A Posteriori Error Bounds for Reduced Basis Approximations of Nonaffine and Nonlinear Parabolic Partial Differential Equations

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Bericht Nr. 306

März 2010

Key words: Reduced basis methods, parabolic PDEs, parameter–dependent systems, nonlinear PDEs, nonaffine parameter dependence, a posteriori error estimation, Galerkin approximation.

AMS subject classifications: 35K15, 35K55, 65M15

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A posteriori error bounds for reduced basis approximations of nonaffine and nonlinear parabolic partial differential equations

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March 31, 2010

Abstract

We present a *posteriori* error bounds for reduced basis approximations of parabolic partial differential equations involving (i) a nonaffine dependence on the parameter and (ii) a nonlinear dependence on the field variable. The method employs the Empirical Interpolation Method in order to construct "affine" coefficient-function approximations of the "nonaffine" (or nonlinear) parametrized functions. Our a posteriori error bounds take both error contributions explicitly into account — the error introduced by the reduced basis approximation and the error induced by the coefficient function interpolation. We show that these bounds are rigorous upper bounds for the approximation error under certain conditions on the function interpolation, thus addressing the demand for certainty of the approximation. As regards efficiency, we develop an efficient offline-online computational procedure for the calculation of the reduced basis approximation and associated error bound. The method is thus ideally suited for the many-query or real-time contexts. We also introduce a new sampling approach to generate the collateral reduced basis space for functions with a nonlinear dependence on the field variable. Numerical results are presented to confirm and test our approach.

1 Introduction

The role of numerical simulation in engineering and science has become increasingly important. System or component behavior is often modeled using

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a set of partial differential equations and associated boundary conditions, the analytical solution to which is generally unavailable. In practice, a discretization procedure such as the finite element method (FEM) is used.

However, as the physical problems become more complex and the mathematical models more involved, current computational methods prove increasingly inadequate, especially in contexts requiring numerous solutions of parametrized partial differential equations for many different values of the parameter. Even for modest-complexity models, the computational cost to solve these problems is prohibitive.

For example, the design, optimization, control, and characterization of engineering components or systems often require repeated, reliable, and realtime prediction of performance metrics, or outputs, $s^{\rm e}$, such as heat fluxes or flowrates¹. These outputs are typically functionals of field variables, $y^{\rm e}$, — such as temperatures or velocities — associated with a parametrized partial differential equation; the parameters, or inputs, μ , serve to identify a particular configuration of the component — such as boundary conditions, material properties, and geometry. The relevant system behaviour is thus described by an implicit input-output relationship, $s^{\rm e}(\mu)$, evaluation of which demands solution of the underlying partial differential equation (PDE).

Our focus here is on parabolic PDEs. For simplicity, we will directly consider a time-discrete framework associated to the time interval $I \equiv]0, t_f]$ $(\bar{I} \equiv [0, t_f])$. We divide \bar{I} into K subintervals of equal length $\Delta t = \frac{t_f}{K}$ and define $t^k \equiv k\Delta t$, $0 \leq k \leq K \equiv \frac{t_f}{\Delta t}$, and $\mathbb{I} \equiv \{t^0, \ldots, t^K\}$; for notational convenience, we also introduce $\mathbb{K} \equiv \{1, \ldots, K\}$. We shall consider Euler-Backward for the time integration although higher-order schemes such as Crank-Nicolson can also be readily treated [13]. The abstract formulation can be stated as follows: given any $\mu \in \mathcal{D} \subset \mathbb{R}^P$, we evaluate the output $s^{ek}(\mu) \equiv s^{e}(t^k; \mu) = \ell(y^{ek}(\mu)), \ \forall k \in \mathbb{K}$, where $y^{ek}(\mu) \equiv y^{e}(t^k; \mu) \in X^e$ satisfies

$$m(y^{ek}(\mu), v) + \Delta t \, a(y^{ek}(\mu), v; \mu) = m(y^{ek-1}(\mu), v) + \Delta t \, f(v; \mu) \, u(t^k),$$

$$\forall v \in X^e, \ \forall k \in \mathbb{K}, \quad (1)$$

with initial condition (say) $y^{e}(t^{0}; \mu) = y_{0}^{e}(\mu) = 0$. Here, \mathcal{D} is the parameter domain in which our *P*-tuple (input) parameter μ resides; X^{e} is an appropriate Hilbert space; $\Omega \subset \mathbb{R}^{d}$ is our spatial domain, a point in which shall be denoted x; $f(\cdot; \mu)$, $\ell(\cdot)$ are X^{e} -continuous bounded linear functionals; $a(\cdot, \cdot; \mu)$ and $m(\cdot, \cdot)$ are X^{e} -continuous and Y^{e} -continuous ($X^{e} \subset Y^{e}$)

¹Here superscript "e" shall refer to "exact." We shall later introduce a "truth approximation" which will bear no superscript.

bounded bilinear forms, respectively; and $u(t^k)$ is the "control input" at time $t = t^k$. We assume here that $\ell(\cdot)$, and $m(\cdot, \cdot)$ do not depend on the parameter; parameter dependence, however, is readily admitted [15].

Since the exact solution is usually unavailable, numerical solution techniques must be employed to solve (1). Classical approaches such as the finite element method can not typically satisfy the requirements of *real-time certified* prediction of the outputs of interest. In the finite element method, the infinite dimensional solution space is replaced by a finite dimensional "truth" approximation space $X \subset X^e$ of size \mathcal{N} : for any $\mu \in \mathcal{D}$, we evaluate the output

$$s^k(\mu) = \ell(y^k(\mu)), \quad \forall k \in \mathbb{K},$$
(2)

where $y^k(\mu) \in X$ satisfies

$$m(y^{k}(\mu), v) + \Delta t \, a(y^{k}(\mu), v; \mu) = m(y^{k-1}(\mu), v) + \Delta t \, f(v; \mu) \, u(t^{k}),$$

$$\forall v \in X, \ \forall k \in \mathbb{K}, \quad (3)$$

with initial condition $y(\mu, t^0) = y_0(\mu) = 0$. We shall assume — hence the appellation "truth" — that the approximation space is sufficiently rich such that the FEM approximation $y^k(\mu)$ (respectively, $s^k(\mu)$) is indistinguishable from the analytic, or exact, solution $y^{ek}(\mu)$ (respectively, $s^{ek}(\mu)$).

Unfortunately, for any reasonable error tolerance, the dimension \mathcal{N} needed to satisfy this condition — even with the application of appropriate (parameterdependent) adaptive mesh refinement strategies — is typically extremely large, and in particular much too large to satisfy the condition of real-time response or the need for numerous solutions. Our goal is the development of numerical methods that permit the *efficient* and *reliable* evaluation of this PDE-induced input-output relationship in real-time or in the limit of many queries — that is, in the design, optimization, control, and characterization contexts. To achieve this goal we pursue the reduced basis method. The reduced basis method was first introduced in the late 1970s for the nonlinear analysis of structures [1, 29] and subsequently abstracted and analyzed [5, 12, 31, 36]; see [37] for a recent review of contributions to the methodology.

The core requirement for the development of efficient offline-online computational strategies, i.e., online \mathcal{N} -independence, is the affine parameter dependence — e.g. the bilinear form $a(w, v; \mu)$ can be expressed as

$$a(w, v; \mu) = \sum_{q=1}^{Q} \Theta^{q}(\mu) a^{q}(w, v), \qquad (4)$$

where the $\Theta^q(\mu) : \mathcal{D} \to \mathbb{R}$ are parameter dependent functions and the $a^q(w, v)$ are parameter-independent bilinear forms. In the recent past, reduced basis approximations and associated a posteriori error estimation for linear and at most quadratically nonlinear elliptic and parabolic PDEs honoring this requirement have been successfully developed [15, 16, 19, 26, 27, 32, 40, 42, 43].

In [14] we extended these results and developed efficient offline-online strategies for *reduced basis approximations* of nonaffine (and certain classes of nonlinear) elliptic and parabolic PDEs. Our approach is based on the Empirical Interpolation Method (EIM) [4] — a technique that recovers the efficient offline-online decomposition even in the presence of nonaffine parameter dependence. We can thus develop an "online \mathcal{N} -independent" computational decomposition even for nonaffine parameter dependence, i.e., where for general $g(x; \mu)$ (here $x \in \Omega$ and $\mu \in \mathcal{D}$) the bilinear form satisfies

$$a(w,v;\mu) \equiv \int_{\Omega} \nabla w \cdot \nabla v + \int_{\Omega} g(x;\mu) \, w \, v.$$
 (5)

A posteriori error bounds for nonaffine linear and certain classes of nonaffine nonlinear elliptic problems have been proposed in [7] and [28], respectively. In this paper, we shall consider the extension of these techniques and develop a posteriori error bounds (i) for nonaffine parabolic problems and (ii) for problems in which g is a nonaffine nonlinear function of the parameter μ (possibly including time), spatial coordinate x, and field variable y we hence treat certain classes of nonlinear problems. We recall that the computational cost to generate the collateral reduced basis space for the function approximation is very high in the parabolic case if the function g is time-varying either through an explicit dependence on time or an implicit dependence via the field variable $y(t^k; \mu)$ [14]. We therefore propose a novel more efficient approach to generate the collateral reduced basis space which is based on a POD(in time)/Greedy(in parameter space) search [16].

A large number of model order reduction (MOR) techniques [2, 8, 9, 25, 30, 35, 39, 44] have been developed to treat (nonlinear) time-dependent problems. One approach is linearization [44] and polynomial approximation [9, 30]: however, due to a lack of efficient representations of nonlinear terms and fast exponential growth (with the degree of the nonlinear approximation order) of computational complexity, these methods are quite expensive and do not address strong nonlinearities efficiently; other approaches for highly nonlinear systems (such as piecewise-linearization) have also been proposed [35, 38] but at the expense of high computational cost and little control over model accuracy. Furthermore, although a priori error bounds

to quantify the error due to model reduction have been derived in the linear case, *a posteriori* error bounds have not yet been adequately considered even for the linear case, let alone the nonlinear case, for most MOR approaches. Finally, it is important to note that most MOR techniques focus mainly on reduced-order modeling of dynamical systems in which time is considered the *only* "parameter;" the development of reduced-order models for problems with a simultaneous dependence of the field variable on parameter and time — our focus here — is much less common [6, 10].

This paper is organized as follows: In Section 2 we present a short review of the empirical interpolation method. The abstract problem formulation, reduced basis approximation, associated *a posteriori* error estimation, and computational considerations for linear coercive parabolic problems with nonaffine parameter dependence are discussed in Section 3. In Section 4 we extend these results to monotonic nonlinear parabolic PDEs. Numerical results are used throughout to test and confirm our theoretical results. We offer concluding remarks in Section 5.

2 Empirical Interpolation Method

The Empirical Interpolation Method (EIM), introduced in [4], serves to construct "affine" coefficient-function approximations of "non-affine" parametrized functions. The method is frequently applied in reduced basis approximations of parametrized partial differential equations with nonaffine parameter dependence [14]; the affine approximation of the equations is crucial for computational efficiency. Here, we briefly summarize the results for the interpolation procedure and the estimator for the interpolation error [4, 14].

2.1 Coefficient-function approximation

We are given a function $g : \Omega \times \mathcal{D} \to \mathbb{R}$ such that, for all $\mu \in \mathcal{D}$, $g(\cdot; \mu) \in L^{\infty}(\Omega)$; here, $\mathcal{D} \subset \mathbb{R}^{P}$ is the parameter domain, $\Omega \subset \mathbb{R}^{2}$ is the spatial domain – a point in which shall be denoted by $x = (x_{(1)}, x_{(2)})$ – and $L^{\infty}(\Omega) \equiv \{v | \operatorname{ess\,sup}_{v \in \Omega} | v(x) | < \infty\}$.

We first define the nested sample sets $S_M^g \equiv \{\mu_1^g \in \mathcal{D}, \ldots, \mu_M^g \in \mathcal{D}\}$, associated reduced basis spaces $W_M^g = \text{span} \{\xi_m \equiv g(x; \mu_m^g), 1 \leq m \leq M\}$, and nested sets of interpolation points $T_M^g = \{x_1, \ldots, x_M\}, 1 \leq M \leq M_{\text{max}}$. We present here a generalization for the construction of the EIM which allows a simultaneous definition of the generating functions W_M^g and associated interpolation points T_M^g [24]. The construction is based on a greedy algorithm [42] and is required for our POD/Greedy algorithm which we will introduce in Section 4.4.

We first choose $\mu_1^g \in \mathcal{D}$, compute $\xi_1 \equiv g(x; \mu_1^g)$, define $W_1^g \equiv \operatorname{span}\{\xi_1\}$, and set $x_1 = \operatorname{arg} \operatorname{ess} \operatorname{sup}_{x \in \Omega} |\xi_1(x)|, q_1 = \xi_1(x)/\xi_1(x_1), \operatorname{and} B_{11}^1 = 1$. We then proceed by induction to generate S_M^g, W_M^g , and T_M^g : for $1 \leq M \leq M_{\max} - 1$, we determine $\mu_{M+1}^g \equiv \operatorname{arg} \max_{\mu \in \Xi_{\operatorname{train}}^g} \|g(\cdot; \mu) - g_M(\cdot; \mu)\|_{L^{\infty}(\Omega)}$, compute $\xi_{M+1} \equiv g(x; \mu_{M+1}^g)$, and define $W_{M+1}^g \equiv \operatorname{span}\{\xi_m\}_{m=1}^{M+1}$; to generate the interpolation points we solve the linear system $\sum_{j=1}^M \sigma_j^M q_j(x_i) = \xi_{M+1}(x_i)$, $1 \leq i \leq M$ and we set $r_{M+1}(x) = \xi_{M+1}(x) - \sum_{j=1}^M \sigma_j^M q_j(x), x_{M+1} =$ arg ess $\operatorname{sup}_{x \in \Omega} |r_{M+1}(x)|$, and $q_{M+1}(x) = r_{M+1}(x)/r_{M+1}(x_{M+1})$. Here, $\Xi_{\operatorname{train}}^g \subset \mathcal{D}$ is a finite but suitably large train sample which shall serve as our \mathcal{D} surrogate, and $g_M(\cdot; \mu) \in W_M^g$ is the EIM interpolant of $g(\cdot; \mu)$ over the set T_M^g for any $\mu \in \mathcal{D}$. Specifically

$$g_M(x;\mu) \equiv \sum_{m=1}^M \varphi_{M\,m}(\mu) q_m,\tag{6}$$

where

$$\sum_{j=1}^{M} B_{ij}^{M} \varphi_{Mj}(\mu) = g(x_i; \mu), \quad 1 \le i \le M,$$
(7)

and the matrix $B^M \in \mathbb{R}^{M \times M}$ is defined such that $B_{ij}^M = q_j(x_i), 1 \leq i, j \leq M$. We note that the determination of the coefficients $\varphi_{Mm}(\mu)$ requires only $\mathcal{O}(M^2)$ computational cost since B^M is lower triangular with unity diagonal and that $\{q_m\}_{m=1}^M$ is a basis for W_M^g [4, 14].

Finally, we define a "Lebesgue constant" [33] $\Lambda_M \equiv \sup_{x \in \Omega} \sum_{m=1}^M |V_m^M(x)|$, where $V_m^M(x) \in W_M^g$ are the characteristic functions of W_M^g satisfying $V_m^M(x_n) \equiv \delta_{mn}, 1 \leq m, n \leq M$; here, δ_{mn} is the Kronecker delta symbol. We recall that (i) the set of all characteristic functions $\{V_m^M\}_{m=1}^M$ is a basis for W_M^g , and (ii) the Lebesgue constant Λ_M satisfies $\Lambda_M \leq 2^M - 1$ [4, 14]. In applications, the actual asymptotic behavior of Λ_M is much lower, as we shall observe subsequently.

2.2 A posteriori error estimation

Given an approximation $g_M(x;\mu)$ for $M \leq M_{\max} - 1$, we define $\mathcal{E}_M(x;\mu) \equiv \hat{\varepsilon}_M(\mu) q_{M+1}(x)$, where $\hat{\varepsilon}_M(\mu) \equiv |g(x_{M+1};\mu) - g_M(x_{M+1};\mu)|$. We also define the interpolation error as

$$\varepsilon_M(\mu) \equiv \|g(\,\cdot\,;\mu) - g_M(\,\cdot\,;\mu)\|_{L^{\infty}(\Omega)}.$$
(8)

In general, $\varepsilon_M(\mu) \ge \hat{\varepsilon}_M(\mu)$, since $\varepsilon_M(\mu) \ge |g(x;\mu) - g_M(x;\mu)|$ for all $x \in \Omega$, and thus also for $x = x_{M+1}$. However, we can prove (see [4, 14, 24])

Proposition 1. If $g(\cdot; \mu) \in W_{M+1}^g$, then (i) $g(x; \mu) - g_M(x; \mu) = \pm \mathcal{E}_M(x; \mu)$ (either $\mathcal{E}_M(x; \mu)$ or $-\mathcal{E}_M(x; \mu)$), and (ii) $\|g(\cdot; \mu) - g_M(\cdot; \mu)\|_{L^{\infty}(\Omega)} = \hat{\varepsilon}_M(\mu)$.

Of course, in general $g(\cdot; \mu) \notin W^g_{M+1}$, and hence our estimator $\hat{\varepsilon}_M(\mu)$ is indeed a lower bound; however, if $\varepsilon_M(\mu) \to 0$ very fast, we expect that the effectivity,

$$\eta_M(\mu) \equiv \frac{\hat{\varepsilon}_M(\mu)}{\varepsilon_M(\mu)},\tag{9}$$

shall be close to unity. Furthermore, the estimator is very inexpensive – one additional evaluation of $g(\cdot;\mu)$ at a single point in Ω . Also note that we can readily improve the rigor of our bound at only modest additional cost: if we assume that $g(\cdot;\mu) \in W^g_{M+k}$, then $\hat{\varepsilon}_M = 2^{k-1} \max_{i \in \{1,\ldots,k\}} |g(x_{M+i};\mu) - g_M(x_{M+i};\mu)|$ is an upper bound for $\varepsilon_M(\mu)$.

In a recent note [11] a new rigorous *a posteriori* error bound for the empirical interpolation method is proposed that does not rely on the assumption $g(\cdot; \mu) \in W_{M+1}^g$. In the following derivation for nonaffine linear problems, we may directly replace the current "next-point" error bound by this new bound, thus obtaining a rigorous error bound for the reduced-basis approximation. Unfortunately, we cannot follow this approach for nonlinear problems and – with the goal of presenting a unified treatment in mind – we therefore employ the "next-point" error bound throughout the subsequent analysis.

3 Nonaffine Linear Parabolic Equations

3.1 Problem statement

3.1.1 Abstract formulation

We first recall the Hilbert spaces $X^{e} \equiv H_{0}^{1}(\Omega)$ — or, more generally, $H_{0}^{1}(\Omega) \subset X^{e} \subset H^{1}(\Omega)$ — and $Y^{e} \equiv L^{2}(\Omega)$, where $H^{1}(\Omega) \equiv \{v \mid v \in L^{2}(\Omega), \nabla v \in (L^{2}(\Omega))^{d}\}$, $H_{0}^{1}(\Omega) \equiv \{v \mid v \in H^{1}(\Omega), v|_{\partial\Omega} = 0\}$, and $L^{2}(\Omega)$ is the space of square integrable functions over Ω [34]; here Ω is a bounded domain in \mathbb{R}^{d} with Lipschitz continuous boundary $\partial\Omega$. The inner product and norm associated with X^{e} (Y^{e}) are given by $(\cdot, \cdot)_{X^{e}}$ ($(\cdot, \cdot)_{Y^{e}}$) and $\|\cdot\|_{X^{e}} = (\cdot, \cdot)_{X^{e}}^{1/2}$ ($\|\cdot\|_{Y^{e}} = (\cdot, \cdot)_{Y^{e}}^{1/2}$), respectively; for example, $(w, v)_{X^{e}} \equiv \int_{\Omega} \nabla w \cdot \nabla v + (w, v)_{Y^{e}} = (w, v)_{Y^{e}}^{1/2}$

 $\int_{\Omega} w \, v, \ \forall \, w, v \in X^{\mathrm{e}}, \text{ and } (w, v)_{Y^{\mathrm{e}}} \equiv \int_{\Omega} w \, v, \ \forall \, w, v \in Y^{\mathrm{e}}.$ The truth approximation subspace $X \subset X^{\mathrm{e}}(\subset Y^{\mathrm{e}})$ shall inherit this inner product and norm: $(\cdot; \cdot)_X \equiv (\cdot; \cdot)_X^{\mathrm{e}}$ and $\|\cdot\|_X \equiv \|\cdot\|_X^{\mathrm{e}};$ we further define $Y \equiv Y^{\mathrm{e}}.$

We directly consider the truth approximation statement defined in (3) with the output given by (2), in which

$$a(w, v; \mu) = a_0(w, v) + a_1(w, v, g(x; \mu)),$$
(10)

and

$$f(v;\mu) = \int_{\Omega} v h(x;\mu) \tag{11}$$

where $a_0(\cdot, \cdot)$ is a continuous (and, for simplicity, parameter-independent) bilinear form and $a_1: X \times X \times L^{\infty}(\Omega)$ is a trilinear form. For simplicity of exposition, we assume here that $h(x; \mu) = g(x; \mu)$.

We shall further assume that $a(\cdot, \cdot; \mu)$ and $m(\cdot, \cdot)$ are continuous

$$\begin{aligned} a(w,v;\mu) &\leq \gamma_a(\mu) \|w\|_X \|v\|_X \leq \gamma_a^0 \|w\|_X \|v\|_X, \ \forall w,v \in X, \ \forall \mu \in \mathcal{D}(12) \\ m(w,v) &\leq \gamma_m^0 \|w\|_Y \|v\|_Y, \ \forall w,v \in X; \end{aligned} \tag{13}$$

coercive,

$$0 < \alpha_a^0 \le \alpha_a(\mu) \equiv \inf_{w \in X} \frac{a(w, w; \mu)}{\|w\|_X^2}, \quad \forall \mu \in \mathcal{D},$$
(14)

$$0 < \alpha_m^0 \equiv \inf_{v \in X} \frac{m(v, v)}{\|v\|_Y^2};$$
(15)

and symmetric, $a(v, w; \mu) = a(w, v; \mu), \forall w, v \in X, \forall \mu \in \mathcal{D}$, and $m(v, w) = m(w, v), \forall w, v \in X, \forall \mu \in \mathcal{D}$. (We (plausibly) suppose that $\gamma_a^0, \gamma_m^0, \alpha_a^0, \alpha_m^0$ may be chosen independent of \mathcal{N} .) We also assume that the trilinear form a_1 satisfies

$$a_1(w, v, z) \le \gamma_{a_1}^0 \|w\|_X \|v\|_X \|z\|_{L^{\infty}(\Omega)}, \quad \forall w, v \in X, \ \forall z \in L^{\infty}(\Omega).$$
(16)

Next, we require that the linear forms $f(\cdot; \mu) : X \to \mathbb{R}$ and $\ell(\cdot) : X \to \mathbb{R}$ be bounded with respect to $\|\cdot\|_Y$. And finally, we require that all linear and bilinear forms are independent of time — the system is thus linear time-invariant (LTI). It follows, since $g(\cdot; \mu) \in L^{\infty}(\Omega)$, that a solution to (3) exists and is unique [34].

3.1.2 Model problem

As a numerical example we consider the following nonaffine diffusion problem defined on the unit square, $\Omega =]0, 1[^2 \in \mathbb{R}^2$: Given $\mu \equiv (\mu_1, \mu_2) \in \mathcal{D} \equiv [-1, -0.01]^2 \subset \mathbb{R}^{P=2}$, we evaluate $y^k(\mu) \in X$ from (3), where $X \subset X^e \equiv H_0^1(\Omega)$ is a linear finite element truth approximation subspace of dimension $\mathcal{N} = 2601$,

and $z = G(x; \mu)$ is a nonaffine function given by

$$G(x;\mu) \equiv \frac{1}{\sqrt{(x_{(1)} - \mu_1)^2 + (x_{(2)} - \mu_2)^2}}.$$
(18)

The output can be written in the form (2), $s^k(\mu) = \ell(y^k(\mu)), \forall k \in \mathbb{K}$, where $\ell(v) \equiv |\Omega|^{-1} \int_{\Omega} v$ — clearly a very smooth functional. We shall consider the time interval I = [0, 2] and a timestep $\Delta t = 0.01$; we thus have K = 200. We also presume the periodic control input $u(t^k) = \sin(2\pi t^k), t^k \in \mathbb{I}$.

Two snapshots of the solution $y^k(\mu)$ at time $t^k = 25\Delta t$ are shown in Figures 1(a) and (b) for $\mu = (-1, -1)$ and $\mu = (-0.01, -0.01)$, respectively. The solution oscillates in time and the peak is offset towards x = (0, 0) for μ near the "corner" (-0.01, -0.01).

3.2 Reduced basis approximation

3.2.1 Formulation

We suppose that we are given the nested Lagrangian [31] reduced basis spaces

$$W_N^y = \operatorname{span}\{\zeta_n, \ 1 \le n \le N\}, \quad 1 \le N \le N_{\max}, \tag{19}$$

where the ζ_n , $1 \leq n \leq N$, are mutually $(\cdot, \cdot)_X$ -orthogonal basis functions. We comment on the POD/Greedy algorithm for constructing the basis functions in Section 3.4.

Our reduced basis approximation $y_{N,M}^k(\mu)$ to $y^k(\mu)$ is then: given $\mu \in \mathcal{D}$, $y_{N,M}^k(\mu) \in W_N^y$, $1 \le k \le K$, satisfies

$$m(y_{N,M}^{k}(\mu), v) + \Delta t \ (a_{0}(y_{N,M}^{k}(\mu), v) + a_{1}(y_{N,M}^{k}(\mu), v; g_{M}(x; \mu))) = m(y_{N,M}^{k-1}(\mu), v) + \Delta t \ f(v; g_{M}(x; \mu)) \ u(t^{k}), \quad \forall v \in W_{N}^{y}, \quad (20)$$

with initial condition $y_{N,M}^0(\mu) = 0$. We then evaluate the output estimate, $s_{N,M}^k(\mu), \ 1 \le k \le K$, from

$$s_{N,M}^k(\mu) \equiv \ell(y_{N,M}^k(\mu)). \tag{21}$$

Note that we directly replaced $g(x; \mu)$ in (10) by the affine approximation $g_M(x; \mu) = \sum_{m=1}^{M} \varphi_{Mm}(\mu) q_m(x)$ from (6) based upon the empirical interpolation approach described in Section 2.

We now express $y_{N,M}^k(\mu) = \sum_{n=1}^N y_{N,Mn}^k(\mu) \zeta_n$, choose as test functions $v = \zeta_j, 1 \le j \le N$, and invoke (6) to obtain

$$\sum_{i=1}^{N} \left\{ m(\zeta_{i},\zeta_{j}) + \Delta t \left(a_{0}(\zeta_{i},\zeta_{j}) + \sum_{m=1}^{M} \varphi_{M\,m}(\mu) \, a_{1}(\zeta_{i},\zeta_{j},q_{m}) \right) \right\} \, y_{N,M\,i}^{k}(\mu) \\ = \sum_{i=1}^{N} m(\zeta_{i},\zeta_{j}) \, y_{N,M\,i}^{k-1}(\mu) + \Delta t \sum_{m=1}^{M} \varphi_{M\,m}(\mu) \, f(\zeta_{j};q_{m}) \, u(t^{k}), \quad 1 \le i \le N.$$

$$(22)$$

where $\varphi_{Mm}(\mu)$, $1 \leq m \leq M$, is determined from (7). We can thus recover online \mathcal{N} -independence even for nonaffine problems: the quantities $m(\zeta_i, \zeta_j)$, $a_0(\zeta_i, \zeta_j)$, $a_1(\zeta_i, \zeta_j, q_m)$, and $f(\zeta_i; q_m)$ are all *parameter independent* and can thus be pre-computed offline, as discussed further in Section 3.2.2.

In [14] we developed a priori estimates for the convergence rate $y_{N,M}^k(\mu) \rightarrow y^k(\mu)$ – the sum of a best approximation result and a perturbation due to the variational crime associated with the interpolation of g. We next summarize the offline-online computational procedure and then turn to the development of our *a posteriori* error bounds.

3.2.2 Computational procedure

We summarize here the offline-online procedure [3, 18, 23, 32]. We first express $y_{N,M}^k(\mu)$ as

$$y_{N,M}^{k}(\mu) = \sum_{n=1}^{N} y_{N,Mn}^{k}(\mu) \zeta_{n},$$
(23)

and choose as test functions $v = \zeta_j$, $1 \leq j \leq N$ in (20). It then follows from (22) that $\underline{y}_{N,M}^k(\mu) = [y_{N,M1}^k(\mu) \ y_{N,M2}^k(\mu) \dots \ y_{N,MN}^k(\mu)]^T \in \mathbb{R}^N$ satisfies

$$(M_N + \Delta t \ A_N(\mu)) \ \underline{y}_{N,M}^k(\mu) = M_N \ \underline{y}_{N,M}^{k-1}(\mu) + \Delta t \ F_N(\mu) \ u(t^k), \quad \forall \ k \in \mathbb{K},$$
(24)

with initial condition $y_{N,Mn}(\mu, t^0) = 0, 1 \leq n \leq N$. Given $\underline{y}_{N,M}^k(\mu), 1 \leq k \leq K$, we finally evaluate the output estimate from

$$s_{N,M}^{k}(\mu) = L_{N}^{T} \underline{y}_{N,M}^{k}(\mu), \quad \forall k \in \mathbb{K}.$$
(25)

Here, $M_N \in \mathbb{R}^{N \times N}$ is a *parameter-independent* SPD matrix with entries

$$M_{N\,i,j} = m(\zeta_i, \zeta_j), \quad 1 \le i, j \le N.$$

$$\tag{26}$$

Furthermore, we obtain from (6) and (10) that $A_N(\mu) \in \mathbb{R}^{N \times N}$ and $F_N(\mu) \in \mathbb{R}^N$ can be expressed as

$$A_N(\mu) = A_{0,N} + \sum_{m=1}^M \varphi_{Mm}(\mu) A_{1,N}^m, \qquad (27)$$

$$F_N(\mu) = \sum_{m=1}^M \varphi_{Mm}(\mu) F_N^m,$$
 (28)

where $\varphi_{Mm}(\mu)$, $1 \leq m \leq M$, is calculated from (7), and the *parameter-independent* quantities $A_{0,N} \in \mathbb{R}^{N \times N}$, $A_{1,N}^m \in \mathbb{R}^{N \times N}$, and $F_N^m \in \mathbb{R}^N$ are given by

$$\begin{aligned}
A_{0,N\,i,j} &= a_0(\zeta_i,\zeta_j), & 1 \le i,j \le N, \\
A_{1,N\,i,j}^m &= a_1(\zeta_i,\zeta_j,q_m), & 1 \le i,j \le N, \ 1 \le m \le M, \\
F_{N\,j}^m &= f(\zeta_j;q_m), & 1 \le j \le N, \ 1 \le m \le M,
\end{aligned}$$
(29)

respectively. Finally, $L_N \in \mathbb{R}^N$ is the output vector with entries $L_{Ni} = \ell(\zeta_i)$, $1 \leq i \leq N$. We note that these quantities must be computed in a stable fashion which is consistent with the finite element quadrature points (see [13], p. 132).

The offline-online decomposition is now clear. In the offline stage — performed only once — we first construct the nested approximation spaces W_M^g and sets of interpolation points T_M^g , $1 \leq M \leq M_{\max}$; we then solve for the ζ_n , $1 \leq n \leq N_{\max}$ and compute and store the μ -independent quantities in (26), (29), and L_N . The computational cost — without taking into account the construction of W_M^g and T_M^g — is therefore $O(KN_{\max})$ solutions of the underlying \mathcal{N} -dimensional "truth" finite element approximation and $O(M_{\max}N_{\max}^2)$ \mathcal{N} -inner products; the storage requirements are also $O(M_{\max}N_{\max}^2)$. In the online stage — performed many times, for each new parameter value μ — we first compute $\varphi_M(\mu)$ from (7) at

cost $O(M^2)$ by multiplying the pre-computed inverse of B^M with the vector $g(x_i;\mu)$, $1 \leq i \leq M$; we then assemble the reduced basis matrix (27) and vector (28); this requires $O(MN^2)$ operations. We then solve (24) for $\underline{y}_{N,M}^k(\mu)$; since the reduced basis matrices are in general full, the operation count (based on LU factorization and our LTI assumption) is $O(N^3 + KN^2)$. Finally, given $\underline{y}_{N,M}^k(\mu)$ we evaluate the output estimate $s_{N,M}^k(\mu)$, $1 \leq k \leq K$, from (25) at a cost of O(KN).

Hence, as required in the many-query or real-time contexts, the online complexity is *independent* of \mathcal{N} , the dimension of the underlying "truth" finite element approximation space. Since $N, M \ll \mathcal{N}$ we expect significant computational savings in the online stage relative to classical discretization and solution approaches.

3.3 A posteriori error estimation

We will now develop a posteriori error estimators which will help us to (i) assess the error introduced by our reduced-basis approximation (relative to the "truth" finite element approximation); and (ii) devise an efficient procedure for generating the reduced-basis space W_N^y . We recall that a posteriori error estimates have been developed for reduced basis approximations of linear affine parabolic problems using a finite element truth discretization in [15]. Subsequently, extensions to finite volume disretizations including bounds for the error in the $L^2(\Omega)$ -norm have also been considered [16].

3.3.1 Preliminaries

To begin, we assume that we are given a positive lower bound for the coercivity constant $\alpha_a(\mu)$: $\hat{\alpha}_a(\mu) : \mathcal{D} \to \mathbb{R}_+$ satisfies

$$\alpha_a(\mu) \ge \hat{\alpha}_a(\mu) \ge \hat{\alpha}_a^0 > 0, \quad \forall \, \mu \in \mathcal{D}.$$
(30)

This bound can be calculated using the Successive Constraint Method (SCM) [17]; however, simpler recipes often suffice [32, 43].

We next introduce the dual norm of the residual

$$\varepsilon_{N,M}^{k}(\mu) \equiv \sup_{v \in X} \frac{R^{\kappa}(v;\mu)}{\|v\|_{X}}, \quad \forall k \in \mathbb{K},$$
(31)

where

$$R^{k}(v;\mu) \equiv f(v;g_{M}(x;\mu)) \ u(t^{k}) - a_{0}(y_{N,M}^{k}(\mu),v) - a_{1}(y_{N,M}^{k}(\mu),v,g_{M}(x;\mu)) - \frac{1}{\Delta t}m(y_{N,M}^{k}(\mu) - y_{N,M}^{k-1}(\mu),v), \quad \forall v \in X, \ \forall k \in \mathbb{K}.$$
(32)

We also introduce the dual norm

$$\Phi_M^{\operatorname{na}k}(\mu) \equiv \sup_{v \in X} \frac{f(v; q_{M+1}) \ u(t^k) - a_1(y_{N,M}^k(\mu), v, q_{M+1})}{\|v\|_X}, \quad \forall \ k \in \mathbb{K}, \quad (33)$$

which reflects the contribution of the nonaffine terms. Finally, we specify the inner products $(v, w)_X \equiv a_0(v, w), \forall v, w \in X$ and $(v, w)_Y \equiv m(v, w),$ $\forall v, w \in X$, recall the definition $\hat{\varepsilon}_M(\mu) = |g(t_{M+1}; \mu) - g_M(t_{M+1}; \mu)|$ from Section 2.2, and define the "spatio-temporal" energy norm, $1 \leq k \leq K$,

$$|||v^{k}(\mu)||| \equiv \left(m(v^{k}(\mu), v^{k}(\mu)) + \sum_{k'=1}^{k} \left(a_{0}(v^{k'}(\mu), v^{k'}(\mu)) + a_{1}(v^{k'}(\mu), v^{k'}(\mu); g(x; \mu))\right) \Delta t\right)^{\frac{1}{2}}.$$
 (34)

3.3.2 Error bound formulation

We obtain the following result for the error bound.

Proposition 2. Suppose that $g(x;\mu) \in W^g_{M+1}$. The error, $e^k(\mu) \equiv y^k(\mu) - y^k_{N,M}(\mu)$, is then bounded by

$$|||e^{k}(\mu)||| \leq \Delta_{N,M}^{y\,k}(\mu), \quad \forall \, \mu \in \mathcal{D}, \; \forall \, k \in \mathbb{K},$$
(35)

where the error bound $\Delta_{N,M}^{y\,k}(\mu) \equiv \Delta_{N,M}^{y}(t^{k};\mu)$ is defined as

$$\Delta_{N,M}^{y\,k}(\mu) \equiv \left(\frac{2\Delta t}{\hat{\alpha}_a(\mu)} \sum_{k'=1}^k \varepsilon_{N,M}^{k'}(\mu)^2 + \frac{2\Delta t}{\hat{\alpha}_a(\mu)} \hat{\varepsilon}_M^2(\mu) \sum_{k'=1}^k \Phi_M^{\mathrm{na}\,k'}(\mu)^2\right)^{\frac{1}{2}}.$$
(36)

Proof. We immediately derive from (3) and (32) that $e^k(\mu)$, $1 \le k \le K$, satisfies

$$m(e^{k}(\mu), v) + \Delta t \left(a_{0}(e^{k}(\mu), v) + a_{1}(e^{k}(\mu), v, g(x; \mu)) \right) = m(e^{k-1}(\mu), v) + \Delta t R(v; \mu, t^{k}) + \Delta t \left(f(v; g(x; \mu) - g_{M}(x; \mu)) u(t^{k}) - a_{1}(y_{N,M}^{k}(\mu), v, g(x; \mu) - g_{M}(x; \mu)) \right), \forall v \in X, \quad (37)$$

where $e(t^0; \mu) = 0$ since $y(t^0; \mu) = y_{N,M}(t^0; \mu) = 0$ by assumption. We now choose $v = e^k(\mu)$, invoke the Cauchy-Schwarz inequality for the cross term

 $m(e^{k-1}(\mu), e^k(\mu))$, and apply (31) to obtain, $1 \le k \le K$,

$$m(e^{k}(\mu), e^{k}(\mu)) + \Delta t \left(a_{0}(e^{k}(\mu), e^{k}(\mu)) + a_{1}(e^{k}(\mu), e^{k}(\mu), g(x;\mu)) \right) \leq m^{\frac{1}{2}}(e^{k}(\mu), e^{k}(\mu)) \ m^{\frac{1}{2}}(e^{k-1}(\mu), e^{k-1}(\mu)) + \Delta t \ \varepsilon_{N,M}^{k}(\mu) \ \|e^{k}(\mu)\|_{X} \\ + \Delta t \left(f(e^{k}(\mu); g(x;\mu) - g_{M}(x;\mu)) \ u(t^{k}) - a_{1}(y_{N,M}^{k}(\mu), e^{k}(\mu), g(x;\mu) - g_{M}(x;\mu)) \right).$$
(38)

From our assumption, $g(x;\mu)\in W^g_{M+1},$ Proposition 1, and (33) it directly follows that

$$f(e^{k}(\mu); g(x; \mu) - g_{M}(x; \mu)) \ u(t^{k}) - a_{1}(y_{N,M}^{k}(\mu), e^{k}(\mu), g(x; \mu) - g_{M}(x; \mu))$$

$$\leq \hat{\varepsilon}_{M}(\mu) \ \sup_{v \in X} \frac{f(v; q_{M+1}) \ u(t^{k}) - a_{1}(y_{N,M}^{k}(\mu), v, q_{M+1})}{\|v\|_{X}} \ \|e^{k}(\mu)\|_{X}$$

$$\leq \hat{\varepsilon}_{M}(\mu) \ \Phi_{M}^{\mathrm{na}\,k}(\mu) \ \|e^{k}(\mu)\|_{X}.$$
(39)

We now recall Young's inequality (for $c \in \mathbb{R}$, $d \in \mathbb{R}$, $\rho \in \mathbb{R}_+$)

$$2 |c| |d| \le \frac{1}{\rho^2} c^2 + \rho^2 d^2, \tag{40}$$

which we apply thrice: first, choosing $c = m^{\frac{1}{2}}(e^k(\mu), e^k(\mu)), d = m^{\frac{1}{2}}(e^{k-1}(\mu), e^{k-1}(\mu)),$ and $\rho = 1$, we obtain

$$2 m^{\frac{1}{2}}(e^{k}(\mu), e^{k}(\mu)) m^{\frac{1}{2}}(e^{k-1}(\mu), e^{k-1}(\mu)) \\ \leq m(e^{k-1}(\mu), e^{k-1}(\mu)) + m(e^{k}(\mu), e^{k}(\mu)); \quad (41)$$

second, choosing $c = \varepsilon_{N,M}^k(\mu)$, $d = ||e^k(\mu)||_X$, and $\rho = (\hat{\alpha}_a(\mu)/2)^{\frac{1}{2}}$ we have

$$2 \varepsilon_N^k(\mu) \|e^k(\mu)\|_X \le \frac{2}{\hat{\alpha}_a(\mu)} \varepsilon_{N,M}^k(\mu)^2 + \frac{\hat{\alpha}_a(\mu)}{2} \|e^k(\mu)\|_X^2;$$
(42)

and third, choosing $c = \hat{\varepsilon}_M(\mu) \Phi_M^{\mathrm{na\,k}}(\mu), d = ||e^k(\mu)||_X$, and $\rho = (\hat{\alpha}_a(\mu)/2)^{\frac{1}{2}}$ gives

$$2 \ \hat{\varepsilon}_{M}(\mu) \ \Phi_{M}^{\mathrm{na}\,k}(\mu) \ \|e^{k}(\mu)\|_{X} \leq \frac{2}{\hat{\alpha}_{a}(\mu)} \ \hat{\varepsilon}_{M}^{2}(\mu) \ \Phi_{M}^{\mathrm{na}\,k}(\mu)^{2} + \frac{\hat{\alpha}_{a}(\mu)}{2} \ \|e^{k}(\mu)\|_{X}^{2};$$
(43)

Combining (38) and (39), and invoking (14) and (41)-(43), we obtain, $1 \le k \le K$,

$$m(e^{k}(\mu), e^{k}(\mu)) - m(e^{k-1}(\mu), e^{k-1}(\mu)) + \Delta t \left(a_{0}(e^{k}(\mu), e^{k}(\mu)) + a_{1}(e^{k}(\mu), e^{k}(\mu), g(x; \mu)) \right) \leq \frac{2\Delta t}{\hat{\alpha}_{a}(\mu)} \left(\varepsilon_{N,M}^{k}(\mu)^{2} + \hat{\varepsilon}_{M}^{2}(\mu) \Phi_{M}^{\mathrm{na\,k}}(\mu)^{2} \right),$$
(44)

where we used the fact that $\hat{\alpha}_a(\mu) \leq \alpha_a(\mu), \forall \mu \in \mathcal{D}$. We now perform the sum from k' = 1 to k and recall that $e(\mu, t^0) = 0$, leading to

$$m(e^{k}(\mu), e^{k}(\mu)) + \sum_{k'=1}^{k} \Delta t \left(a_{0}(e^{k'}(\mu), e^{k'}(\mu)) + a_{1}(e^{k'}(\mu), e^{k'}(\mu), g(x; \mu)) \right)$$

$$\leq \frac{2\Delta t}{\hat{\alpha}_{a}(\mu)} \sum_{k'=1}^{k} \left(\varepsilon_{N,M}^{k'}(\mu)^{2} + \hat{\varepsilon}_{M}^{2}(\mu) \Phi_{M}^{\mathrm{na}k'}(\mu)^{2} \right), \quad \forall k \in \mathbb{K}, \quad (45)$$

which is the result stated in Proposition 2.

We note from (36) that our error bound comprises the affine as well as the nonaffine error contributions. We may thus choose N and M such that both contributions balance, i.e., neither N nor M should be chosen unnecessarily high. We also recall that our (crucial) assumption $g(x;\mu) \in$ W_{M+1}^g cannot be confirmed in actual practice — in fact, we generally have $g(x;\mu) \notin W_{M+1}^g$ and hence our error bound (36) is *not* completely rigorous, since $\hat{\varepsilon}_M(\mu) \leq \epsilon_M(\mu)$. We comment on both of these issues again in detail

We can now define the (simple) output bound in

in Section 3.5 when discussing numerical results.

Proposition 3. Suppose that $g(x; \mu) \in W_{M+1}^g$. The error in the output of interest is then bounded by

$$|s^{k}(\mu) - s^{k}_{N,M}(\mu)| \le \Delta^{sk}_{N,M}(\mu), \quad \forall k \in \mathbb{K}, \ \forall \mu \in \mathcal{D},$$
(46)

where the output bound $\Delta^{s\,k}_{N,M}(\mu)$ is defined as

$$\Delta_{N,M}^{s\,k}(\mu) \equiv \sup_{v \in X} \frac{\ell(v)}{\|v\|_Y} \Delta_{N,M}^{y\,k}(\mu) \,. \tag{47}$$

Proof. From (2) and (21) we obtain

$$\begin{aligned} s^{k}(\mu) - s^{k}_{N,M}(\mu)| &= |\ell(y^{k}(\mu)) - \ell(y^{k}_{N,M}(\mu))| \\ &= |\ell(e^{k}(\mu))| \le \sup_{v \in X} \frac{\ell(v)}{\|v\|_{Y}} \|e^{k}(\mu)\|_{Y}. \end{aligned}$$

The result immediately follows since $||e^k(\mu)||_Y \leq \Delta_{N,M}^{yk}(\mu), 1 \leq k \leq K$. \Box

Since our focus here is on developing *a posteriori* error bounds for nonaffine and (subsequently) nonlinear problems, we do not consider primaldual techniques. However, incorporating these techniques analogous to [15] is also possible.

3.3.3 Computational procedure

We now turn to the development of offline-online computational procedures for the calculation of $\Delta_{N,M}^{yk}(\mu)$ and $\Delta_{N,M}^{sk}(\mu)$. The necessary computations for the offline and online stage are detailed in A. Here, we only summarize the computational costs involved.

In the offline stage we first compute the quantities \mathcal{F} , $\mathcal{A}^{0,1}$, and \mathcal{M} from (88) and (91) and then evaluate the Λ from (90) and (92); this requires (to leading order) $O(M_{\max}N_{\max})$ expensive "truth" finite element solutions, and $O(M_{\max}^2 N_{\max}^2)$ \mathcal{N} -inner products. In the online stage — given a new parameter value μ and associated reduced basis solution $\underline{y}_{N,M}^k(\mu)$, $1 \leq k \leq K$ — the computational cost to evaluate $\Delta_{N,M}^{y\,k}(\mu)$ and $\Delta_{N,M}^{s\,k}(\mu)$, $1 \leq k \leq K$, is $O(KM^2N^2)$. Thus, all online calculations needed are *independent* of \mathcal{N} .

3.4 Sampling Procedure

The sampling procedure is a two stage process. We first construct the sample set S_M^g , associated space W_M^g , and set of interpolation points T_M^g for the nonaffine function as described in Section 2. We then invoke a POD/Greedy sampling procedure — a combination of the Proper Orthogonal Decomposition (POD) in time with a Greedy selection procedure in parameter space [16, 20] — to generate W_N^g .

Let $\text{POD}_X(\{y^k(\mu), 1 \leq k \leq K\}, R)$ return the *R* largest POD modes, $\{\chi_i, 1 \leq i \leq R\}$, with respect to the $(\cdot, \cdot)_X$ inner product. We recall that the POD modes, χ_i , are mutually *X*-orthogonal such that $\mathcal{P}_R = \text{span}\{\chi_i, 1 \leq i \leq R\}$ satisfies the optimality property

$$\mathcal{P}_{R} = \arg \inf_{Y_{R} \subset \operatorname{span}\{y^{k}(\mu), 1 \le k \le K\}} \left(\frac{1}{K} \sum_{k=1}^{K} \inf_{w \in Y_{R}} \|y^{k}(\mu) - w\|_{X}^{2}\right), \quad (48)$$

where Y_R denotes a linear space of dimension R. Here, we are only interested in the largest POD mode which we obtain using the method of snapshots [39]. To this end, we solve the eigenvalue problem $C\psi^i = \lambda^i \psi^i$ for $(\psi^1 \in \mathbb{R}^K, \lambda^1 \in \mathbb{R})$ associated with the largest eigenvalue of C, where $C_{ij} = (y^i(\mu), y^j(\mu))_X$, $1 \le i, j \le K$; we then obtain the first POD mode from $\chi_1 = \sum_{k=1}^K \psi_k^1 y^k(\mu)$.

The POD/Greedy procedure proceeds as follows: we first choose a $\mu^* \in \mathcal{D}$ and set $S_0^y = \{0\}, W_0^y = \{0\}, N = 0$. Then, for $1 \leq N \leq N_{\max}$, we first compute the projection error $e_{N,\text{proj}}^k(\mu) = y^k(\mu^*) - \text{proj}_{X,W_{N-1}}(y^k(\mu^*)), 1 \leq k \leq K$, where $\text{proj}_{X,W_N}(w)$ denotes the X-orthogonal projection of $w \in X$ onto W_N , and we expand the parameter sample $S_N^y \leftarrow S_{N-1}^y \cup \{\mu^*\}$ and the reduced basis space $W_N^y \leftarrow W_{N-1}^y \cup \text{POD}_X(\{e_{N,\text{proj}}^k(\mu^*), 1 \leq k \leq K\}, 1)$, and set $N \leftarrow N + 1$. Finally, we choose the next parameter value from $\mu^* \leftarrow \arg \max_{\mu \in \Xi_{\text{train}}} \Delta_{N,M_{\max}}^{yK}(\mu)/|||y_N^K(\mu)|||$, i.e., we perform a greedy search over Ξ_{train} for the largest relative *a posteriori* error bound at the final time. Here, $\Xi_{\text{train}} \subset \mathcal{D}$ is a finite but suitably large train sample. In general, we may also specify a desired error tolerance, $\epsilon_{\text{tol,min}}$, and stop the procedure as soon as $\max_{\mu \in \Xi_{\text{train}}} \Delta_{N,M_{\max}}^{yK}(\mu)/|||y_N^K(\mu)||| \leq \epsilon_{\text{tol,min}}$ is satisfied; N_{\max} is then indirectly determined through the stopping criterion.

We note that during the POD/Greedy sampling procedure we shall use the "best" possible approximation $g_M(x;\mu)$ of $g(x;\mu)$ so as to minimize the error induced by the empirical interpolation procedure, i.e., we set $M = M_{\text{max}}$. In cases where the control input $u(t^k)$ is unknown, we appeal to the LTI property and generate the reduced basis space based on an impulse input [15]. Extensions of the sampling procedure to treat non-zero initial conditions and multiple inputs may also be considered [13].

3.5 Numerical Results

We now present numerical results for our model problem of Section 3.1.2. We choose for $\Xi_{\text{train}} \subset \mathcal{D}$ a deterministic grid of 40×40 parameter points over \mathcal{D} and we take $\mu_1^g = (-0.01, -0.01)$. Next, we pursue the empirical interpolation procedure described in Section 2 to construct S_M^g , W_M^g , T_M^g , and B^M , $1 \leq M \leq M_{\text{max}}$, for $M_{\text{max}} = 57$.

We first present the results for the empirical interpolation of $G(x; \mu)$ from (18). To this end, we introduce a parameter test sample Ξ_{Test} of size $Q_{\text{Test}} =$ 225, and define the maximum error $\varepsilon_{M,\max} = \max_{\mu \in \Xi_{\text{Test}}} \varepsilon_M(\mu)$, the average effectivity $\bar{\eta}_M = Q_{\text{Test}}^{-1} \sum_{\mu \in \Xi_{\text{Test}}} \eta_M(\mu)$, where $\eta_M(\mu)$ is the effectivity defined in (9), and \varkappa_M is the condition number of B^M . We present in Table 1 $\varepsilon_{M,\max}$, Λ_M , $\bar{\eta}_M$, and \varkappa_M as a function of M. We observe that $\varepsilon_{M,\max}$ converges rapidly with M; that the Lebesgue constant grows very slowly; that the error estimator effectivity is less than but reasonably close to unity; and that B^M is quite well-conditioned for our choice of basis.

M	$\varepsilon_{M,\max}$	Λ_M	$\bar{\eta}_M$	\varkappa_M
8	$2.05\mathrm{E}\!-\!01$	1.98	0.17	3.73
16	$8.54\mathrm{E}\!-\!03$	2.26	0.85	6.01
24	$6.53\mathrm{E}\!-\!04$	3.95	0.50	8.66
32	$1.29\mathrm{E}\!-\!04$	5.21	0.73	12.6
40	$1.37\mathrm{E}{-}05$	5.18	0.43	16.6
48	$4.76\mathrm{E}\!-\!06$	10.2	0.19	20.0

Table 1: Numerical results for empirical interpolation of $G(x;\mu)$: $\varepsilon_{M,\max}$, Λ_M , $\bar{\eta}_M$, and \varkappa_M as a function of M.

We next turn to the reduced basis approximation and construct the reduced basis space W_N^y according to the POD/Greedy sampling procedure in Section 3.4; we sample on Ξ_{train} with $M = M_{\text{max}}$ and obtain $N_{\text{max}} = 45$ for $\epsilon_{\text{tol,min}} = 1 \text{ E} - 6$.

In Figure 2 we plot, as a function of N and M, the maximum relative error in the energy norm $\epsilon_{N,M,\max,\mathrm{rel}}^y = \max_{\mu \in \Xi_{\mathrm{Test}}} |||e^K(\mu)|||/|||y^K(\mu_y)|||$, where $\mu_y \equiv \arg\max_{\mu \in \Xi_{\mathrm{Test}}} |||y^K(\mu)|||$. We observe that the reduced-basis approximation converges very rapidly. We also note the "plateau" in the curves for M fixed and the "drops" in the $N \to \infty$ asymptotes as M increases: for fixed M the error due to the coefficient function approximation, $g_M(x;\mu) - g(x;\mu)$, will ultimately dominate for large N; increasing M renders the coefficient function approximation more accurate, which in turn leads to a drop in the error. We further note that the separation points, or "knees," of the N-M-convergence curves reflect a balanced contribution of both error terms; neither N nor M limit the convergence of the reduced basis approximation.

In Table 2 we present, as a function of N and M, $\epsilon_{N,M,\max,\text{rel}}^y$, the maximum relative error bound $\Delta_{N,M,\max,\text{rel}}^y$, and the average effectivity $\bar{\eta}_{N,M}^y$; here, $\Delta_{N,M,\max,\text{rel}}^y$ is the maximum over Ξ_{Test} of $\Delta_{N,M}^{yk}(\mu)/|||y^K(\mu_y)|||$ and $\bar{\eta}_{N,M}^y$ is the average over $\Xi_{\text{Test}} \times \mathbb{I}$ of $\Delta_{N,M}^{yk}(\mu)/|||y^k(\mu) - y_{N,M}^k(\mu)|||$. Note that the tabulated (N, M) values correspond roughly to the "knees" of the *N*-*M*-convergence curves. We observe very rapid convergence of the reduced basis approximation and error bound.

The effectivity serves as a measure of rigour and sharpness of the error bound: we would like $\bar{\eta}_{N,M}^y \ge 1$, i.e., $\Delta_{N,M}^{yk}(\mu)$ be a true upper bound for the error in the energy-norm; and ideally we have $\bar{\eta}_{N,M}^y \approx 1$ so as to obtain

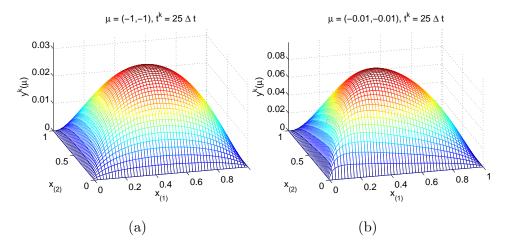


Figure 1: Solution $y^k(\mu)$ at $t^k = 25\Delta t$ for (a) $\mu = (-1, -1)$ and (b) $\mu = (-0.01, -0.01)$.

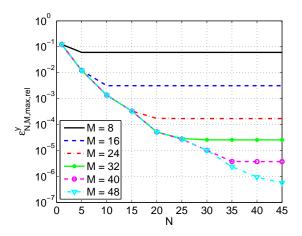


Figure 2: Convergence of the reduced basis approximation: $\epsilon^y_{N,M,\max,\text{rel}}$.

a sharp bound for the error. We recall, however, that in actual practice we cannot confirm the assumption $g(x;\mu) \in W^g_{M+1}$ from Proposition 2 and thus $\bar{\eta}^y_{N,M} \geq 1$ may not hold. Specifically, if we choose (N,M) such that the function interpolation limits the convergence we do obtain effectivities less than 1, e.g., for (N,M) = (25,24) (instead of (25,32) in Table 2) we obtain $\bar{\eta}^y_{N,M} = 0.83$. A judicious choice for N and M is thus important for rigour and safety.

We next turn to the output estimate and present, in Table 2, the maximum relative output error $\epsilon_{N,M,\max,\mathrm{rel}}^s$, the maximum relative output bound $\Delta_{N,M,\max,\mathrm{rel}}^s$, and the average output effectivity $\bar{\eta}^s$; here, $\epsilon_{N,M,\max,\mathrm{rel}}^s$ is the maximum over Ξ_{Test} of $|s(\mu, t_s^k(\mu)) - s_{N,M}(\mu, t_s^k(\mu))| / |s(\mu, t_s^k(\mu))|$, $\Delta_{N,M,\max,\mathrm{rel}}^s$ is the maximum over Ξ_{Test} of $\Delta_{N,M}^s(\mu, t_s^k(\mu)) / |s(\mu, t_s^k(\mu))|$, and $\bar{\eta}^s$ is the average over Ξ_{Test} of $\Delta_{N,M}^s(\mu, t_\eta(\mu)) / |s(\mu, t_s(\mu))| - s_{N,M}(\mu, t_\eta(\mu))|$, where $t_s^k(\mu) \equiv \arg \max_{t^k \in \mathbb{I}} |s(\mu, t^k)|$ and $t_\eta(\mu) \equiv \arg \max_{t^k \in \mathbb{I}} |s(\mu, t^k)|$. Again, we observe very rapid convergence of the reduced basis output approximation and output bound — for only N = 15 and M = 24 the output error bound is already less than 0.3%. The output effectivities are still acceptable for smaller values of (N, M), but deteriorate for larger values.

In Table 3 we present, as a function of N and M, the online computational times to calculate $s_{N,M}^k(\mu)$ and $\Delta_{N,M}^{s\,k}(\mu)$ for $1 \leq k \leq K$. The values are normalized with respect to the computational time for the direct calculation of the truth approximation output $s^k(\mu) = \ell(y^k(\mu)), 1 \leq k \leq K$. The computational savings for an accuracy of less than 0.3 percent (N = 15, M = 24) in the output bound is approximately a factor of 30. We note that the time to calculate $\Delta_{N,M}^{s\,k}(\mu)$ exceeds that of calculating $s_N^k(\mu)$ considerably — this is due to the higher computational cost, $O(KM^2N^2)$, to evaluate $\Delta_{N,M}^{y\,k}(\mu)$. Thus, although the previous observations suggests to choose M large so that the error contribution due to the nonaffine function approximation is small, we should choose M as small as possible to retain the computational efficiency of our method. We emphasize that the reduced basis entry does *not* include the extensive offline computations — and is thus only meaningful in the real-time or many-query contexts.

4 Nonlinear Parabolic Equations

In this section we extend the previous results to nonaffine *nonlinear* parabolic problems. We first introduce the abstract statement and reduced basis approximation, we then develop the *a posteriori* error bounds and subsequently introduce a new construction to define the generating functions for the non-

Table 2: Convergence rates and effectivities as a function of N and M for the nonaffine problem.

\overline{N}	M	$\epsilon^y_{N,M, ext{max,rel}}$	$\Delta^y_{N,M, ext{max,rel}}$	$\bar{\eta}_{N,M}^y$	$\epsilon^s_{N,M,\mathrm{max,rel}}$	$\Delta^s_{N,M,\mathrm{max,rel}}$	$\bar{\eta}_{N,M}^s$
$\overline{5}$	16	$1.22\mathrm{E}\!-\!02$	$1.74\mathrm{E}\!-\!02$	1.42	$3.30\mathrm{E}\!-\!03$	$1.01\mathrm{E}\!-\!01$	29.1
15	24	$3.32\mathrm{E}\!-\!04$	$4.75\mathrm{E}{-}04$	1.09	$1.57\mathrm{E}{-}04$	$2.77\mathrm{E}\!-\!03$	27.5
25	32	$2.91\mathrm{E}-05$	$4.30\mathrm{E}\!-\!05$	1.44	$1.88\mathrm{E}\!-\!05$	$2.50\mathrm{E}\!-\!04$	85.4
35	40	$3.78\mathrm{E}\!-\!06$	$3.50\mathrm{E}\!-\!06$	1.11	$3.22\mathrm{E}\!-\!06$	$2.04\mathrm{E}\!-\!05$	137
45	48	$5.66\mathrm{E}\!-\!07$	$8.17\mathrm{E}{-}07$	1.39	$8.14\mathrm{E}{-}08$	$4.76\mathrm{E}\!-\!06$	553

Table 3: Online computational times (normalized with respect to the time to solve for $s^k(\mu)$, $1 \le k \le K$) for the nonaffine problem.

\overline{N}	M	$s_{N,M}^k(\mu), \ \forall k \in \mathbb{K}$	$\Delta_{N,M}^{sk}(\mu), \; \forall k \in \mathbb{K}$	$s^k(\mu), \ \forall k \in \mathbb{K}$
$\overline{5}$	16	$2.70\mathrm{E}\!-\!03$	$1.84\mathrm{E}{-02}$	1
15	24	$3.18\mathrm{E}\!-\!03$	$3.01\mathrm{E}\!-\!02$	1
25	32	$3.96\mathrm{E}\!-\!03$	$4.57\mathrm{E}{-}02$	1
35	40	$4.71\mathrm{E}{-}03$	$7.16\mathrm{E}\!-\!02$	1
45	48	$5.52\mathrm{E}{-}03$	$1.02\mathrm{E}\!-\!01$	1

linear term. Finally, we discuss numerical results obtained for a model problem.

4.1 Problem statement

4.1.1 Abstract formulation

We consider a time-discrete framework associated to the time interval $I \equiv [0, t_f]$ as introduced in Section 1; \overline{I} is divided into K subintervals of equal length $\Delta t = \frac{t_f}{K}$, that t^k is defined by $t^k \equiv k\Delta t$, $0 \leq k \leq K \equiv \frac{t_f}{\Delta t}$; furthermore, $\mathbb{I} \equiv \{t^0, \ldots, t^k\}$ and $\mathbb{K} \equiv \{1, \ldots, K\}$. The "truth" approximation is then: given a parameter $\mu \in \mathcal{D}$, we evaluate the output of interest

$$s^{k}(\mu) = \ell(y^{k}(\mu)), \quad \forall k \in \mathbb{K}$$

$$\tag{49}$$

where the field variable $y^k(\mu) \in X$, $1 \leq k \leq K$, satisfies the weak form of the nonlinear parabolic partial differential equation

$$m(y^{k}(\mu), v) + \Delta t \ a^{L}(y^{k}(\mu), v) + \Delta t \ \int_{\Omega} g(y^{k}(\mu); x; \mu) v$$

= $m(y^{k-1}(\mu), v) + \Delta t \ f(v) \ u(t^{k}), \quad \forall v \in X,$ (50)

with initial condition (say) $y(\mu, t^0) = 0$. Here, μ and \mathcal{D} are the input and input domain; $u(t^k)$ denotes the control input; and $g(w; x; \mu) : \mathbb{R} \times \Omega \times \mathcal{D} \to \mathbb{R}$ is a nonlinear nonaffine function continuous in its arguments, increasing in its first argument, and satisfies, for all $y \in \mathbb{R}$, $yg(y; x; \mu) \ge 0$ for any $x \in \Omega$ and $\mu \in \mathcal{D}$. We note that the field variable, $y^k(\mu)$, is of course also a function of the spatial coordinate x. In the sequel we will use the notation $y(x, t^k; \mu)$ to signify this dependence whenever it is crucial.

We shall make the following assumptions. We assume that $a^{L}(\cdot, \cdot)$ and $m(\cdot, \cdot)$ are continuous

$$a^{L}(w,v) \leq \gamma_{a}^{0} ||w||_{X} ||v||_{X}, \quad \forall w,v \in X,$$
 (51)

$$m(w,v) \leq \gamma_m^0 \|w\|_Y \|v\|_Y, \quad \forall w,v \in X;$$

$$(52)$$

coercive,

$$0 < \alpha_a^0 \equiv \inf_{w \in X} \frac{a^L(w, w)}{\|w\|_X^2}, \qquad (53)$$

$$0 < \alpha_m^0 \equiv \inf_{v \in X} \frac{m(v, v)}{\|v\|_Y^2};$$
 (54)

and symmetric, $a^{L}(v, w) = a^{L}(w, v), \forall w, v \in X$, and m(v, w) = m(w, v), $\forall w, v \in X$. (We (plausibly) suppose that $\gamma_{a}^{0}, \gamma_{m}^{0}, \alpha_{a}^{0}, \alpha_{m}^{0}$ may be chosen independent of \mathcal{N} .) We also require that the linear forms $f(\cdot) : X \to \mathbb{R}$ and $\ell(\cdot) : X \to \mathbb{R}$ be bounded with respect to $\|\cdot\|_{Y}$. The problem is thus well-posed [22].

Since the focus of this section is the treatment of the nonlinearity $g(w; x; \mu)$ we assume that the bilinear and linear forms m, a^L and b, ℓ are parameter independent; a parameter dependence of either form is readily admitted. Note also that our results presented here directly carry over to the case where g is also an explicit function of (discrete) time t^k .

4.1.2 Model problem

We turn to a numerical example. We consider the following nonlinear diffusion problem defined on the unit square, $\Omega =]0,1[^2 \in \mathbb{R}^2$: Given $\mu =$ $(\mu_1, \mu_2) \in \mathcal{D}^{\mu} \equiv [0.01, 10]^2$, we evaluate $y^k(\mu) \in X$ from (50), where $X \subset X^e \equiv H_0^1(\Omega)$ is a linear finite element truth approximation subspace of dimension $\mathcal{N} = 2601$,

$$m(w,v) \equiv \int_{\Omega} w \, v, \ a^{L}(w,v) \equiv \int_{\Omega} \nabla w \cdot \nabla v, \ f(v) \equiv 100 \int_{\Omega} v \, \sin(2\pi x_{1}) \, \cos(2\pi x_{2})$$
(55)

and the nonlinearity is given by

$$g(y^{k}(\mu);\mu) = \mu_{1} \frac{e^{\mu_{2} y^{k}(\mu)} - 1}{\mu_{2}}.$$
(56)

The output $s^k(\mu)$ is evaluated from (49) with $\ell(v) = \int_{\Omega} v$. We presume the periodic control input $u(t^k) = \sin(2\pi t^k)$, $t^k \in \mathbb{I}$. We shall consider the time interval $\overline{I} = [0, 2]$ and a timestep $\Delta t = 0.01$; we thus have K = 200.

We note that μ_2 represent the strength of the nonlinearity whereas μ_1 represents the strength of the sink term in (56); as $\mu_2 \to 0$ we have $g(w;\mu) \to \mu_1 w$. The solution thus tends to the solution for the linear problem as μ_2 tends to zero. Two snapshots of the solution $y^k(\mu)$ at time $t^k = 25\Delta t$ are shown for $\mu = (0.01, 0.01)$ and $\mu = (10, 10)$ in Figures 3(a) and (b), respectively. We observe that the solution has two negative peaks and two positive peaks with similar height for $\mu = (0.01, 0.01)$ (which oscillate back and forth in time). As μ_2 increases, the height of the negative peaks remains largely unchanged, while the positive peaks get rectified as shown in Figure 3(b). The exponential nonlinearity has a damping effect on the positive peak always being smaller than the negative peaks.

4.2 Reduced basis approximation

4.2.1 Formulation

We suppose that we are given the nested collateral reduced basis space $W_M^g = \operatorname{span}\{\xi_n, 1 \le n \le M\} = \operatorname{span}\{q_1, \ldots, q_M\}, 1 \le M \le M_{\max}$ and nested set of interpolation points $T_M^g = \{x_1, \ldots, x_M\}, 1 \le M \le M_{\max}$; we will propose a procedure to construct W_M^g and T_M^g in Section 4.4. Then, for given $w^k(\mu) \in X$ and M, we approximate $g(w^k(\mu); x; \mu)$ by $g_M^{w^k}(x; \mu) = \sum_{m=1}^M \varphi_{Mm}^k(\mu)q_m(x)$, where

$$\sum_{j=1}^{M} B_{ij}^{M} \varphi_{Mj}^{k}(\mu) = g(w(x_i, t^k; \mu); x_i; \mu), \quad 1 \le i \le M;$$
(57)

note that $\varphi_M^k(\mu) \equiv \varphi_M(t^k;\mu)$ now also depends on the (discrete) time t^k . We also introduce the nested Lagrangian reduced basis spaces $W_N^y =$ span{ ζ_n , $1 \le n \le N$ }, $1 \le N \le N_{\text{max}}$, where the ζ_n , $1 \le n \le N$, are mutually $(\cdot, \cdot)_X$ -orthogonal basis functions. We construct W_N^y according to the POD/Greedy procedure outlined in Section 3.4 with $M = M_{\text{max}}$.

Our reduced basis approximation $y_{N,M}^k(\mu)$ to $y^k(\mu)$ is then obtained by a standard Galerkin projection: given $\mu \in \mathcal{D}, y_{N,M}^k(\mu) \in W_N^y$ satisfies

$$m(y_{N,M}^{k}(\mu), v) + \Delta t \ a^{L}(y_{N,M}^{k}(\mu), v) + \Delta t \ \int_{\Omega} g_{M}^{y_{N,M}^{k}}(x; \mu) \ v$$

= $m(y_{N,M}^{k-1}(\mu), v) + \Delta t \ f(v) \ u(t^{k}), \quad \forall \ v \in W_{N}^{y}, \ \forall \ k \in \mathbb{K},$ (58)

with initial condition $y_{N,M}(\mu, t^0) = 0$. We evaluate the output approximation from

$$s_{N,M}^k(\mu) = \ell(y_{N,M}^k(\mu)), \quad \forall k \in \mathbb{K}.$$
(59)

We note that the need to incorporate the empirical interpolation method into the reduced basis approximation only exists for high-order polynomial or non-polynomial nonlinearities [14]. If g is a low-order (or at most quadratically) polynomial nonlinearity in $y^k(\mu)$, we can expand the nonlinear terms into their power series and develop an efficient, i.e., online \mathcal{N} -independent, offline-online computational decomposition using the standard Galerkin procedure [40, 41].

4.2.2Computational procedure

In this section we develop the offline-online computational decomposition to recover online \mathcal{N} -independence even in the nonlinear case. We first express $y_{N,M}^k(\mu)$ as

$$y_{N,M}^{k}(\mu) = \sum_{n=1}^{N} y_{N,Mn}^{k}(\mu) \zeta_{n},$$
(60)

and choose as test functions $v = \zeta_j$, $1 \le j \le N$, in (58). It then follows from the affine representation of $g_M^{y_{N,M}^k}$ that $\underline{y}_{N,M}^k(\mu) =$ $[y_{N,M1}^k(\mu) \ y_{N,M2}^k(\mu) \ \dots \ y_{N,MN}^k(\mu)]^T \in \mathbb{R}^N, \ 1 \le k \le K, \ \text{satisfies}$

$$(M_N + \Delta t \ A_N) \ \underline{y}_{N,M}^k(\mu) + \Delta t \ C^{N,M} \ \varphi_M^k(\mu) = M_N \ \underline{y}_{N,M}^{k-1}(\mu) + \Delta t \ B_N \ u(t^k)$$
(61)

with initial condition $y_{N,Mn}(t^0;\mu) = 0, \ 1 \le n \le N$. Here, the coefficients $\varphi_M^k(\mu) = [\varphi_{M1}^k(\mu) \ \varphi_{M2}^k(\mu) \ \dots \ \varphi_{MM}^k(\mu)]^T \in \mathbb{R}^M$ are determined from (57)

with $w^k = y_{N,M}^k$; $M_N \in \mathbb{R}^{N \times N}$, $A_N \in \mathbb{R}^{N \times N}$, and $C^{N,M} \in \mathbb{R}^{N \times M}$, are parameter-independent matrices with entries $M_{N\,i,j} = m(\zeta_i, \zeta_j)$, $1 \le i, j \le N$, $A_{N\,i,j} = a(\zeta_i, \zeta_j)$, $1 \le i, j \le N$, and $C_{i,j}^{N,M} = \int_{\Omega} \zeta_i q_j$, $1 \le i \le N$, $1 \le j \le M$, respectively; and $F_N \in \mathbb{R}^N$ is a parameter independent vector with entries $F_{N\,i} = f(\zeta_i)$, $1 \le i \le N$.

We can now substitute $\varphi^k_{M\,m}(\mu)$ from (57) into (61) to obtain the non-linear algebraic system

$$(M_N + \Delta t \ A_N) \ \underline{y}_{N,M}^k(\mu) + \Delta t \ D^{N,M} \ g(Z^{N,M} \ \underline{y}_{N,M}^k(\mu); \underline{x}_M; \mu)$$
$$= M_N \ \underline{y}_{N,M}^{k-1}(\mu) + \Delta t \ B_N \ u(t^k), \quad \forall \ k \in \mathbb{K},$$
(62)

where $D^{N,M} = C^{N,M}(B^M)^{-1} \in \mathbb{R}^{N \times M}, Z^{N,M} \in \mathbb{R}^{M \times N}$ is a parameterindependent matrix with entries $Z_{i,j}^{N,M} = \zeta_j(x_i), 1 \leq i \leq M, 1 \leq j \leq N$, and $\underline{x}_M = [x_i \dots x_M]^T \in \mathbb{R}^M$ is the set of interpolation points. We now solve for $\underline{y}_{N,M}^k(\mu)$ at each timestep using a Newton iterative scheme: given the solution for the previous timestep, $\underline{y}_{N,M}^{k-1}(\mu)$, and a current iterate $\underline{y}_{N,M}^k(\mu)$, we find an increment $\delta \underline{y}_{N,M}$ such that

$$\begin{pmatrix} M_N + \Delta t \ A_N + \Delta t \overline{E}^N \end{pmatrix} \ \delta \underline{y}_{N,M}$$

= $M_N \ \underline{y}_{N,M}^{k-1}(\mu) + \Delta t \ B_N(\mu) \ u(t^k) - (M_N + \Delta t \ A_N) \ \underline{y}_{N,M}^k(\mu)$
 $- \Delta t \ D^{N,M} \ g(Z^{N,M} \ \underline{y}_{N,M}^k(\mu); \underline{x}_M; \mu),$ (63)

where $\bar{E}^N \in \mathbb{R}^{N \times N}$ must be calculated at every Newton iteration from

$$\bar{E}_{i,j}^{N} = \sum_{m=1}^{M} D_{i,m}^{N,M} g_1 \left(\sum_{n=1}^{N} \bar{y}_{N,Mn}^{k}(\mu) \zeta_n(x_m); x_m; \mu \right) \zeta_j(x_m), \quad 1 \le i, j \le N,$$
(64)

where g_1 is the partial derivative of g with respect to the first argument. Finally, we evaluate the output estimate from

$$s_{N,M}^{k}(\mu) = L_{N}^{T} \ \underline{y}_{N,M}^{k}(\mu), \quad \forall k \in \mathbb{K},$$
(65)

where $L_N \in \mathbb{R}^N$ is the output vector with entries $L_{Ni} = \ell(\zeta_i), \ 1 \le i \le N$.

The offline-online decomposition is now clear. In the offline stage — performed only *once* — we first construct the nested approximation spaces W_M^g and sets of interpolation points T_M^g , $1 \le M \le M_{\text{max}}$; we then solve for the ζ_n , $1 \le n \le N_{\text{max}}$ and compute and store the μ -independent quantities

 M_N , A_N , B^M , $D^{N,M}$, B_N , and $Z^{N,M}$. In the online stage — performed many times, for each new parameter value μ — we solve (63) for $\underline{y}_{N,M}^k(\mu)$ and evaluate the output estimate $s_{N,M}^k(\mu)$ from (65). The operation count is dominated by the Newton update at each timestep: we first assemble \overline{E}^N from (64) at cost $O(MN^2)$ — note that we perform the sum in the parenthesis of (64) first before performing the outer sum — and then invert the left hand side of (63) at cost $O(N^3)$. The operation count in the online stage is thus $O(MN^2 + N^3)$ per Newton iteration per timestep. We thus recover \mathcal{N} -independence in the online stage.

4.3 A posteriori error estimation

4.3.1 Preliminaries

We now turn to the development of our *a posteriori* error estimator; by construction, the error estimator is rather similar to the nonaffine parabolic case in Section 3. To begin, we recall that the bilinear form a^L is assumed to be parameter independent here; we can thus use the coercivity constant α_a and have no need for the lower bound $\hat{\alpha}_a(\mu)$ required earlier. We next introduce the dual norm of the residual

$$\varepsilon_{N,M}^{k}(\mu) \equiv \sup_{v \in X} \frac{R^{k}(v;\mu)}{\|v\|_{X}}, \quad \forall k \in \mathbb{K},$$
(66)

where

$$R^{k}(v;\mu) \equiv f(v) \ u(t^{k}) - \frac{1}{\Delta t} m(y_{N,M}^{k}(\mu) - y_{N,M}^{k-1}(\mu), v) - a^{L}(y_{N,M}^{k}(\mu), v) - \int_{\Omega} g_{M}^{y_{N,M}^{k}}(x;\mu) \ v, \quad \forall \ v \in X, \ \forall \ k \in \mathbb{K},$$
(67)

is the residual associated to the nonlinear parabolic problem. We also require the dual norm

$$\vartheta_M^q \equiv \sup_{v \in X} \frac{\int_\Omega q_{M+1} v}{\|v\|_X}.$$
(68)

and the error bound $\hat{\varepsilon}^k_M(\mu)$ for the nonlinear function approximation given by

$$\hat{\varepsilon}_{M}^{k}(\mu) \equiv |g(y_{N,M}^{k}(x_{M+1};\mu);x_{M+1};\mu) - g_{M}^{y_{N,M}^{k}}(x_{M+1};\mu)|.$$
(69)

We note that, contrary to the nonaffine case, the error bound $\hat{\varepsilon}_{M}^{k}(\mu)$ is now also a function of (discrete) time. Finally, we define the "spatio-temporal"

energy norm, $1 \le k \le K$,

$$|||v^{k}(\mu)||| \equiv \left(m(v^{k}(\mu), v^{k}(\mu)) + \sum_{k'=1}^{k} a^{L}(v^{k'}(\mu), v^{k'}(\mu)) \Delta t\right)^{\frac{1}{2}}, \quad \forall v \in X.$$
(70)

4.3.2 Error bound formulation

We obtain the following result for the error in the energy norm.

Proposition 4. Suppose that $g(y_{N,M}^k(\mu); x; \mu) \in W_{M+1}^g$, $1 \le k \le K$. The error, $e^k(\mu) \equiv y^k(\mu) - y_{N,M}^k(\mu)$, is then bounded by

$$|||e^{k}(\mu)||| \leq \Delta_{N,M}^{y\,k}(\mu), \quad \forall \, \mu \in \mathcal{D}, \; \forall \, k \in \mathbb{K},$$
(71)

where the error bound $\Delta_{N,M}^{y\,k}(\mu)$ is defined as

$$\Delta_{N,M}^{y\,k}(\mu) \equiv \left(\frac{2\Delta t}{\alpha_a} \sum_{k'=1}^k \varepsilon_{N,M}^{k'}(\mu)^2 + \frac{2\Delta t}{\alpha_a} \vartheta_M^{q-2} \sum_{k'=1}^k \hat{\varepsilon}_M^{k'}(\mu)^2\right)^{\frac{1}{2}}.$$
 (72)

Proof. We immediately derive from (50) and (67) that $e^k(\mu) = y^k(\mu) - y^k_{N,M}(\mu), 1 \le k \le K$, satisfies

$$m(e^{k}(\mu), v) + \Delta t \, a^{L}(e^{k}(\mu), v) + \Delta t \, \int_{\Omega} \left(g(y^{k}(\mu); x; \mu) - g(y^{k}_{N,M}(\mu); x; \mu) \right) v$$

= $m(e^{k-1}(\mu), v) + \Delta t \, R(v; \mu, t^{k}) + \Delta t \, \int_{\Omega} \left(g^{y^{k}_{N,M}}_{M}(x; \mu) - g(y^{k}_{N,M}(\mu); x; \mu) \right) v,$
 $\forall v \in X, \quad (73)$

where $e(t^0; \mu) = 0$ since $y(t^0; \mu) = y_{N,M}(t^0; \mu) = 0$ by assumption. We now choose $v = e^k(\mu)$ in (73), immediately note from the monotonicity of g that

$$\int_{\Omega} \left(g(y^k(\mu); x; \mu) - g(y^k_{N,M}(\mu); x; \mu) \right) \, e^k(\mu) \ge 0; \tag{74}$$

invoke (66) and the Cauchy-Schwarz inequality for the cross term $m(e^{k-1}(\mu), e^k(\mu))$ to obtain, $1 \le k \le K$,

$$m(e^{k}(\mu), e^{k}(\mu)) + \Delta t \ a^{L}(e^{k}(\mu), e^{k}(\mu)) \\\leq m^{\frac{1}{2}}(e^{k-1}(\mu), e^{k-1}(\mu)) \ m^{\frac{1}{2}}(e^{k}(\mu), e^{k}(\mu)) + \Delta t \ \varepsilon_{N,M}^{k}(\mu) \ \|e^{k}(\mu)\|_{X} \\+ \Delta t \ \int_{\Omega} \left(g_{M}^{y_{N,M}^{k}}(x;\mu) - g(y_{N,M}^{k}(\mu);x;\mu)\right) \ e^{k}(\mu).$$
(75)

We will now apply (40) twice: first, choosing $c = m^{\frac{1}{2}}(e^k(\mu), e^k(\mu)), d = m^{\frac{1}{2}}(e^{k-1}(\mu), e^{k-1}(\mu))$, and $\rho = 1$, we obtain

$$2 m^{\frac{1}{2}}(e^{k}(\mu), e^{k}(\mu)) m^{\frac{1}{2}}(e^{k-1}(\mu), e^{k-1}(\mu)) \\ \leq m(e^{k-1}(\mu), e^{k-1}(\mu)) + m(e^{k}(\mu), e^{k}(\mu));$$
(76)

and second, choosing $c = \varepsilon_{N,M}^k(\mu)$, $d = ||e^k(\mu)||_X$, and $\rho = (\alpha_a/2)^{\frac{1}{2}}$ we have

$$2 \varepsilon_{N,M}^{k}(\mu) \|e^{k}(\mu)\|_{X} \leq \frac{2}{\alpha_{a}} \varepsilon_{N,M}^{k}(\mu)^{2} + \frac{\alpha_{a}}{2} \|e^{k}(\mu)\|_{X}^{2}.$$
 (77)

We now note from our assumption $g(y_{N,M}^k(\mu);x;\mu)\in W^g_{M+1}$ and Proposition 1 that

$$g_M^{y_{N,M}^k}(x;\mu) - g(y_{N,M}^k(\mu);x;\mu) = \hat{\varepsilon}_M^k(\mu) \, q_{M+1}(x); \tag{78}$$

it thus follows that

$$2 \int_{\Omega} \left(g_{M}^{y_{N,M}^{k}}(x;\mu) - g(y_{N,M}^{k}(\mu);x;\mu) \right) e^{k}(\mu) \\ \leq 2 \sup_{v \in X} \left\{ \frac{\int_{\Omega} \left(g_{M}^{y_{N,M}^{k}}(x;\mu) - g(y_{N,M}^{k}(\mu);x;\mu) \right) v}{\|v\|_{X}} \right\} \|e^{k}(\mu)\|_{X} \\ \leq 2 \hat{\varepsilon}_{M}^{k}(\mu) \sup_{v \in X} \left\{ \frac{\int_{\Omega} q_{M+1}v}{\|v\|_{X}} \right\} \|e^{k}(\mu)\|_{X} \\ \leq 2 \hat{\varepsilon}_{M}^{k}(\mu) \vartheta_{M}^{q} \|e^{k}(\mu)\|_{X} \\ \leq \frac{2}{\alpha_{a}} \hat{\varepsilon}_{M}^{k}(\mu)^{2} \vartheta_{M}^{q-2} + \frac{\alpha_{a}}{2} \|e^{k}(\mu)\|_{X}^{2},$$
(79)

where we applied (40) with $c = \hat{\varepsilon}_M^k(\mu) \,\vartheta_M^q$, $d = \|e^k(\mu)\|_X$, and $\rho = (\alpha_a/2)^{\frac{1}{2}}$ in the last step. Finally, from (75), (76), (77), (79), invoking (53) and summing from 1 to k we obtain the bound

$$m(e^{k}(\mu), e^{k}(\mu)) + \Delta t \sum_{k'=1}^{k} a(e^{k'}(\mu), e^{k'}(\mu)) \\ \leq \frac{2\Delta t}{\alpha_{a}} \sum_{k'=1}^{k} \left(\varepsilon_{N,M}^{k'}(\mu)^{2} + \vartheta_{M}^{q-2} \hat{\varepsilon}_{M}^{k'}(\mu)^{2} \right)$$
(80)

which is the result stated in Proposition 4.

We can now define the (simple) output bound

Proposition 5. Suppose that $g(y_{N,M}^k(\mu); x; \mu) \in W_{M+1}^g$, $1 \le k \le K$. The error in the output is then bounded by

$$|s^{k}(\mu) - s^{k}_{N,M}(\mu)| \le \Delta^{s\,k}_{N,M}(\mu), \quad \forall \, k \in \mathbb{K}, \ \forall \, \mu \in \mathcal{D},$$
(81)

where the output bound is defined as

$$\Delta_{N,M}^{sk}(\mu) \equiv \sup_{v \in X} \frac{\ell(v)}{\|v\|_Y} \Delta_{N,M}^{yk}(\mu), \quad \forall k \in \mathbb{K}, \ \forall \mu \in \mathcal{D}.$$
(82)

Proof. The result directly follows from (49), (59), and the fact that the error satisfies $||e^k(\mu)\rangle||_Y \leq \Delta_{N,M}^{yk}(\mu), 1 \leq k \leq K$, for all $\mu \in \mathcal{D}$.

We note from (72) that our error bound comprises two terms: the contribution from the linear (affine) terms and from the nonlinear (nonaffine) function approximation. Similar to the linear nonaffine case, we may thus choose N and M such that both contributions balance, i.e., neither N nor M should be chosen unnecessarily high. However, our choice should also take the rigor of the error bound into account.

The rigor is related to the condition that $g(y_{N,M}^k(\mu); x; \mu) \in W_{M+1}^g$, $1 \leq k \leq K$, which is *very* unlikely to hold in the nonlinear case: first, because W_M^g is constructed based on $g(y^k(\mu); x; \mu)$ and not $g(y_{N,M}^k(\mu); x; \mu)$, and second, particularly because of the time-dependence of $g(y_{N,M}^k(\mu); x; \mu)$. A judicious choice of N and M can control the trade-off between safety and efficiency — we opt for safety by choosing N and M such that the rigorous part $\varepsilon_{N,M}^k(\mu)$ dominates over the non-rigorous part, $\vartheta_M^q \hat{\varepsilon}_M^k(\mu)$; we opt for efficiency by choosing N and M such that both terms balance.

4.3.3 Computational procedure

The offline-online decomposition for the calculation of $\Delta_{N,M}^{y\,k}(\mu)$ (and $\Delta_{N,M}^{s\,k}(\mu)$) follows directly from the corresponding procedure for nonaffine problems discussed in Sections 3.3.3. We will therefore omit the details and only summarize the computational costs involved in the online stage. In the online stage — given a new parameter value μ and associated reduced basis solution $\underline{y}_{N,M}^k(\mu)$, $1 \leq k \leq K$ — the computational cost to evaluate $\Delta_{N,M}^{y\,k}(\mu)$ (and hence $\Delta_{N,M}^{s\,k}(\mu)$) is $O(K(N+M)^2)$ and thus *independent* of \mathcal{N} .

4.4 Sampling Procedure

We first consider the construction of W_M^g and T_M^g . We present an extension of the construction procedure described in Section 2 for nonaffine (stationary) functions to nonaffine time-varying functions. Although we directly consider the case where the function is time-varying through an implicit dependence on time *via* the field variable $y^k(\mu)$, our method can also be applied to functions with an explicit dependence on time.

We recall that our previous approach of constructing the collateral reduced basis space W_M^g in the nonlinear case is computationally very expensive [14]. The reason is twofold: first, we need to calculate and store the "truth" solution $y^k(\mu)$ at all times $t^k \in \mathbb{I}$ on the training sample Ξ_{train}^g in parameter space. And second, construction of W_M^g requires the solution of a linear program² for all parameter-time pairs, $(t^k; \mu) \in \tilde{\Xi}_{\text{train}}^g \equiv \mathbb{I} \times \Xi_{\text{train}}^g$, since the function g is time-varying, as is inherently the case in the nonlinear context.

Our new approach combines the procedure described in Section 2.1 for nonaffine stationary functions with the POD/Greedy algorithm of Section 3.4. Although we cannot avoid the first problem related to our previous construction, i.e., calculation and storage of $y^k(\mu)$ on Ξ_{train}^g , we do to a great extent alleviate the second problem. Furthermore, we believe that our new approach is more coherent — as compared to the construction of W_N^y — and more robust. To this end, we recall the definition of the interpolation error (8) generalized to time-varying functions

$$\varepsilon_{M}^{k}(\mu) \equiv \|g(y^{k}(\mu); x; \mu) - g_{M}^{y^{k}}(x; \mu)\|_{L^{\infty}(\Omega)}.$$
(83)

where $g_M^{y^k}(x;\mu) = \sum_{m=1}^M \varphi_{Mm}^k(\mu)q_m(x)$, and $\varphi_M^k(\mu)$ is calculated from (57) for $w^k = y^k(\mu)$. We also recall the function $\text{POD}_Y(\{y^k(\mu), 1 \le k \le K\}, R)$ which returns the R largest POD modes, $\{\chi_i, 1 \le i \le R\}$, now with respect to the Y inner product. Again, we are only interested in the largest POD mode which we obtain using the method of snapshots [39].

The POD/Greedy-EIM procedure proceeds by induction: we first choose a $\mu^* \in \mathcal{D}$ and set $S_0^g = \{0\}, W_0^g = \{0\}, M = 0$. Then, for $1 \leq M \leq M_{\max}$, we first compute the error $e_{M,\text{EIM}}^k(\mu) = g(y^k(\mu^*); x; \mu^*) - g_M^{y^k}(x; \mu^*), 1 \leq k \leq K$, and we expand the parameter sample $S_M^g \leftarrow S_{M-1}^g \cup \{\mu^*\}$ and

²The construction of W_M^g in [14] is based on a greedy selection process: we choose the next parameter value μ^* — and hence generating function $\xi \equiv g(y^k(\mu^*); x; \mu)$ — as the one that maximizes the best approximation error in the $L^{\infty}(\Omega)$ -norm over the train sample.

the collateral reduced basis space $W_M^g \leftarrow W_{M-1}^g \cup \text{POD}_Y(\{e_{M,\text{EIM}}^k(\mu^*), 1 \leq k \leq K\}, 1)$, and set $M \leftarrow M + 1$. We then generate the next interpolation point x_M , basis function q_M , and update $B_{ij}^M = q_j(x_i), 1 \leq i, j \leq M$ according to the procedure described in Section 2.1. Finally, we choose the next parameter value from $\mu^* \leftarrow \arg \max_{\mu \in \Xi_{\text{train}}} \sum_{k=1}^K \varepsilon_M^k(\mu)$, where $\varepsilon_M^k(\mu)$ is defined in (83).

Given W_M^g , T_M^g , and B^M , we can then construct W_N^y following the POD/Greedy procedure outlined in Section 3.4. We shall again use the "best" possible approximation $g_M^{y_{N,M}^k}(x;\mu)$ of $g(y_{N,M}^k;x;\mu)$ so as to minimize the error induced by the empirical interpolation procedure, i.e., we set $M = M_{\text{max}}$.

Finally, we note that we cannot appeal to the LTI property anymore to generate W_N^y (and W_M^g), i.e., a reduced basis space trained on an impulse response will, in general, not yield good approximation properties for arbitrary control inputs $u(t^k)$. However, model reduction techniques for nonlinear control systems face the same problem — $u(t^k)$ is usually not known in advance in the control context — and methods to train the reduced-order model on a "generalized" impulse input have been proposed for nonlinear systems [21]. We can directly employ these approaches to also generate the reduced basis approximation. Furthermore, our *a posteriori* error bound serves as a measure of fidelity especially in the online stage and we can thus detect an unacceptable deviation from the truth approximation in real-time.

4.5 Numerical Results

We now present numerical results for the model problem introduced in Section 4.1.2. We choose for $\Xi_{\text{train}} \subset \mathcal{D}$ a deterministic grid of 12×12 parameter points over \mathcal{D} and we take $\mu_1^g = (10, 10)$. Next, we pursue the POD/Greedy-EIM procedure described in Section 4.4 to construct S_M^g, W_M^g, T_M^g , and B^M , $1 \leq M \leq M_{\text{max}}$, for $M_{\text{max}} = 191$. We plot the parameter sample S_M^g in Figure 4(a). We observe that the parameter sample is spread throughout \mathcal{D} but strongly biased towards larger values of μ_2 corresponding to a more dominant nonlinearity.

We next turn to the reduced basis approximation and construct the reduced basis space W_N^y according to the POD/Greedy sampling procedure in Section 3.4; we sample on Ξ_{train} with $M = M_{\text{max}}$ and obtain $N_{\text{max}} = 55$ for $\epsilon_{\text{tol,min}} = 1 \text{ E}-6$. We plot the parameter sample S_N^y in Figure 4(b). We observe again that the parameter sample is biased towards larger values of μ_2 and that most samples are located on the "boundaries" of the parameter domain \mathcal{D} .

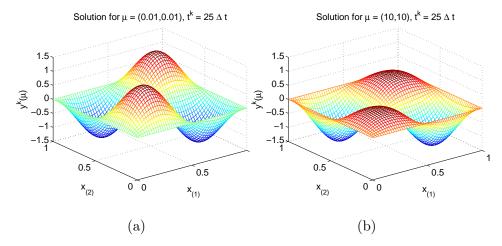


Figure 3: Solution $y^k(\mu)$ at $t^k = 25\Delta t$ for (a) $\mu = (-1, -1)$ and (b) $\mu = (-0.01, -0.01)$.

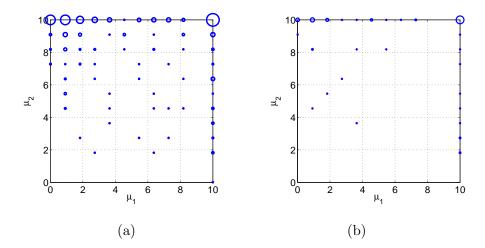


Figure 4: Parameter samples (a) S_M^g and (b) S_N^y . The diameter of the circles scale with the frequency of the corresponding parameter in the sample.

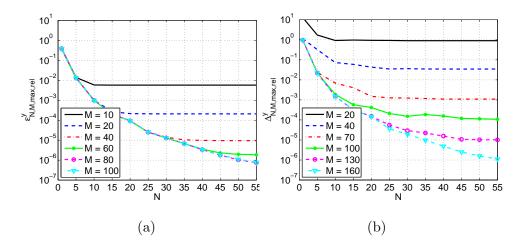


Figure 5: Convergence of the reduced basis approximation for the nonlinear model problem: (a) $\epsilon_{N,M,\text{max,rel}}^y$ and (b) $\Delta_{N,M,\text{max,rel}}^y$.

In Figure 5(a) and (b) we plot, as a function of N and M, the maximum relative error in the energy norm $\epsilon_{N,M,\max,\text{rel}}^y$ and maximum relative error bound $\Delta_{N,M,\max,\text{rel}}^y$ over a test sample Ξ_{test} of size 225, respectively (see Section 3.5 for the definition of these quantities). We observe very rapid convergence of the reduced basis approximation. Furthermore, the errors behave similar as in the nonaffine example: the error levels off at smaller and smaller values as we increase M; increasing M effectively brings the error curves down. We also observe that increasing M above 80 has no (visible) effect on the convergence of the error, whereas the error bound still shows a considerable decrease up to M = 160. In order to obtain sharp error bounds we thus have to choose M conservatively.

In Table 4 we present, as a function of N and M, $\epsilon_{N,M,\max,\text{rel}}^y$, $\Delta_{N,M,\max,\text{rel}}^y$, and $\bar{\eta}_{N,M}^y$; and for the output $\epsilon_{N,M,\max,\text{rel}}^s$, $\Delta_{N,M,\max,\text{rel}}^s$, $\bar{\eta}^s$ (see Section 3.5 for the definition of these quantities). Note that the choice of (N, M) is based on the convergence of the error bound in Figure 5(b). We observe very rapid convergence of the reduced basis (output) approximation and (output) error bound. The effectivities, $\bar{\eta}_{N,M}^y$, are greater but close to 1 throughout, we thus obtain sharp upper bounds for the true error. Due to our conservative choice of M the error contribution due to the function approximation is much smaller than the reduced-basis contribution; we therefore do not obtain effectivities smaller than 1 here. The output effectivities are considerably larger but still acceptable thanks to the fast convergence of the reduced-basis approximation – for only N = 20 and M = 100 the relative output error bound is less than 1%.

In Table 5 we present, as a function of N and M, the online computational times to calculate $s_{N,M}^k(\mu)$ and $\Delta_{N,M}^{s\,k}(\mu)$ for $1 \leq k \leq K$. The values are normalized with respect to the computational time for the direct calculation of the truth approximation output $s^k(\mu) = \ell(y^k(\mu)), \ 1 \leq k \leq K$. The computational savings are considerable despite the output effectivities of O(100): for an accuracy of less than 1% in the output bound (N = 20, M = 100) the reduction in online time is approximately a factor of 3600.

Table 4: Convergence rate and effectivities as a function of N and M for the nonlinear problem.

\overline{N}	M	$\epsilon^y_{N,M, ext{max,rel}}$	$\Delta^y_{N,M, ext{max,rel}}$	$\bar{\eta}_{N,M}^y$	$\epsilon^s_{N,M,\mathrm{max,rel}}$	$\Delta^s_{N,M,\mathrm{max,rel}}$	$\bar{\eta}^s_{N,M}$
1	40	$3.83\mathrm{E}{-}01$	$1.15\mathrm{E}+00$	2.44	$9.99\mathrm{E}\!-\!01$	$2.49\mathrm{E}+01$	14.1
5	60	$1.32\mathrm{E}\!-\!02$	$4.59\mathrm{E}\!-\!02$	2.43	$5.35\mathrm{E}\!-\!03$	$1.00\mathrm{E}+00$	130
10	80	$9.90\mathrm{E}\!-\!04$	$3.41\mathrm{E}\!-\!03$	2.10	$2.57\mathrm{E}\!-\!04$	$7.42\mathrm{E}\!-\!02$	146
20	100	$9.40\mathrm{E}\!-\!05$	$4.16\mathrm{E}\!-\!04$	2.77	$1.43\mathrm{E}\!-\!05$	$9.06\mathrm{E}\!-\!03$	436
30	120	$1.30\mathrm{E}\!-\!05$	$7.34\mathrm{E}\!-\!05$	2.48	$5.34\mathrm{E}\!-\!06$	$1.60\mathrm{E}\!-\!03$	307
40	140	$3.36\mathrm{E}\!-\!06$	$8.75\mathrm{E}\!-\!06$	1.64	$2.85\mathrm{E}\!-\!06$	$1.90\mathrm{E}\!-\!04$	205

Table 5: Online computational times (normalized with respect to the time to solve for $s^k(\mu)$, $1 \le k \le K$) for the nonlinear problem.

\overline{N}	M	$s_{N,M}(\mu, t^k), \ \forall k \in \mathbb{K}$	$\Delta^s_{N,M}(\mu,t^k), \; \forall k \in \mathbb{K}$	$s(\mu, t^k), \ \forall k \in \mathbb{K}$
1	40	$5.42\mathrm{E}\!-\!05$	$9.29\mathrm{E}\!-\!05$	1
5	60	$9.67\mathrm{E}\!-\!05$	$8.58\mathrm{E}\!-\!05$	1
10	80	$1.19\mathrm{E}\!-\!04$	$9.37\mathrm{E}\!-\!05$	1
20	100	$1.71\mathrm{E}\!-\!04$	$1.05\mathrm{E}\!-\!04$	1
30	120	$2.42\mathrm{E}\!-\!04$	$1.18\mathrm{E}\!-\!04$	1
40	140	$3.15\mathrm{E}\!-\!04$	$1.35\mathrm{E}{-}04$	1

5 Conclusions

We have presented *a posteriori* error bounds for reduced basis approximations of nonaffine and certain classes of nonlinear parabolic partial differential equations. We employed the Empirical Interpolation Method to construct affine coefficient-function approximations of the nonaffine and nonlinear parametrized functions, thus permitting an efficient offline-online computational procedure for the calculation of the reduced basis approximation and the associated error bounds. The error bounds take both error contributions — the error introduced by the reduced basis approximation and the error induced by the coefficient function interpolation — explicitly into account and are rigorous upper bounds under certain conditions on the function approximation. The POD/Greedy sampling procedure is commonly used to generate the reduced basis space for time-dependent problems. Here, we extended these ideas to the Empirical Interpolation Method and introduced a new sampling approach to construct the collateral reduced basis space for time-varying functions. The new sampling approach is more efficient than our previous approach and thus also allows to consider higher parameter dimensions.

We presented numerical results that showed the very fast convergence of the reduced basis approximations and associated error bounds. We note that there exists an optimal, i.e., most online-efficient, choice of N vs. Mwhere neither error contribution limits the convergence of the reduced basis approximation. Although our results showed that we can obtain upper bounds for the error with a judicious choice of N and M, our error bounds are, unfortunately, provably rigorous only under a very restrictive condition on the function interpolation. In the nonaffine case we can easily lift this restriction by replacing our current bound for the interpolation error with the new rigorous bound proposed in a recent note[11]; in the nonlinear case, however, the new bound is not applicable and the restriction remains. This is the topic of current research.

Our results also showed that the computational savings to calculate the output estimate and bound in the online stage compared to direct calculation of the truth output are considerable — especially in the nonlinear case where we obtained a speed-up of $O(10^3)$. We note that the offline computations in the nonlinear case are also more extensive, primarily due to the precomputation and storage of the truth solutions required to generate W_M^g . However, if a high premium on real-time performance or a many-query context can justify or outweigh the offline cost, the reduced basis approach presented here can be very gainfully employed.

A Computational procedure: a posteriori error bounds

We summarize the development of offline-online computational procedures for the calculation of $\Delta_{N,M}^{y\,k}(\mu)$. We first note from standard duality arguments that

$$\varepsilon_{N,M}^{k}(\mu) \equiv \sup_{v \in X} \frac{R^{k}(v;\mu)}{\|v\|_{X}}$$
$$= \|\hat{e}^{k}(\mu)\|_{X}, \qquad (84)$$

where $\hat{e}^k(\mu) \in X$ is given by

$$(\hat{e}^k(\mu), v)_X = R(v; \mu, t^k), \qquad \forall v \in X;$$
(85)

(85) is effectively a Poisson problem for each $t^k \in \mathbb{I}$. From (32), (10), and (6) it thus follows that $\hat{e}^k(\mu)$ satisfies

$$(\hat{e}^{k}(\mu), v)_{X} = \sum_{m=1}^{M} \varphi_{M m}(\mu) f(v; q_{m}) u(t^{k}) - \sum_{n=1}^{N} \left\{ \frac{1}{\Delta t} \left(y_{N,M n}^{k}(\mu) - y_{N,M n}^{k-1}(\mu) \right) m(\zeta_{n}, v) + y_{N,M n}^{k}(\mu) a_{0}(\zeta_{n}, v) + \sum_{m=1}^{M} \varphi_{M m}(\mu) y_{N,M n}^{k}(\mu) a_{1}(\zeta_{n}, v, q_{m}) \right\}, \ \forall v \in X.$$
(86)

It is clear from linear superposition that we can express $\hat{e}^k(\mu)$ as

$$\hat{e}^{k}(\mu) = \sum_{q=m}^{M} \varphi_{M\,m}(\mu) \, y(t^{k}) \, \mathcal{F}_{m} \\ -\sum_{n=1}^{N} \left\{ \frac{1}{\Delta t} \, \left(y_{N,M\,n}^{k}(\mu) - y_{N,M\,n}^{k-1}(\mu) \right) \, \mathcal{M}_{n} \right. \\ \left. + \left(\mathcal{A}_{n}^{0} + \sum_{m=1}^{M} \varphi_{M\,m}(\mu) \, \mathcal{A}_{m,n}^{1} \right) y_{N,M\,n}^{k}(\mu) \right\}, \quad (87)$$

where we calculate $\mathcal{F}_m \in X$, $\mathcal{A}_n^0 \in X$, $\mathcal{A}_{m,n}^1 \in X$, and $\mathcal{M}_n \in X$ from

$$(\mathcal{F}_{m}, v)_{X} = f(v; q_{m}), \qquad \forall v \in X, \ 1 \leq m \leq M_{\max},$$

$$(\mathcal{A}_{n}^{0}, v)_{X} = a_{0}(\zeta_{n}, v), \qquad \forall v \in X, \ 1 \leq n \leq N_{\max},$$

$$(\mathcal{A}_{m,n}^{1}, v)_{X} = a_{1}(\zeta_{n}, v, q_{m}), \quad \forall v \in X, \ 1 \leq n \leq N_{\max}, \ 1 \leq m \leq M_{\max},$$

$$(\mathcal{M}_{n}, v)_{X} = m(\zeta_{n}, v), \qquad \forall v \in X, \ 1 \leq n \leq N_{\max};$$

$$(88)$$

note \mathcal{B} , $\mathcal{A}^{0,1}$, and \mathcal{M} are parameter independent. From (84) and (88) it follows that

$$\varepsilon_{N,M}^{k}(\mu)^{2} = \sum_{m,m'=1}^{M} \varphi_{M\,m}(\mu) \,\varphi_{m'}(\mu) \,u(t^{k}) \,u(t^{k}) \,\Lambda_{mm'}^{ff}$$

$$+ \sum_{m=1}^{M} \sum_{n=1}^{N} \varphi_{M\,m}(\mu) \,u(t^{k}) \left(\left(\Lambda_{mn}^{a_{0}f} + \sum_{m'=1}^{M} \varphi_{m'}(\mu) \,\Lambda_{mnm'}^{a_{1}f} \right) y_{N,M\,n}^{k}(\mu) \right)$$

$$+ \left(y_{N,M\,n}^{k}(\mu) - y_{N,M\,n}^{k-1}(\mu) \right) \,\Lambda_{mn}^{mf} \right)$$

$$+ \sum_{n,n'=1}^{N} \left\{ y_{N,M\,n}^{k}(\mu) \,y_{N,M\,n'}^{k}(\mu) \left(\Lambda_{nn'}^{a_{0}a_{0}} + \sum_{m=1}^{M} \varphi_{M\,m}(\mu) \Lambda_{nn'm}^{a_{0}a_{1}} \right)$$

$$+ y_{N,M\,n}^{k}(\mu) \left(y_{N,M\,n'}^{k}(\mu) - y_{N,M\,n'}^{k-1}(\mu) \right) \left(\Lambda_{nn'}^{a_{0}m} + \sum_{m=1}^{M} \varphi_{M\,m}(\mu) \Lambda_{nn'm}^{a_{1}m} \right)$$

$$+ \left(y_{N,M\,n}^{k}(\mu) - y_{N,M\,n}^{k-1}(\mu) \right) \left(y_{N,M\,n'}^{k}(\mu) - y_{N,M\,n'}^{k-1}(\mu) \right) \Lambda_{nn'}^{mm}$$

$$+ \sum_{m,m'=1}^{M} \varphi_{M\,m}(\mu) \,\varphi_{m'}(\mu) \,y_{N,M\,n}^{k}(\mu) \,y_{N,M\,n'}^{k}(\mu) \,\Lambda_{nn'mm'}^{a_{1}a_{1}} \right\},$$

$$(89)$$

where the parameter-independent quantities Λ are defined as

$$\Lambda_{mm'}^{ff} = (\mathcal{F}_{m}, \mathcal{F}_{m'})_{X}, \qquad 1 \le m, m' \le M_{\max};$$

$$\Lambda_{mn}^{a_{0}f} = -2 (\mathcal{F}_{m}, \mathcal{A}_{n}^{0})_{X}, \qquad 1 \le m \le M_{\max}, \ 1 \le n \le N_{\max};$$

$$\Lambda_{mnm'}^{a_{1}f} = -2 (\mathcal{F}_{m}, \mathcal{A}_{m',n}^{1})_{X}, \qquad 1 \le m, m' \le M_{\max}, \ 1 \le n \le N_{\max};$$

$$\Lambda_{mn}^{mf} = -\frac{2}{\Delta t} (\mathcal{F}_{m}, \mathcal{M}_{n})_{X}, \qquad 1 \le m \le M_{\max}, \ 1 \le n \le N_{\max};$$

$$\Lambda_{nn'}^{a_{0}a_{0}} = (\mathcal{A}_{n}^{0}, \mathcal{A}_{n'}^{0})_{X}, \qquad 1 \le m \le M_{\max}, \ 1 \le n, n' \le N_{\max};$$

$$\Lambda_{nn'm}^{a_{0}a_{1}} = 2(\mathcal{A}_{n}^{0}, \mathcal{A}_{m,n'}^{1})_{X}, \qquad 1 \le m \le M_{\max}, \ 1 \le n, n' \le N_{\max};$$

$$\Lambda_{nn'm}^{a_{0}a_{1}} = (\mathcal{A}_{m,n}^{1}, \mathcal{A}_{m',n'}^{1})_{X}, \qquad 1 \le m, m' \le M_{\max}, \ 1 \le n, n' \le N_{\max};$$

$$\Lambda_{nn'}^{a_{0}m} = \frac{2}{\Delta t} (\mathcal{A}_{n}^{0}, \mathcal{M}_{n'})_{X}, \qquad 1 \le n, n' \le N_{\max};$$

$$\Lambda_{nn'm}^{a_{1}m} = \frac{2}{\Delta t} (\mathcal{A}_{n,n}^{1}, \mathcal{M}_{n'})_{X}, \qquad 1 \le n, n' \le N_{\max};$$

$$\Lambda_{nn'm}^{a_{1}m} = \frac{2}{\Delta t} (\mathcal{A}_{n,n}^{1}, \mathcal{M}_{n'})_{X}, \qquad 1 \le n, n' \le N_{\max};$$

$$\Lambda_{nn'}^{mm} = \frac{1}{\Delta t^{2}} (\mathcal{M}_{n}, \mathcal{M}_{n'})_{X}, \qquad 1 \le n, n' \le N_{\max}.$$
(90)

(90) The evaluation of $\Phi_M^{\operatorname{na}k}(\mu)$ is very similar; to this end, we first calculate $\mathcal{F}_{M+1} \in X$ and $\mathcal{A}_{M+1,n}^1 \in X$ from

$$(\mathcal{F}_{M+1}, v)_X = f(v; q_{M+1}), \quad \forall v \in X, (\mathcal{A}_{M+1,n}^1, v)_X = a_1(\zeta_n, v; q_{M+1}), \quad \forall v \in X, \ 1 \le n \le N_{\max};$$
 (91)

It then follows from (33) and standard duality arguments that

$$\Phi_{M}^{na\,k}(\mu)^{2} = y(t^{k})^{2} \Lambda_{M+1\,M+1}^{ff} + \sum_{n=1}^{N} y_{N,M\,n}^{k}(\mu) \left\{ y(t^{k}) \Lambda_{n\,M+1\,M+1}^{a_{1}f} + \sum_{n'=1}^{N} y_{N,M\,n'}^{k}(\mu) \Lambda_{nn'M+1\,M+1}^{a_{1}a_{1}} \right\}$$

where the parameter-independent quantities Λ are defined as

$$\Lambda_{M+1M+1}^{ff} = (\mathcal{F}_{M+1}, \mathcal{F}_{M+1})_X;$$

$$\Lambda_{nM+1M+1}^{a_{1f}} = -2 (\mathcal{F}_{M+1}, \mathcal{A}_{M+1,n}^1)_X, \quad 1 \le n \le N_{\max};$$

$$\Lambda_{nn'M+1M+1}^{a_{1a_1}} = (\mathcal{A}_{M+1,n}^1, \mathcal{A}_{M+1,n'}^1)_X, \quad 1 \le n, n' \le N_{\max}.$$
(92)

The offline-online decomposition is now clear. In the offline stage we first compute the quantities \mathcal{F} , $\mathcal{A}^{0,1}$, and \mathcal{M} from (88) and (91) and then evaluate the Λ from (90) and (92); this requires (to leading order) $O(M_{\max}N_{\max})$

expensive "truth" finite element solutions, and $O(M_{\max}^2 N_{\max}^2) \mathcal{N}$ -inner products. In the online stage — given a new parameter value μ and associated reduced basis solution $\underline{y}_{N,M}^k(\mu), \forall k \in \mathbb{K}$ — the computational cost to evaluate $\Delta_{N,M}^{y\,k}(\mu)$ and $\Delta_{N,M}^{s\,k}(\mu), \forall k \in \mathbb{K}$, is $O(KM^2N^2)$. Thus, all online calculations needed are *independent* of \mathcal{N} .

Acknowledgment

I would like to thank Professor Anthony T. Patera of MIT and Professor Yvon Maday of University Paris VI for their many invaluable contributions to this work. This work was supported by the Excellence Inititiative of the German federal and state governments, by DARPA and AFOSR under Grant F49620-03-1-0356, DARPA/GEAE and AFOSR under Grant F49620-03-1-0439, and the Singapore-MIT Alliance.

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