36E{+}2$
48	$1.89E{-}4$	$2.51E{-}4$	$1.42E{+}0$	$6.25E{-}5$	$1.76E{-}4$	$5.28E{+}0$	$6.66E{-}3$	$5.88E{-}1$	$4.22E{+}2$
56	$8.71E{-}5$	$1.05E{-}4$	$1.67E{+}0$	$1.60E{-}5$	$6.79E{-}5$	$7.58E{+}0$	$1.68E{-}3$	$4.79E{-}1$	$2.79E{+}2$

TABLE 3. Constrained case with optimal sampling: state predictability, adjoint predictability, and control errors, error bounds, and effectivities as a function of N.

	State			Adjoint			Cost Functional		
N	$\epsilon^{y,*}_{N,\max,\text{rel}}$	$\Delta^{y,*}_{N,\max,\text{rel}}$	$\bar{\eta}^{y,*}_{N}$	$\epsilon^{p,*}_{N,\max,\text{rel}}$	$\Delta^{p,*}_{N,\max,\text{rel}}$	$\bar{\eta}^{p,*}_{N}$	$\epsilon^{J,*}_{N,\max,\text{rel}}$	$\Delta^{J,*}_{N,\max,\text{rel}}$	$\bar{\eta}^{J,*}_{N}$
8	$6.79E{-}2$	$4.77E{+}0$	$7.28E{+}1$	$2.74E{-}2$	$8.25E{+}0$	$1.39E{+}2$	$3.12E{-}2$	$2.98E{+}1$	$6.06E{+}2$
16	$2.49E{-}2$	$6.84E{-}1$	$5.21E{+}1$	$1.07E{-}2$	$1.29E{+}0$	$1.63E{+}2$	$1.45E{-}2$	$4.85E{+}0$	$3.95E{+}3$
24	$3.74E{-}3$	$7.80E{-}2$	$3.33E{+}1$	$1.67E{-}3$	$1.29E{-}1$	$9.98E{+}1$	$5.26E{-}4$	$8.37E{-}1$	$5.25E{+}3$
32	$1.39E{-}3$	$2.35E{-}2$	$3.06E{+}1$	$2.74E{-}4$	$4.35E{-}2$	$1.38E{+}2$	$4.57E{-}4$	$2.75E{-}1$	$1.46E{+}3$
40	$3.95E{-}4$	$7.66E{-}3$	$3.39E{+}1$	$1.39E{-}4$	$1.16E{-}2$	$1.35E{+}2$	$4.82E{-}5$	$9.12E{-}2$	$5.98E{+}3$
48	$1.89E{-}4$	$3.75E{-}3$	$3.98E{+}1$	$6.25E{-}5$	$4.34E{-}3$	$1.59E{+}2$	$4.11E{-}5$	$4.05E{-}2$	$1.34E{+}4$
56	$8.71E{-}5$	$1.36E{-}3$	$4.57E{+}1$	$1.60E{-}5$	$2.40E{-}3$	$2.33E{+}2$	$2.60E{-}5$	$3.18E{-}2$	$2.35E{+}4$

TABLE 4. Constrained case with optimal sampling: state optimality, adjoint optimality, and cost functional errors, error bounds, and effectivities as a function of N.

Finally, we recall our discussion concerning the control error bound at the end of Section 3.1.2. We pointed out that one reason for overestimating the error bound (3.4) are the additional contributions from time steps where we cannot guarantee the sign of ξ; these intervals were marked with Δ_I in Figure 1. In Table 5 we present, as a function of N, the maximum number of time steps contained in Δ_I for the first ($\Delta_{I,1}$) and second ($\Delta_{I,2}$) control component. Here, the maximum is taken over Ξ_{test}. We note that $\max \Delta_{I,1}$ and $\max \Delta_{I,2}$ — and hence the corresponding contributions to the error bound (3.35) — tend to zero very fast.

N	8	16	24	32	40	48	56	64	72
$\max \Delta_{I,1}$	85	36	9	3	2	1	1	1	0
$\max \Delta_{I,2}$	78	29	8	2	2	1	1	0	0

TABLE 5. Maximal size of the interval Δ_I for the first and second control component.

4.3. **Impulse sampling without control constraints**

In this final section we consider the impulse sampling approach discussed in Section 3.4.2. We focus on the unconstrained case and again present analogous results as in the previous two sections. The predictability and control errors, bounds, and effectivities are shown in Table 6, the optimality and cost functional errors, bounds, and effectivities are presented in Table 7.

We immediately note that the effectivities of the state and adjoint predictability and optimality error bounds are very similar to the ones in Section 4.1. However, the rate of convergence of the error and bound itself is much smaller. To achieve a certain desired accuracy we require almost twice as many basis functions with the impulse sampling compared to the optimal sampling. In contrast, the convergence of the error in the optimal control is the same as before (note that the maximum relative control error for $N = 48$ is $1.76\,\mathrm{E}{-}7$ now compared to $2.55\,\mathrm{E}{-}7$ in Table 1). Again, since the control error bound is proportional to the adjoint predictability error bound, this means an even larger increase in the effectivities of the control error bound. The results for the cost functional are again very similar to the ones in Section 4.1. The convergence of the error and bound is slower — again, we need to choose N almost twice as large as before to obtain a certain desired accuracy — but the effectivities are the same as the ones we obtained using the optimal sampling approach. Following our discussion in Section 3.4.2, however, we expect that one can recover the "optimal" convergence by generating a derived reduced basis following the ideas in [10].

	State			Adjoint			Control		
N	$\epsilon^y_{N,\max,\mathrm{rel}}$	$\tilde{\Delta}^y_{N,\max,\mathrm{rel}}$	$\bar{\eta}^y_N$	$\epsilon^p_{N,\max,\mathrm{rel}}$	$\tilde{\Delta}^p_{N,\max,\mathrm{rel}}$	$\bar{\eta}^p_N$	$\epsilon^{u,*}_{N,\max,\mathrm{rel}}$	$\Delta^{u,*}_{N,\max,\mathrm{rel}}$	$\bar{\eta}^{u,*}_N$
8	$5.44E{-}1$	$6.60E{-}1$	$1.17E{+}0$	$2.39E{-}1$	$9.96E{-}1$	$5.52E{+}0$	$1.27E{-}1$	$4.25E{+}0$	$3.33E{+}2$
16	$4.36E{-}2$	$4.94E{-}2$	$1.16E{+}0$	$1.53E{-}2$	$9.72E{-}2$	$4.00E{+}0$	$8.89E{-}4$	$1.23E{+}0$	$5.07E{+}2$
32	$9.58E{-}3$	$1.05E{-}2$	$1.13E{+}0$	$1.47E{-}3$	$1.63E{-}2$	$7.79E{+}0$	$1.65E{-}5$	$1.24E{-}1$	$7.00E{+}3$
48	$1.04E{-}3$	$1.17E{-}3$	$1.17E{+}0$	$1.72E{-}4$	$2.50E{-}3$	$1.04E{+}1$	$1.76E{-}7$	$3.15E{-}2$	$9.61E{+}4$
64	$2.76E{-}4$	$3.29E{-}4$	$1.15E{+}0$	$4.74E{-}5$	$7.89E{-}4$	$1.09E{+}1$	$1.51E{-}8$	$7.90E{-}3$	$3.03E{+}5$
80	$9.34E{-}5$	$1.09E{-}4$	$1.21E{+}0$	$7.47E{-}6$	$2.80E{-}4$	$1.65E{+}1$	$7.85E{-}10$	$2.81E{-}3$	$1.65E{+}6$
96	$2.42E{-}5$	$2.96E{-}5$	$1.20E{+}0$	$3.42E{-}6$	$7.94E{-}5$	$1.14E{+}1$	$1.17E{-}10$	$7.94E{-}4$	$2.99E{+}6$

TABLE 6. Unconstrained case with impulse sampling: state predictability, adjoint predictability, and control errors, error bounds, and effectivities as a function of N.

APPENDIX A. PROOFS

A.1. **Proof of Lemma 3.2**

Proof. Let y_1 be the solution of the state equation for the control input $\tilde{u} - u^*$,

$$m(y_1^k - y_1^{k-1}, \phi) + \tau a(y_1^k, \phi; \mu) = \tau \sum_{i=1}^{m} b_i(\phi)(\tilde{u}_i^k - u_i^{*,k}), \quad \forall \phi \in Y, \quad 1 \le k \le K, \tag{A.1}$$

	State			Adjoint			Cost Functional		
N	$\epsilon_{N,\max,\mathrm{rel}}^{y,*}$	$\Delta_{N,\max,\mathrm{rel}}^{y,*}$	$\bar{\eta}_N^{y,*}$	$\epsilon_{N,\max,\mathrm{rel}}^{p,*}$	$\Delta_{N,\max,\mathrm{rel}}^{p,*}$	$\bar{\eta}_N^{p,*}$	$\epsilon_{N,\max,\mathrm{rel}}^{J,*}$	$\Delta_{N,\max,\mathrm{rel}}^{J,*}$	$\bar{\eta}_N^{J,*}$
8	$5.48E{-}1$	$1.06E{+}1$	$3.01E{+}1$	$2.39E{-}1$	$2.91E{+}1$	$2.24E{+}2$	$2.25E{-}2$	$4.06E{+}0$	$1.46E{+}3$
16	$4.36E{-}2$	$3.76E{+}0$	$2.99E{+}1$	$1.53E{-}2$	$1.11E{+}1$	$1.23E{+}2$	$2.14E{-}4$	$2.71E{-}1$	$4.19E{+}2$
32	$9.58E{-}3$	$3.78E{-}1$	$2.73E{+}1$	$1.47E{-}3$	$1.12E{+}0$	$1.88E{+}2$	$3.68E{-}6$	$2.75E{-}3$	$2.43E{+}3$
48	$1.04E{-}3$	$9.63E{-}2$	$2.79E{+}1$	$1.72E{-}4$	$2.85E{-}1$	$3.53E{+}2$	$4.54E{-}8$	$1.66E{-}4$	$2.25E{+}3$
64	$2.76E{-}4$	$2.23E{-}2$	$2.74E{+}1$	$4.74E{-}5$	$6.18E{-}2$	$4.10E{+}2$	$2.56E{-}9$	$1.18E{-}5$	$3.43E{+}3$
80	$9.34E{-}5$	$7.92E{-}3$	$2.84E{+}1$	$7.47E{-}6$	$2.20E{-}2$	$6.23E{+}2$	$1.05E{-}10$	$1.46E{-}6$	$3.81E{+}3$
96	$2.42E{-}5$	$2.24E{-}3$	$2.89E{+}1$	$3.42E{-}6$	$6.25E{-}3$	$5.21E{+}2$	$2.14E{-}11$	$1.19E{-}7$	$3.89E{+}3$

TABLE 7. Unconstrained case with impulse sampling: state optimality, adjoint optimality, and cost functional errors, error bounds, and effectivities as a function of N.

with initial condition $y_1^0 = 0$. We now choose $\phi = p^{*,k}$ and sum from $k = 1$ to K to obtain

$$\sum_{k=1}^{K} m(y_1^k - y_1^{k-1}, p^{*,k}) + \tau \sum_{k=1}^{K} a(y_1^k, p^{*,k}; \mu) = \tau \sum_{k=1}^{K} \sum_{i=1}^{m} b_i(p^{*,k})(\tilde{u}_i^k - u_i^{*,k}), \tag{A.2}$$

which we can rewrite in the form

$$\sum_{k=1}^{K-1} m(y_1^k, p^{*,k} - p^{*,k+1}) + \tau \sum_{k=1}^{K-1} a(y_1^k, p^{*,k}; \mu) + m(y_1^K, p^{*,K}) + \tau a(y_1^K, p^{*,K}; \mu)$$

$$= \tau \sum_{k=1}^{K} \sum_{i=1}^{m} b_i(p^{*,k})(\tilde{u}_i^k - u_i^{*,k}). \tag{A.3}$$

We next consider the adjoint equation (2.8c) and choose as test function $\varphi = y_1^k$ to obtain

$$m(y_1^k, p^{*,k} - p^{*,k+1}) + \tau a(y_1^k, p^{*,k}; \mu) = \tau \sigma_1 (y_d^k - y^{*,k}, y_1^k)_{L^2(D)}, \quad 1 \leq k \leq K-1. \tag{A.4}$$

Furthermore, the final condition (2.8d) with test function $\varphi = y_1^K$ yields

$$m(y_1^K, p^{*,K}) + \tau a(y_1^K, p^{*,K}; \mu) = \tau \sigma_1 (y_d^K - y^{*,K}, y_1^K)_{L^2(D)} + \sigma_2 (y_d^K - y^{*,K}, y_1^K)_{L^2(D)}. \tag{A.5}$$

From (A.3) and (A.5) it follows that

$$\sum_{k=1}^{K-1} m(y_1^k, p^{*,k} - p^{*,k+1}) + \tau \sum_{k=1}^{K-1} a(y_1^k, p^{*,k}; \mu)$$

$$= \tau \sum_{k=1}^{K} \sum_{i=1}^{m} b_i(p^{*,k})(\tilde{u}_i^k - u_i^{*,k}) - \tau \sigma_1 (y_d^K - y^{*,K}, y_1^K)_{L^2(D)} - \sigma_2 (y_d^K - y^{*,K}, y_1^K)_{L^2(D)}. \tag{A.6}$$

We next sum (A.4) from $k = 1$ to $K - 1$ to find

$$\sum_{k=1}^{K-1} m(y_1^k, p^{*,k} - p^{*,k+1}) + \tau \sum_{k=1}^{K-1} a(y_1^k, p^{*,k}; \mu) = \tau \sigma_1 \sum_{k=1}^{K-1} (y_d^k - y^{*,k}, y_1^k)_{L^2(D)}. \tag{A.7}$$

Since the left-hand sides of (A.7) and (A.6) are equal it follows that

$$\tau \sum_{k=1}^{K} \sum_{i=1}^{m} b_i(p^{*,k})(\tilde{u}_i^k - u_i^{*,k}) = \tau\sigma_1 \sum_{k=1}^{K} (y_d^k - y^{*,k}, y_1^k)_{L^2(D)} + \sigma_2(y_d^K - y^{*,K}, y_1^K)_{L^2(D)}. \tag{A.8}$$

Following the same steps as above, we let y_2 be the solution of the state equation for the control input $u^* - \tilde{u}$ ($y_2 = -y_1$), choose as test function $\phi = \tilde{p}^k$, and sum from $k = 1$ to K to obtain (compare (A.3))

$$\sum_{k=1}^{K-1} m(y_2^k, \tilde{p}^k - \tilde{p}^{k+1}) + \tau \sum_{k=1}^{K-1} a(y_2^k, \tilde{p}^k; \mu) + m(y_2^K, \tilde{p}^K) + \tau a(y_2^K, \tilde{p}^K; \mu) = \tau \sum_{k=1}^{K} \sum_{i=1}^{m} b_i(\tilde{p}^k)(u_i^{*,k} - \tilde{u}_i^k). \tag{A.9}$$

We now consider the adjoint equation for $\tilde{p}^k$ with test function $\varphi = y_2^k$ and — analogous to (A.8) — arrive at

$$\tau \sum_{k=1}^{K} \sum_{i=1}^{m} b_i(\tilde{p}^k)(u_i^{*,k} - \tilde{u}_i^k) = \tau\sigma_1 \sum_{k=1}^{K} (y_d^k - \tilde{y}^k, y_2^k)_{L^2(D)} + \sigma_2(y_d^K - \tilde{y}^K, y_2^K)_{L^2(D)}. \tag{A.10}$$

It follows from the linearity of the state equation that

$$y_1 = \tilde{y} - y^* \quad \text{and} \quad y_2 = y^* - \tilde{y}. \tag{A.11}$$

Finally, summing (A.8) and (A.10) and invoking (A.11) yields

$$\begin{aligned}
\tau \sum_{k=1}^{K} \sum_{i=1}^{m} b_i(p^{*,k} - \tilde{p}^k)(\tilde{u}_i^k - u_i^{*,k}) &= \tau\sigma_1 \sum_{k=1}^{K} (y_d^k - y^{*,k}, y_1^k)_{L^2(D)} + \sigma_2(y_d^K - y^{*,K}, y_1^K)_{L^2(D)} \\
&\quad + \tau\sigma_1 \sum_{k=1}^{K} (y_d^k - \tilde{y}^k, y_2^k)_{L^2(D)} + \sigma_2(y_d^K - \tilde{y}^K, y_2^K)_{L^2(D)} \\
&= \tau\sigma_1 \sum_{k=1}^{K} (y_d^k - y^{*,k}, \tilde{y}^k - y^{*,k})_{L^2(D)} + \sigma_2(y_d^K - y^{*,K}, \tilde{y}^K - y^{*,K})_{L^2(D)} \\
&\quad - \tau\sigma_1 \sum_{k=1}^{K} (y_d^k - \tilde{y}^k, \tilde{y}^k - y^{*,k})_{L^2(D)} - \sigma_2(y_d^K - \tilde{y}^K, \tilde{y}^K - y^{*,K})_{L^2(D)} \\
&= \tau\sigma_1 \sum_{k=1}^{K} \|\tilde{y}^k - y^{*,k}\|_{L^2(D)} + \sigma_2\|\tilde{y}^K - y^{*,K}\|_{L^2(D)} \geq 0, \tag{A.12}
\end{aligned}$$

which is the result stated in Lemma 3.2. □

A.2. Proof of Lemma 3.5

Proof. We immediately derive from (2.8c), (2.8d) and (3.11), (3.12) that $\tilde{e}^{p,k} = p^k(y(u_N^*)) - p_N^{*,k}(y_N^*(u_N^*))$ satisfies

$$m(\varphi, \tilde{e}^{p,k} - \tilde{e}^{p,k+1}) + \tau a(\varphi, \tilde{e}^{p,k}; \mu) = \tau r^{p,k}(\varphi; \mu) + \tau\sigma_1(y_N^{*,k} - \tilde{y}^k, \varphi)_{L^2(D)}, \quad \forall \varphi \in Y, \quad K - 1 \geq k \geq 1, \tag{A.13}$$

with final condition

$$m(\varphi, \tilde{e}^{p,K}) + \tau a(\varphi, \tilde{e}^{p,K}; \mu) = \tau r^{p,K}(\varphi; \mu) + \tau\sigma_1(y_N^{*,K} - \tilde{y}^K, \varphi)_{L^2(D)} + \sigma_2(y_N^{*,K} - \tilde{y}^K, \varphi)_{L^2(D)}, \quad \forall \varphi \in Y. \tag{A.14}$$

We now choose $\varphi = \tilde{e}^{p,k}$ in (A.13) and $\varphi = \tilde{e}^{p,K}$ in (A.14) to obtain

$$m(\tilde{e}^{p,k}, \tilde{e}^{p,k}) + \tau a(\tilde{e}^{p,k}, \tilde{e}^{p,k}; \mu) = m(\tilde{e}^{p,k}, \tilde{e}^{p,k+1}) + \tau r^{p,k}(\tilde{e}^{p,k}; \mu) + \tau \sigma_1(y_N^{*,k} - \tilde{y}^k, \tilde{e}^{p,k})_{L^2(D)}, \quad K - 1 \geq k \geq 1, \tag{A.15}$$

and

$$m(\tilde{e}^{p,K}, \tilde{e}^{p,K}) + \tau a(\tilde{e}^{p,K}, \tilde{e}^{p,K}; \mu) = \tau r^{p,K}(\tilde{e}^{p,K}; \mu) + \tau \sigma_1(y_N^{*,K} - \tilde{y}^K, \tilde{e}^{p,K})_{L^2(D)}$$
$$+ \sigma_2(y_N^{*,K} - \tilde{y}^K, \tilde{e}^{p,K})_{L^2(D)}, \quad \forall \varphi \in Y. \tag{A.16}$$

We first consider (A.15) and note that we can bound the first and third term on the right-hand side using Cauchy-Schwarz and Young's inequality by

$$2m(\tilde{e}^{p,k}, \tilde{e}^{p,k+1}) \leq m(\tilde{e}^{p,k}, \tilde{e}^{p,k}) + m(\tilde{e}^{p,k+1}, \tilde{e}^{p,k+1}), \tag{A.17}$$

and

$$2\tau\sigma_1(y_N^{*,k} - \tilde{y}^k, \tilde{e}^{p,k})_{L^2(D)} \leq 2\tau\sigma_1 C_D^2 \|y_N^{*,k} - \tilde{y}^k\|_Y \|\tilde{e}^{p,k}\|_Y \leq C_D^4 \frac{2\tau\sigma_1^2}{\alpha_{\mathrm{LB}}(\mu)} \|y_N^{*,k} - \tilde{y}^k\|_Y^2 + \frac{\tau\alpha_{\mathrm{LB}}(\mu)}{2} \|\tilde{e}^{p,k}\|_Y^2, \tag{A.18}$$

where we also used the definition of C_D. Furthermore, using the definition of the dual norm and Young's inequality the second term on the right-hand side of (A.15) can be bounded by

$$2\tau r^{p,k}(\tilde{e}^{p,k}; \mu) \leq 2\tau \|r^{p,k}(\cdot; \mu)\|_{Y'} \|\tilde{e}^{p,k}\|_Y \leq \frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \|r^{p,k}(\cdot; \mu)\|_{Y'}^2 + \frac{\tau\alpha_{\mathrm{LB}}(\mu)}{2} \|\tilde{e}^{p,k}\|_Y^2. \tag{A.19}$$

It thus follows from (A.15), (A.17), (A.18), (A.19), and invoking (1.7) and (1.11) that

$$m(\tilde{e}^{p,k}, \tilde{e}^{p,k}) - m(\tilde{e}^{p,k+1}, \tilde{e}^{p,k+1}) + \tau a(\tilde{e}^{p,k}, \tilde{e}^{p,k}; \mu) \leq \frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \|r^{p,k}(\cdot; \mu)\|_{Y'}^2 + C_D^4 \frac{2\tau\sigma_1^2}{\alpha_{\mathrm{LB}}(\mu)} \|y_N^{*,k} - \tilde{y}^k\|_Y^2. \tag{A.20}$$

We next consider the final condition (A.16) where we bound the last term on the right-hand side using Cauchy-Schwarz and Young's inequality by

$$2\sigma_2(y_N^{*,K} - \tilde{y}^K, \tilde{e}^{p,K})_{L^2(D)} \leq 2\sigma_2 \|y_N^{*,K} - \tilde{y}^K\|_{L^2(D)} \|\tilde{e}^{p,K}\|_{L^2(D)}$$
$$\leq \sigma_2^2 \|y_N^{*,K} - \tilde{y}^K\|_{L^2(D)}^2 + \|\tilde{e}^{p,K}\|_{L^2(D)}^2. \tag{A.21}$$

It thus follows from (A.16), (A.18) and (A.19) for $k = K$, (A.21), and invoking (1.7) and (1.11) that

$$m(\tilde{e}^{p,K}, \tilde{e}^{p,K}) + \tau a(\tilde{e}^{p,K}, \tilde{e}^{p,K}; \mu) \leq \frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \|r^{p,K}(\cdot; \mu)\|_{Y'}^2$$
$$+ C_D^4 \frac{2\tau\sigma_1^2}{\alpha_{\mathrm{LB}}(\mu)} \|y_N^{*,K} - \tilde{y}^K\|_Y^2 + \sigma_2^2 \|y_N^{*,K} - \tilde{y}^K\|_{L^2(D)}^2, \tag{A.22}$$

where we also used the fact that $\|\cdot\|_{L^2(D)} \leq \|\cdot\|_{L^2(\Omega)} = m(\cdot, \cdot)$. We now perform the sum from $k' = k$ to $K - 1$ of (A.20) and add (A.22), leading to

$$m(\tilde{e}^{p,k}, \tilde{e}^{p,k}) + \tau \sum_{k'=k}^{K} a(\tilde{e}^{p,k}, \tilde{e}^{p,k}; \mu) \leq \frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=k}^{K} \|r^{p,k'}(\cdot; \mu)\|_{Y'}^2$$
$$+ C_D^4 \frac{2\tau\sigma_1^2}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=k}^{K} \|y_N^{*,k'} - \tilde{y}^{k'}\|_Y^2 + \sigma_2^2 \|y_N^{*,K} - \tilde{y}^K\|_{L^2(D)}^2. \tag{A.23}$$

Finally, we note that we can bound the sum of the error $\tilde{e}^{y,k} = y_N^{*,k} - \tilde{y}^k$ by

$$\tau \sum_{k'=k}^{K} \|\tilde{e}^{y,k'}\|_Y^2 \le \frac{\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=k}^{K} a(\tilde{e}^{y,k'}, \tilde{e}^{y,k'}; \mu) \le \frac{1}{\alpha_{\mathrm{LB}}(\mu)} \left(m(\tilde{e}^{y,K}, \tilde{e}^{y,K}) + \tau \sum_{k'=1}^{K} a(\tilde{e}^{y,k'}, \tilde{e}^{y,k'}; \mu) \right)$$

$$\le \frac{1}{\alpha_{\mathrm{LB}}(\mu)} \left(\tilde{\Delta}_N^{y,K}(\mu) \right)^2 \tag{A.24}$$

and from (1.15) that

$$\|y_N^{*,K} - \tilde{y}^K\|_{L^2(D)}^2 \le \frac{1}{2} \left(\tilde{\Delta}_N^{y,K}(\mu) \right)^2. \tag{A.25}$$

The desired result then follows from (A.23), (A.24), and (A.25).   □

A.3. Proof of Lemma 3.9

Proof. Since the proof follows along the same lines as the proof of Lemma 3.5 we only sketch the main steps. We immediately derive from (2.8a) and (3.10) that $e^{y,*,k} = y^{*,k}(u^*) - y_N^{*,k}(u_N^*)$ satisfies

$$m(e^{y,*,k} - e^{y,*,k-1}, \phi) + \tau a(e^{y,*,k}, \phi; \mu) = \tau r^{y,k}(\phi; \mu) + \tau \sum_{i=1}^{m} b_i(\phi)(u_i^{*,k} - u_{N,i}^{*,k}), \quad \forall \phi \in Y, \quad 1 \le k \le K, \tag{A.26}$$

with initial condition $e^{y,*,0} = 0$ since $y^{*,0} = y_N^{*,0} = 0$ by assumption. We now choose $\phi = e^{y,*,k}$, again apply Cauchy-Schwarz, Young's inequality, and the definition of the dual norm — analogous to (A.17) and (A.19) — and invoke (1.7) and (1.11) to obtain

$$m(e^{y,*,k}, e^{y,*,k}) - m(e^{y,*,k-1}, e^{y,*,k-1}) + \tau a(e^{y,*,k}, e^{y,*,k}; \mu)$$

$$\le \frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \|r^{y,k}(\cdot; \mu)\|_{Y'}^2 + \frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \left(\sum_{i=1}^{m} \|b_i\|_{Y'} (u_i^{*,k} - u_{N,i}^{*,k}) \right)^2 \tag{A.27}$$

We now perform the sum from $k' = 1$ to k, recall that $e^{y,*,0} = 0$, and invoke Proposition 3.6 resp. 3.8, leading to

$$m(e^{y,*,k}, e^{y,*,k}) + \tau \sum_{k'=1}^{k} a(e^{y,*,k'}, e^{y,*,k'}; \mu)$$

$$\le \frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=1}^{k} \|r^{y,k'}(\cdot; \mu)\|_{Y'}^2 + \frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=1}^{k} \left(\sum_{i=1}^{m} \|b_i\|_{Y'}^2 \right) \left(\sum_{i=1}^{m} (u_i^{*,k'} - u_{N,i}^{*,k'})^2 \right)$$

$$\le \frac{2\tau}{\alpha_{\mathrm{LB}}(\mu)} \sum_{k'=1}^{k} \|r^{y,k'}(\cdot; \mu)\|_{Y'}^2 + \frac{2}{\alpha_{\mathrm{LB}}(\mu)} \left(\sum_{i=1}^{m} \|b_i\|_{Y'}^2 \right) \left(\Delta_N^{u,*}(\mu) \right)^2, \tag{A.28}$$

which is the result stated in Lemma 3.9.   □

References

[1] N. Altmüller and L. Grüne. Distributed and boundary model predictive control for the heat equation. *GAMM Mitteilungen*, 35(2):131–145, 2012.

[2] A. C. Antoulas. *Approximation of Large-Scale Dynamical Systems*. Advances in Design and Control. SIAM, 2005.

[3] N. Arada, E. Casas, and F. Tröltzsch. Error estimates for the numerical approximation of a semilinear elliptic control problem. *Computational Optimization and Applications*, 23:201–229, 2002.

[4] J. A. Atwell and B. B. King. Proper orthogonal decomposition for reduced basis feedback controllers for parabolic equations. *Mathematical and Computer Modelling*, 33(1-3):1–19, 2001.

[5] R. Becker, H. Kapp, and R. Rannacher. Adaptive finite element methods for optimal control of partial differential equations: Basic concept. *SIAM Journal on Control and Optimization*, 39:113–132, 2000.

[6] P. Benner, V. Mehrmann, and D. Sorensen, editors. *Dimension reduction of large-scale systems*, volume 45 of *Lecture Notes in Computational Science and Engineering*, Berlin, 2005. Springer.

[7] E. Casas and F. Tröltzsch. Error estimates for the finite-element approximation of a semilinear elliptic control problem. *Control Cybernet*, 90:695–712, 2002.

[8] L. Dedè. Reduced basis method and a posteriori error estimation for parametrized linear-quadratic optimal control problems. *SIAM Journal on Scientific Computing*, 32(2):997–1019, 2010.

[9] L. Dedè. Reduced basis method and error estimation for parametrized optimal control problems with control constraints. *Journal of Scientific Computing*, 50(2):287–305, 2012.

[10] J. Eftang, D. Huynh, D. Knezevic, and A. Patera. A two-step certified reduced basis method. *Journal of Scientific Computing*, 51:28–58, 2012.

[11] A.-L. Gerner and K. Veroy. Certified reduced basis methods for parametrized saddle point problems. Accepted for publication in SIAM Journal on Scientific Computing, 2012.

[12] M. A. Grepl and M. Kärcher. Reduced basis a posteriori error bounds for parametrized linear-quadratic elliptic optimal control problems. *Comptes Rendus Mathematique*, 349(15-16):873–877, 2011.

[13] M. A. Grepl and A. T. Patera. A posteriori error bounds for reduced-basis approximations of parametrized parabolic partial differential equations. *ESAIM: Mathematical Modelling and Numerical Analysis*, 39(1):157–181, 2005.

[14] B. Haasdonk and M. Ohlberger. Reduced basis method for finite volume approximations of parametrized linear evolution equations. *ESAIM: Mathematical Modelling and Numerical Analysis*, 42(02):277–302, 2008.

[15] W. Hager. Multiplier methods for nonlinear optimal control. *SIAM Journal on Numerical Analysis*, 27(4):1061–1080, 1990.

[16] M. Hinze, R. Pinnau, M. Ulbrich, and S. Ulbrich. *Optimization with PDE Constraints*, volume 23 of *Mathematical Modelling: Theory and Applications*. Springer, 2009.

[17] D. B. P. Huynh, G. Rozza, S. Sen, and A. T. Patera. A successive constraint linear optimization method for lower bounds of parametric coercivity and inf-sup stability constants. *Comptes Rendus Mathematique*, 345(8):473–478, 2007.

[18] K. Ito and K. Kunisch. Receding horizon optimal control for infinite dimensional systems. *ESAIM: Control, Optimisation and Calculus of Variations*, 8:741–760, 2002.

[19] K. Ito and K. Kunisch. Reduced-order optimal control based on approximate inertial manifolds for nonlinear dynamical systems. *SIAM Journal on Numerical Analysis*, 46(6):2867–2891, 2008.

[20] K. Ito and S. S. Ravindran. A reduced basis method for control problems governed by pdes. In W. Desch, F. Kappel, and K. Kunisch, editors, *Control and Estimation of Distributed Parameter Systems*, volume 126 of *International Series of Numerical Mathematics*, pages 153–168. Birkhäuser Basel, 1998.

[21] K. Ito and S. S. Ravindran. A reduced-order method for simulation and control of fluid flows. *Journal of Computational Physics*, 143(2):403 – 425, 1998.

[22] K. Ito and S. S. Ravindran. A reduced basis method for optimal control of unsteady viscous flows. *International Journal of Computational Fluid Dynamics*, 15:97–113, 2001.

[23] M. Kärcher. The reduced-basis method for parametrized linear-quadratic elliptic optimal control problems. Master's thesis, Technische Universität München, April 2011.

[24] M. Kärcher and M. A. Grepl. A certified reduced basis method for parametrized elliptic optimal control problems. Technical report, submitted to ESAIM: Control, Optimisation and Calculus of Variations, 2012.

[25] K. Kunisch and S. Volkwein. Control of the Burgers equation by a reduced-order approach using proper orthogonal decomposition. *Journal of Optimization Theory and Applications*, 102:345–371, 1999.

[26] K. Kunisch, S. Volkwein, and L. Xie. HJB-POD based feedback design for the optimal control of evolution problems. *SIAM Journal on Applied Dynamical Systems*, 3:701–722, 2004.

[27] G. Leugering, S. Engell, A. Griewank, M. Hinze, R. Rannacher, V. Schulz, M. Ulbrich, and S. Ulbrich, editors. *Constrained Optimization and Optimal Control for Partial Differential Equations*. (International Series of Numerical Mathematics). Birkhäuser Basel, 2012.

[28] J. L. Lions. *Optimal Control of Systems Governed by Partial Differential Equations*. Springer, 1971.

[29] L. Machiels, Y. Maday, I. B. Oliveira, A. T. Patera, and D. V. Rovas. Output bounds for reduced-basis approximations of symmetric positive definite eigenvalue problems. *Comptes Rendus Mathematique*, 331(2):153–158, 2000.

[30] K. Malanowski, C. Buskens, and H. Maurer. *Convergence of approximations to nonlinear optimal control problems*, volume 195, pages 253–284. CRC Press, 1997.

[31] F. Negri, G. Rozza, A. Manzoni, and A. Quarteroni. Reduced basis method for parametrized elliptic optimal control problems. Technical report, Submitted, 2012.

[32] I. B. Oliveira. *A "HUM" Conjugate Gradient Algorithm for Constrained Nonlinear Optimal Control: Terminal and Regulator Problems*. PhD thesis, Massachusetts Institute of Technology, 2002.

[33] C. Prud'homme, D. V. Rovas, K. Veroy, L. Machiels, Y. Maday, A. T. Patera, and G. Turinici. Reliable real-time solution of parametrized partial differential equations: Reduced-basis output bound methods. *Journal of Fluids Engineering*, 124(1):70–80, 2002.

[34] A. Quarteroni, G. Rozza, L. Dedè, and A. Quaini. Numerical approximation of a control problem for advection-diffusion processes. In F. Ceragioli, A. Dontchev, H. Futura, K. Marti, and L. Pandolfi, editors, *System Modeling and Optimization*, volume 199 of *IFIP International Federation for Information Processing*, pages 261–273. Springer, 2006.

[35] A. M. Quarteroni and A. Valli. *Numerical Approximation of Partial Differential Equations*, volume 23 of *Springer Series in Computational Mathematics*. Springer, 2008.

[36] J. B. Rawlings and D. Q. Mayne. *Model Predictive Control: Theory and Design*. Nob Hill Publishing, 2009.

[37] D. V. Rovas. *Reduced-Basis Output Bound Methods for Parametrized Partial Differential Equations*. PhD thesis, Massachusetts Institute of Technology, February 2003.

[38] G. Rozza, D. B. P. Huynh, and A. T. Patera. Reduced basis approximation and a posteriori error estimation for affinely parametrized elliptic coercive partial differential equations. *Archives of Computational Methods in Engineering*, 15(3):229–275, 2008.

[39] G. Rozza and K. Veroy. On the stability of the reduced basis method for Stokes equations in parametrized domains. *Computer Methods in Applied Mechanics and Engineering*, 196(7):1244 – 1260, 2007.

[40] W. Schilders, H. van der Vorst, and J. Rommes, editors. *Model order reduction: Theory, research aspects and applications*, volume 13 of *Mathematics in Industry*. Springer-Verlag, Berlin, 2008.

[41] T. Tonn, K. Urban, and S. Volkwein. Comparison of the reduced-basis and pod a posteriori error estimators for an elliptic linear-quadratic optimal control problem. *Mathematical and Computer Modelling of Dynamical Systems*, 17(4):355–369, 2011.

[42] F. Tröltzsch. *Optimal Control of Partial Differential Equations: Theory, Methods and Applications*, volume 112 of *Graduate Studies in Mathematics*. American Mathematical Society, 2010.

[43] F. Tröltzsch and S. Volkwein. POD a-posteriori error estimates for linear-quadratic optimal control problems. *Computational Optimization and Applications*, 44:83–115, 2009.

[44] K. Veroy, D. V. Rovas, and A. T. Patera. A posteriori error estimation for reduced-basis approximation of parametrized elliptic coercive partial differential equations: "convex inverse" bound conditioners. *ESAIM: Control, Optimisation and Calculus of Variations*, 8:1007–1028, 2002. Special Volume: A tribute to J.L. Lions.