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Reduced-Order Galerkin Approximations in PDE-Constrained Optimization

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1 Introduction

Optimal control problems for partial differential equations are often hard to tackle numerically because their discretization leads to very large scale optimization problems. Therefore different techniques of model reduction were developed to approximate these problems by smaller ones that are tractable with less effort.

One popular model reduction technique for large-scale state-space systems is the *moment matching approximation* considered first in [15, 16]. This method is based on projecting the dynamical system onto Krylov subspaces computed by an Arnoldi- or Lanczos process. Krylov methods prove to be efficient for large-scale sparse systems, since only matrix-vector multiplications are required. The moment matching method shows the drawbacks that stability and passivity are not necessarily preserved in the reduced-order system and that there is no global approximation error bound; see, e.g., [6, 19]. *Balanced truncation* [54] is another well studied model reduction technique for state-space systems. This method utilizes the solutions to the two Lyapunov equations, the so-called controllability and observability Gramians. The balanced truncation method is based on transforming the state-space system into a balanced form so that its controllability and observability Gramians become diagonal and equal. Moreover, the states that are difficult to reach or to observe, are truncated. The advantage of this method is that it preserves the asymptotic stability in the reduced-order system. Furthermore, a-priori error bounds are available. Recently, the theory of balanced truncation model reduction was extended to descriptor systems; see, e.g., [38] and [21]. Both the moment matching approximation and the balanced truncation approach do not rely on snapshots, which have to be taken more or less arbitrarily. For an overview we refer the reader to [2]. However, up to now, both strategies can be applied more or less only to linear, time-invariant dynamical systems and do not yet cover time variant or nonlinear models. There are attempts to deal

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with time variant equations by approximating them through piecewise constant models, but these investigations are still in an early stage; see, e.g., [8].

Recently the application of *reduced-order models* to linear time varying and nonlinear systems, in particular to nonlinear control systems, has received an increasing amount of attention. The reduced-order approach is based on projecting the dynamical system onto subspaces consisting of basis elements that contain characteristics of the expected solution. This is in contrast to, e.g., finite element techniques, where the basis elements of the subspaces do not relate to the physical properties of the system that they approximate. The *reduced basis* (RB) method, as developed in [17, 41] and [27], is one such reduced-order method where the basis elements correspond to the dynamics of expected control regimes. Currently *Proper orthogonal decomposition* (POD) is probably the mostly used and most successful model reduction technique for nonlinear optimal control problems, where the basis functions contain information from the solutions of the dynamical system at pre-specified time-instances, so-called snapshots. Due to a possible linear dependence or almost linear dependence the snapshots themselves are not appropriate as a basis. Hence a singular value decomposition is carried out and the leading generalized eigenfunctions are chosen as a basis, referred to as the POD basis. POD is successfully used in a variety of fields including fluid dynamics, coherent structures [1, 3] and inverse problems [7]. Moreover in [5] POD is successfully applied to compute reduced-order controllers. The relationship between POD and balancing was considered in [36, 47, 53]. An error analysis for non-linear dynamical systems in finite dimensions were carried out in [43] and a missing point estimation in models described by POD was studied in [4].

Reduced order models are used in PDE-constrained optimization in various ways. In optimal control problems it is sometimes necessary to compute a feedback control law instead of a fixed optimal control. In the implementation of these feedback laws models of reduced order can play an important and very useful role, see [5, 44]. Another useful application is the use in optimization problems, where a PDE solver is part of the function evaluation. Obviously, thinking of a gradient evaluation or even a step-size rule in the optimization algorithm, an expensive function evaluation leads to an enormous amount of computing time. Here, the reduced order model can replace the system given by a PDE in the objective function. It is quite common that a PDE can be replaced by a 5- or 10-dimensional system of ordinary differential equations. This results computationally in a very fast method for optimization compared to the effort for the computation of a single solution of a PDE. There is a large amount of literature in engineering applications in this regard, we mention only the papers [37, 40]. Recent applications can also be found in finance using the RB model [42] and the POD model [48] in the context of calibration for models in option pricing.

To explain the reduced-order modelling we choose the following generic nonlinear optimal control problem: Minimize the cost functional

$$J(y,u) = \frac{1}{2}\int_0^T \int_\Omega |y(t,\mathbf{x}) - y_d(t,\mathbf{x})|^2 \,\mathrm{d}\mathbf{x}\mathrm{d}t + \frac{\kappa}{2}\sum_{i=1}^m \int_0^T |u_i(t)|^2 \,\mathrm{d}t \tag{1a}$$

subject to the semilinear parabolic partial differential equation

$$\begin{aligned} y_t(t,\mathbf{x}) - \Delta y(t,\mathbf{x}) + f(t,\mathbf{x},y(t,\mathbf{x})) &= \sum_{i=1}^{m} u_i(t) b_i(\mathbf{x}) && \text{for all } (t,\mathbf{x}) \in (0,T)\times\Omega, \\ y(t,\mathbf{x}) &= 0 && \text{for all } (t,\mathbf{x}) \in (0,T)\times\Gamma, \\ y(0,\mathbf{x}) &= y_0(\mathbf{x}) && \text{for all } \mathbf{x} \in \Omega \end{aligned} \tag{1b}$$

and to the control constraints

$$u \in U_{ad} = \left\{ \tilde{u} \in U \,\middle|\, u_{a,i} \le \tilde{u}_i \le u_{b,i} \text{ in } (0,T) \text{ for } 1 \le i \le m \right\} \tag{1c}$$

with the control space

$$U = L^2(0,T) := \underbrace{L^2(0,T) \times \ldots \times L^2(0,T)}_{m\text{-times}}$$

We suppose that $\Omega \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, is a bounded open set with Lipschitz-continuous boundary Γ, that the desired state y_d belongs to $L^2(Q)$ and κ is a positive regularization parameter. In (1b) let $T > 0$, $f : [0,T] \times \Omega \times \mathbb{R} \to \mathbb{R}$, and $y_0 \in L^2(\Omega)$. Finally, $u_a, u_b \in L^\infty(0,T)^m$ holds and $b_1, \ldots, b_m \in L^2(\Omega)$ are given shape functions. In [11, 45] sufficient conditions for f are given so that (1) admits a local optimal solution $x^* = (y^*, u^*)$.

The paper is organized as follows: The following section contains an introduction into reduced order models. First we formulate the solution concept of a PDE in variational form and the Galerkin approximation as a numerical solution scheme. Then we introduce the POD method for the continuous and discrete case in time. We address the method of snapshots and related issues like their optimal location. In a final subsection we give an extended motivation of the RB method.

In the third section we address some research issues when using POD bases for optimization problems with PDEs. Updating strategies for the POD basis are discussed in the first two subsections. Another aspect in optimizing the choice of the POD basis is part of section 3.3, which is more recent research like the a-posteriori error estimates in the last section. We complement the statements with numerical results for a tracking problem with a semilinear parabolic PDE.

2 Reduced-order modelling

In this section we introduce the POD method for our model equation (1b) and explain briefly the RB method. Moreover, the reduced-order Galerkin approximation for (1b) is derived.

2.1 The variational formulation

For $T > 0$ let $Q = (0,T) \times \Omega$ and $\Sigma = (0,T) \times \Gamma$. By $H = L^2(\Omega)$ we denote the Lebesgue space of measurable and square integrable functions endowed with the common inner product

$$\langle \varphi, \psi \rangle_H = \int_\Omega \varphi\psi \,\mathrm{d}\mathbf{x} \quad \text{for } \varphi, \psi \in H$$

and the induced norm $\|\varphi\|_H = \sqrt{\langle\varphi,\varphi\rangle_H}$. Let $V = H_0^1(\Omega)$ be the Hilbert space

$$V = \left\{ \varphi : \Omega \to \mathbb{R} \,\middle|\, \varphi \text{ Lebesgue-measurable, } \|\varphi\|_H^2 + \sum_{i=1}^{d} \|\varphi_{\mathbf{x}_i}\|_H^2 < \infty \text{ and } \varphi\big|_\Gamma = 0 \right\},$$

where $\varphi_{\mathbf{x}_i}$ denotes the weak partial derivative of φ with respect to $\mathbf{x}_i$, $1 \le i \le d$. The inner product in V is given by

$$\langle\varphi,\psi\rangle_V = \langle\varphi,\psi\rangle_H + \sum_{i=1}^{d} \langle\varphi_{\mathbf{x}_i},\psi_{\mathbf{x}_i}\rangle_H \quad \text{for } \varphi,\psi \in V$$

with norm $\|\varphi\|_V = \sqrt{\langle\varphi,\varphi\rangle_V}$. The dual space of V is denoted by V'. The Hilbert space $L^2(0,T;H)$ contains all measurable functions $\varphi : [0,T] \to H$ such that

$$\|\varphi\|_{L^2(0,T;H)} = \Big(\int_0^T \|\varphi(t)\|_H^2 \,\mathrm{d}t \Big)^{1/2} < \infty.$$

Analogously, the Hilbert space $L^2(0,T;V)$ is defined. We introduce

$$W(0,T) = \big\{ \varphi \in L^2(0,T;V) \,\big|\, \varphi_t \in L^2(0,T;V') \big\}.$$

It is well-known that $W(0,T)$ is a Hilbert space and that $W(0,T)$ is continuously embedded in $C([0,T];H)$, the space of all measurable and continuous functions from $[0,T]$ to H; see [12], for instance.

We define the notion of a weak solution to our semilinear parabolic equation (1b): We call $y \in W(0,T)$ a *weak* or *variational solution* to (1b) if $y(0,\cdot) = y_0$ holds in H and if y satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle y(t),\varphi\rangle_H + \int_\Omega (\nabla y(t)\cdot\nabla\varphi + f(t,\cdot,y(t))\varphi)\mathrm{d}\mathbf{x} = \sum_{i=1}^{m} u_i(t) \int_\Gamma b_i\varphi \,\mathrm{d}\mathbf{x} \tag{2}$$

for all $\varphi \in V$ and (almost) all $t \in (0,T]$. The existence of a unique weak solution can be found in [11, 45], for example.

To solve (2) numerically, we apply a Galerkin approximation. For that purpose, let $\{\varphi_i\}_{i=1}^N$ denote a set of linear independent ansatz functions in V, for example the finite element functions, e.g. [10]. We set $V^N = \operatorname{span}\{\varphi_1,\ldots,\varphi_N\} \subset V$. The function

$$y^N(t,\cdot) = \sum_{i=1}^{N} c_i(t)\varphi_i \in V^N, \quad t \in [0,T],$$

is called an approximation of the weak solution y in (2) provided

$$\begin{aligned} &\langle y^N(0),\varphi_i\rangle_H = \langle y_0,\varphi_i\rangle_H, \\ &\frac{\mathrm{d}}{\mathrm{d}t}\langle y^N(t),\varphi_i\rangle_H + \int_\Omega (\nabla y^N(t)\cdot\nabla\varphi_i + f(t,\cdot,y^N(t))\varphi_i)\mathrm{d}\mathbf{x} = \sum_{j=1}^{m} u_j(t) \int_\Gamma b_j\varphi_i \,\mathrm{d}\mathbf{x} \end{aligned} \tag{3}$$

for $1 \leq i \leq N$ and almost all $t \in (0,T]$. Notice that (3) yields an N-dimensional initial value problem for the coefficient vector $t \mapsto c(t) = (c_1(t), \ldots, c_N(t))^T \in \mathbb{R}^N$ of the form

$$\dot{c}(t) = F(t, c(t)) \text{ for } t \in (0,T] \quad \text{and} \quad c(0) = c_0$$

with an appropriate $F : [0,T] \times \mathbb{R}^N \to \mathbb{R}^N$ and $c_0 \in \mathbb{R}^N$.

In the following we will present a reduced-order approach that is based on projecting (1b) onto subspaces consisting of basis elements containing characteristics of the expected solution. This is in contrast to e.g. finite element techniques, where the elements of the subspaces are uncorrelated to the physical properties of the system that they approximate. In this work we focus on the POD and the RB method.

2.2 The POD method

We suppose that for given $u \in U_{ad}$ the function y is a weak solution of (1b) satisfying $y \in C([0,T];V)$. Set $\mathcal{V} = \operatorname{span}\{y(t) \,|\, t \in [0,T]\} \subset V \subset X$, where X denote either the space H or the (smoother) space V. If $y_0 \neq 0$ holds, then $\operatorname{span}\{y_0\} \subset \mathcal{V}$ and $L = \dim \mathcal{V} \geq 1$, but $\mathcal{V}$ may have infinite dimension. For given $\ell \geq 1$ we consider the minimization problem

$$\begin{cases} \min \displaystyle\int_0^T \Big\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i \rangle_X \psi_i \Big\|_X^2 \, \mathrm{d}t \\ \text{subject to (s.t.)} \quad \langle \psi_i, \psi_j \rangle_X = \delta_{ij}, \ 1 \leq i,j \leq \ell. \end{cases} \tag{4}$$

The solution $\{\psi_i\}_{i=1}^{\ell}$ to (4) is called a *POD basis of rank* ℓ. Equivalently, the POD basis of rank ℓ can be introduced by the following maximization problem:

$$\max \int_0^T \sum_{i=1}^{\ell} \left| \langle y(t), \psi_i \rangle_X \right|^2 \mathrm{d}t \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle_X = \delta_{ij}, \ 1 \leq i,j \leq \ell.$$

Remark 2.1 In many applications (especially in fluid dynamics) the modified space $\bar{V} = \operatorname{span}\{y(t) - \bar{y} \,|\, t \in [0,T]\}$ with an offset $\bar{y} \in X$ is utilized to compute the POD basis. One possible choice for $\bar{y}$ is the mean value $\bar{y} = 1/T \int_0^T y(t) \, \mathrm{d}t$. $\Diamond$

It is well-known that the solution of (4) is given as follows [26]: the ψ_i's solve the symmetric eigenvalue problem

$$\mathcal{R}\psi_i = \lambda_i \psi_i, \quad \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_\ell \geq 0, \tag{5}$$

where $\mathcal{R} : X \to \mathcal{V} \subset X$ is the linear, bounded, nonnegative, self-adjoint and compact operator

$$\mathcal{R}\psi = \int_0^T \langle y(t), \psi \rangle_X y(t) \, \mathrm{d}t \quad \text{for } \psi \in X. \tag{6}$$

Remark 2.2 (Discrete POD method) In real computations the whole trajectory $y(t)$ is not available for all $t \in [0,T]$. For that purpose let $0 = t_1 < t_2 < \ldots < t_n = T$ be a given snapshot grid in $[0,T]$ and let $y_j = y(t_j)$ denote the approximations for y at time instance

t_j, $j = 1, \ldots, n$. We set $\mathcal{V}^n = \operatorname{span}\{y_1, \ldots, y_n\}$ with $L^n = \dim \mathcal{V}^n \leq n$. Then, for given $\ell \leq n$ we consider the minimization problem

$$\min \sum_{j=1}^{n} \alpha_j \left\| y_j - \sum_{i=1}^{\ell} \langle y_j, \psi_i^n \rangle_X \, \psi_i^n \right\|_X^2 \quad \text{s.t.} \quad \langle \psi_i^n, \psi_j^n \rangle_X = \delta_{ij}, \; 1 \leq i, j \leq \ell \tag{7}$$

instead of (4). In (7), α_j represent the trapezoidal weights

$$\alpha_1 = \frac{t_2 - t_1}{2}, \quad \alpha_j = \frac{t_{j+1} - t_{j-1}}{2} \text{ for } 2 \leq j \leq n-1, \quad \alpha_n = \frac{t_n - t_{n-1}}{2}.$$

The solution of (7) is given by the solution of the eigenvalue problem

$$\mathcal{R}^n \psi_i^n = \sum_{j=1}^{n} \alpha_j \, \langle y_j, \psi_i^n \rangle_X \, y_j = \lambda_i^n \psi_i^n, \quad i = 1, \ldots, \ell, \tag{8}$$

where $\mathcal{R}^n : X \to \mathcal{V}^n \subset X$ is linear, bounded, compact, self-adjoint and non-negative. Thus, there exists an orthonormal set $\{\psi_i^n\}_{i=1}^{L^n}$ of eigenfunctions and corresponding non-negative eigenvalues $\{\lambda_i^n\}_{i=1}^{L^n}$ satisfying

$$\mathcal{R}^n \psi_i^n = \lambda_i^n \psi_i^n, \quad \lambda_1^n \geq \lambda_2^n \geq \ldots \geq \lambda_{L^n}^n > 0. \tag{9}$$

We refer to [33], where the relationship between (9) and (5) is investigated. ◊

The ψ_i can be computed by the following procedure using the singular value decomposition:

1) Solve the symmetric eigenvalue problem

   $$\mathcal{K} v_i = \lambda_i v_i, \quad i = 1, \ldots, \ell,$$

   where $\mathcal{K} : L^2(0,T) \to L^2(0,T)$ is the linear, bounded, nonnegative, selfadjoint and compact operator given by $(\mathcal{K}v)(t) = \int_0^T \langle y(s), y(t) \rangle_X v(s) \, \mathrm{d}s$ for $v \in L^2(0,T)$.

2) Set $\psi_i = 1/\sqrt{\lambda_i} \int_0^T y(t) v(t) \, \mathrm{d}t \in \mathcal{V} \subset X$ for $i = 1, \ldots, \ell$.

Remark 2.3 (Method of snapshots) For the discrete POD method – see Remark 2.2 – one can compute the POD basis by using the correlation matrix $\mathcal{K}^n = ((\langle y_j, y_i \rangle_X)) \in \mathbb{R}^{n \times n}$ (instead of the operator $\mathcal{K}$). This procedure is called the *method of snapshots* [50]. Depending on the size of the eigenvalue problems (for $\mathcal{R}^n$ and $\mathcal{K}^n$) we solve (8) or apply the method of snapshots. For a discussion of this issue and numerical strategies we refer to [3, 31]. ◊

If the POD basis $\{\psi_i\}_{i=1}^{\ell}$ is computed, the associated POD Galerkin approximation of (1b) can be derived. Analogous to Section 2.1 we set set $V^\ell = \operatorname{span}\{\psi_1, \ldots, \psi_\ell\} \subset V$. The function

$$y^\ell(t) = \sum_{i=1}^{\ell} c_i^\ell(t) \psi_i \in V^\ell, \quad t \in [0,T],$$

is called an approximation for the weak solution y to (2) provided

$$\begin{aligned} &\langle y^\ell(0), \psi_i \rangle_H = \langle y_0, \psi_i \rangle_H, \\ &\frac{\mathrm{d}}{\mathrm{d}t} \langle y^\ell(t), \psi_i \rangle_H + \int_\Omega \nabla y^\ell(t) \cdot \nabla \psi_i + f(t, \cdot, y^\ell(t)) \psi_i \, \mathrm{d}\mathbf{x} = \sum_{j=1}^{m} u_j(t) \int_\Gamma b_j \psi_i \, \mathrm{d}\mathbf{x} \end{aligned} \tag{10}$$

for $1 \leq i \leq \ell$ and (almost) all $t \in (0, T]$. Notice that (10) yields an ℓ-dimensional initial value problem for the coefficient vector $t \mapsto c^\ell(t) = (c_1^\ell(t), \ldots, c_\ell^\ell(t))^T \in \mathbb{R}^\ell$ of the form

$$\dot{c}^\ell(t) = G(t, c^\ell(t)) \text{ for } t \in (0, T] \quad \text{and} \quad c^\ell(0) = c_0^\ell$$

with an appropriate $G : [0, T] \times \mathbb{R}^\ell \to \mathbb{R}^\ell$ and $b_0 \in \mathbb{R}^\ell$. We call (10) a reduced-order model for (3). Since the POD basis $\{\psi_i\}_{i=1}^\ell$ contains information of the underlying dynamical system, we expect that (10) is a sufficiently accurate approximation for (2) with $\ell \ll N$.

We refer to [32, 33], where, for fixed u, a-priori error estimates for the difference between the weak solution y to (2) and the POD solution y^ℓ to (9) are derived for linear and certain evolution problems. These results are extended in [25] to a laser surface hardening problem, in [49] to evolution problems with time-dependent coefficients and in [28] to elliptic equations.

Example 2.4 In (1b) we choose the domain $\Omega = (0, 1) \times (0, 1) \subset \mathbb{R}^2$, the subdomains $\Omega_1 = (0, 0.5) \times (0, 0.5)$, $\Omega_2 = (0.5, 1) \times (0, 0.5)$, $\Omega_3 = (0.5, 1) \times (0, 0.5)$, $\Omega_3 = (0.5, 1) \times (0.5, 1)$ and the shape functions $b_i = \chi_{\Omega_i}$, $1 \leq i \leq m = 4$, where χ_{Ω_i} denotes the characteristic function for the set Ω_i. Moreover, let

$$\begin{aligned} y_0(\mathbf{x}) &= 2b_1(\mathbf{x}) - 2b_2(\mathbf{x}) + b_3(\mathbf{x}) - 4b_4(\mathbf{x}), \\ f(t, \mathbf{x}, v) &= v^3 - 1 - \sin(4\pi x_1)\cos(8\pi x_2) - \sin(6\pi x_1)\cos(4\pi x_2) \\ &\quad - \sin(2\pi x_1)\cosh(x_2) - x_1 x_2^2 \end{aligned}$$

for $(t, \mathbf{x}) \in Q$, $\mathbf{x} = (x_1, x_2)$, and $v \in \mathbb{R}$. Then, we solve (1b) by applying a standard finite difference scheme for the spatial discretization and a semi-implicit scheme for the temporal discretization (implicit in the linear term $y_t - \Delta y$ and explicit in the nonlinear term y^3). The POD basis is computed as described above using for simplicity $u_i = 0, i = 1, ..., 4$. The decay of the first 20 eigenvalues λ_i is shown in the left plot of Figure 1. Utilizing the computed POD basis we derive the reduced-order model (10). In the right plot of Figure 1 we present the relative error of the POD solution for different values of ℓ. We observe that the error decreases for increasing ℓ. ◊

Remark 2.5 (Optimal snapshot location) In Remark 2.2 we introduce a discrete variant of the POD method. The paper [35] is devoted to optimizing the choice of the time instances $\{t_j\}_{j=1}^n$ in such a manner that the error between the POD-solution and the trajectory of the dynamical system is minimized. Numerical examples show that the proposed criterion has an effect on the choice of the time instances and further they demonstrate the feasibility of the method in determining optimal snapshot locations for diffusion equations. ◊

Remark 2.6 A difficulty related to POD-based model reduction may result from the evaluation of the nonlinearity on the POD subspace [4]. In this respect, reduced-basis elements [18, 46] offer an interesting alternative. ◊

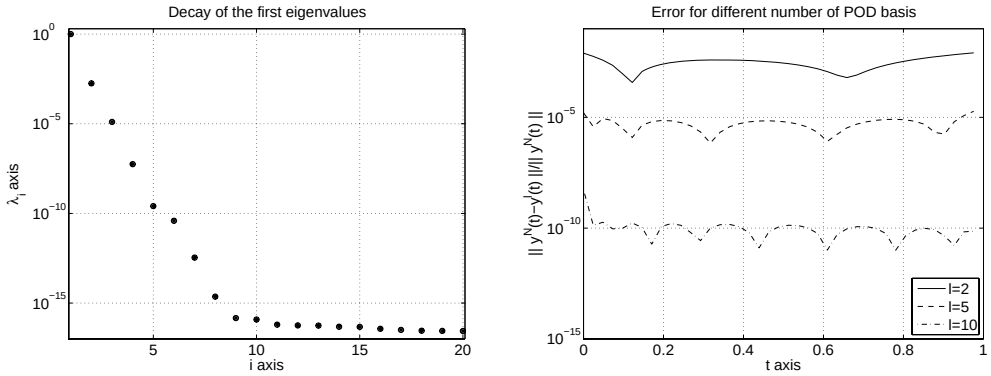

Fig. 1 Example 2.4: Decay of the first 20 eigenvalues λ_i (left plot) and relative error $t \mapsto \|y^N(t) - y^\ell(t)\|_{L^2(\Omega)}/\|y^N(t)\|_{L^2(\Omega)}$ for the POD Galerkin solution (right plot) with the control input $u_i(t) = 0$ for $t \in [0, T]$ and $i = 1, \ldots, 4$.

2.3 The RB method

The RB method has proven to be a very efficient reduced-order method for semilinear (parametrized) elliptic and parabolic equations involving certain nonlinearities. We refer to [41] for a detailed description of the method and, e.g., [17, 18, 20, 46]. An optimal control and inverse problem application are considered in [27] and [39], respectively.

For the RB method one uses also a snapshot grid similar to the POD method (Remark 2.2). However, in the contrast to POD, the solution of (1b) is recorded only at some specified time instances that yield the reduced basis. To be more precise, let $\mathcal{S}^\ell = \{t_{i_1}, \ldots, t_{i_\ell}\}$ be a set of fixed time instances in $[0, T]$, where $i_1, \ldots, i_\ell \in \{1, \ldots, n\}$ with $i_j \neq i_k$ for $j \neq k$ and $\ell \leq n$. We set $V^\ell = \operatorname{span}\{\psi_j = y(t_{i_j}) \text{ for } j = 1, \ldots, \ell\} \subset X$, i.e., V^ℓ is spanned by the solution to (1b) at the time instances $\{t_{i_j}\}_{j=1}^\ell$. Note that for algebraic stability of the reduced-order model the basis $\{\psi_i\}_{i=1}^\ell$ is orthonormalized w.r.t. $\|\cdot\|_X$ by a Gram-Schmidt procedure. To identify time instances in $\mathcal{S}^\ell$, which lead to a 'good' resulting basis $\{\psi_i\}_{i=1}^\ell$ the standard greedy procedure is often applied; see, e.g., [39]. Essentially, a new time instance is identified by determining the solution of

$$t_{i_{\ell+1}} = \operatorname*{arg\,max}_{t \in \{t_j\}_{j=1}^n \setminus \mathcal{S}^\ell} \Delta_y^\ell(t),$$

where $\Delta_y^\ell(t) \in \mathbb{R}$ is a rigorous and fast computable error estimator for the error $\|y(t) - y^\ell(t)\|_X$. Here, $y(t)$ is the solution to (1b) at time t and $y^\ell(t)$ is the reduced-order solution at time t using ℓ RB basis functions for the Galerkin projection. While for the application of the POD method it is sufficient to have unique solvability of (1b), for the RB method one has to compute (an estimate) for the inf-sup constant of the elliptic operator $-\Delta + 3y^2$ with $y \in C(\overline{\Omega})$. Furthermore, for the POD method the basis $\{\psi_i\}_{i=1}^\ell$ is computed, s.t. the *mean* error to the snapshots is minimized, whereas for the RB method the basis $\{\psi_i\}_{i=1}^\ell$ is chosen such that the *maximum* error to the snapshots is minimized.

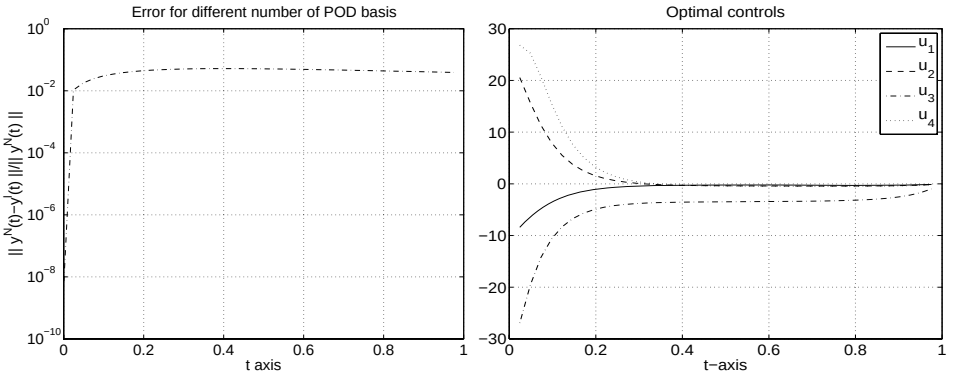

Fig. 2 Relative error $t \mapsto \|y^N(t) - y^\ell(t)\|_{L^2(\Omega)} / \|y^N(t)\|_{L^2(\Omega)}$ for the POD Galerkin solution with $\ell = 10$, where the POD basis is computed from a different input function $u(t)$ (left plot) with the control input $u_1(t) = e^{-t}$ and $u_i(t) = 0$ for $t \in [0, T]$ and $i = 2, 3, 4$ and optimal controls $u^{\ell,i}(t)$, $1 \leq i \leq 4$ and $t \in [0, T]$, for Example 3.1 (right plot).

3 POD Basis for optimal control problems

A standard discretization of the optimal control problem (1) may lead to a large-scale optimization problem which cannot be solved with the currently available computer power or may not be solvable under real-time requirements. An alternative approach is to find a suboptimal solution approach utilizing a reduced-order method like the POD or RB method. The associated suboptimal control problem is obtained by replacing the dynamical system (1b) by the reduced-order model (9) or the RB model. In fact, we arrive at the minimization problem

$$\min J(y^\ell, u) \quad \text{s.t.} \quad (y^\ell, u) \text{ satisfies (10) and } u \in U_{ad}. \tag{11}$$

At this stage the question arises which snapshots to use for the reduced-order model, since it is by no means clear that the reduced-order model computed with snapshots related to a control u is also able to resolve the presumably completely different dynamics related to a different control v. In Example 2.4 we compute a POD basis using $u_i(t) = 0$ in $(0, T)$ for $i = 1, \ldots, 4$ and based on this information we design an associated reduced-order model. If we only change u_1 to be $u_1(t) = e^{-t}$ we observe that the POD solution to (10) has a significantly larger error; compare Figure 1 (right plot) and Figure 2 (left plot). To cope with this difficulty we present different strategies in this section.

3.1 Adaptive strategies for POD

In [1] the authors use an adaptive optimization algorithm. It successfully updates the snapshot samples on which the POD surrogate model is to be based upon up. Starting from a reduced-order model, the suboptimal control is used to find an updated POD basis. This provides the basis for a new reduced-order approximation of (1) and the new suboptimal control is computed. The algorithm is stopped if subsequent suboptimal controls differ less than a given tolerance. A related idea is presented in [44]. We also refer to [13], where the adaptive procedure is combined with the idea to incorporate also information of the dual equation

in the derivation of the POD reduced-order model. It turns out that this strategy leads to a significant improvement of the numerical results.

3.2 Trust-Region POD method

In the paper [3] an optimization based approach was presented in order to deal with the problem of adapting the reduced order model. That paper deals especially with POD models but it can be modified easily to handle other reduced order models.

The TRPOD (Trust Region POD) approach is based on trust region methods which are used in optimization for globalizing locally convergent algorithms. This way one can design a method which gives some update strategies that are based on a mathematically rigorous theory. Instead of using a quadratic approximation of the objective function as the model function for the original function $J(y,u)$ we use the nonlinear function $J_{red}(y^\ell,u)$ based on the reduced order model, see [14]. Let (y_*^ℓ,u_*) be the solution of (11) based on a reduced model obtained at a point (y_k,u_k). The decision, if the model needs to be updated, is based on value of

$$\rho = \frac{J_{red}(y_*^\ell,u_*) - J_{red}(y_k,u_k)}{J(y_*^\ell,u_*) - J(y_k,u_k)}.$$

If that value of ρ deviates significantly from 1, the model needs to be updated somehow. One problem with this approach is that for the computation of ρ we need to evaluate the original cost function J at (y_*^ℓ,u_*). In order to avoid that, in a multilevel strategy was developed in [30], where a hierarchy of problems is considered and the expensive function evaluations only occur at the highest level, when we already have a very good guess for the optimal point. While this variant is currently under research, the TRPOD approach has been used in engineering applications, [9].

3.3 OS-POD strategy

Note that the reduced-order model (11) for (1) depends on the state y used in the computation of the POD basis $\{\psi_i\}_{i=1}^\ell$ through the operator $\mathcal{R}$; see (5) and (6). Hence, (11) is dependent on the reference control u in (1b) used to get the state y. This may deter from one of the main advantages of the POD approach for model reduction, which consists in the fact that unlike typical finite element basis functions the elements of the POD basis reflect the dynamics of the system. In the optimal control context this feature gets lost if the dynamics of the state corresponding to the reference control is significantly different from that of the trajectory corresponding to the optimal control of (1) or the POD Galerkin approximation (11). To eliminate this drawback the authors propose to consider [34]

$$\min J(y^\ell,u) \quad \text{s.t.} \quad (y^\ell,u,y,\psi_i,\lambda_i) \text{ satisfy (10), (5), (2), and (1c).} \tag{12}$$

Problem (12) is an optimization problem in the variables $z = (y^\ell,u,y,\psi_i,\lambda_i)$. For the optimal solution $(y^{\ell,*},u^*,y^*,\psi_i^*,\lambda_i^*)$ problem (12) has the property that the associated POD reduced system is computed from the trajectory corresponding to the optimal solution to (1). It is clear that (12) is more complicated than the original problem which e.g. has the effect that the optimality system for (12) involves two adjoint equations, see [34]. The adjoint equation for (10) is the common one. It contains the linearization of the cost J with respect to the state

variable y^ℓ as forcing function. The second adjoint equation results from (2) and contains as forcing term information the linear approximation of $\mathcal{R}$. The gradient of the reduced functional $u \mapsto J(y^\ell(u), u))$ can be expressed in terms of the solutions to these two adjoints. This can be utilized for practical realizations of (12). It suggests a splitting of the variables z into $z_1 = (y^\ell, u)$ and $z_2 = (y, \psi_i, \lambda_i)$. Minimizing $J(y^\ell, u)$ with respect to the former for fixed z_2 results in the common POD-optimization problem for which first order, gradient based, or second order methods can be used. Minimization with respect to the second set of variables requires one additional forward and one adjoint sweep of the full system if gradient information is used. Thus, for practical realization of (12) a splitting scheme is suggested, where minimization with respect to the z_1 is done more accurately than with respect to z_2. The benefit for this extra work is that the POD basis is updated in the direction of the minimum of J. This proposed methodology is supported and illustrated by several numerical examples.

3.4 A-posteriori POD error estimates for linear-quadratic control problems

In contrast to methods of balanced truncation type, the POD method is somehow lacking a reliable a-priori error analysis. In [24] the authors derive a-priori estimates for linear-quadratic optimal control problems, but the POD basis is computed utilizing the (exact) optimal solution to (1). In practice, this optimal solution is not known a-priori. Thus, unless its snapshots are generating a sufficiently rich state space, it is not clear how far the optimal solution of the POD problem deviates from the exact one.

In [52], the main focus is on an a-posteriori analysis for the POD method applied to optimal control problems for linear elliptic and parabolic partial differential equations. A perturbation method estimates how far the suboptimal control, computed by the POD method, is from the (unknown) exact one. More precisely, we consider linear-quadratic problems, e.g. of the type (1) with $f(t, \mathbf{x}, v) = 3y(t, \mathbf{x})^2 v - g(t, \mathbf{x})$, where $y \in C(\overline{Q})$ and $g \in L^\infty(Q)$ are given. Note that a term $3y^2 v$ remains if we compute the linearization of (1b) with respect to y. Let $u^* = (u_1^*, \dots, u_4^*)$ be the exact optimal control and $u^{\ell,*} = (u_1^{\ell,*}, \dots, u_4^{\ell,*})$ the suboptimal control obtained by a POD Galerkin approximation with ℓ POD ansatz functions. Then,

$$\begin{aligned} \|u^* - u^{\ell,*}\|^2_{L^2(0,T;\mathbb{R}^4)} &= \int_0^T \sum_{i=1}^4 \left|u_i^*(t) - u_i^{\ell,*}(t)\right|^2 \mathrm{d}t \\ &\leq \frac{1}{\kappa^2} \int_0^T \sum_{i=1}^4 \left|\zeta_i^\ell(t)\right|^2 \mathrm{d}t = \frac{1}{\kappa^2} \|\zeta^\ell\|^2_{L^2(0,T;\mathbb{R}^4)}, \end{aligned} \tag{13}$$

where $\zeta^\ell = (\zeta_1^\ell, \dots, \zeta_4^\ell)$ is a an element that measures the violation of the optimality system for the full model by the suboptimal control $u^{\ell,*}$. For the computation of the variable ζ^ℓ only the suboptimal control $u^{\ell,*}$ is needed but no information on the unknown exact optimal control u^*. With the function ζ^ℓ, the POD-control $u^{\ell,*}$ solves an optimal control problem with linear perturbation ζ^ℓ in the objective functional,

$$\min \frac{1}{2} \int_0^T \int_\Omega |y(t, \mathbf{x}) - y_d(t, \mathbf{x})|^2 \, \mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^T \frac{\kappa}{2} \sum_{i=1}^4 \left(|u_i(t)|^2 + \zeta_i^\ell(t) u_i(t)\right) \mathrm{d}t$$

subject to (1b) and (1c). It is easy to deduce the estimate of the type (13). Notice that the a-posteriori error analysis is not restricted to the POD method. Especially, we can use this

approach also for the RB method. We refer to [51], where this a-posteriori error analysis is successfully applied to a linear-quadratic elliptic optimal control problem. Moreover, in [29] this technique is used for a bilinear elliptic optimal control problem. The authors apply an inexact SQP method, where the linear-quadratic optimal control problems at each level of the optimization method are solved inexactly by a POD Galerkin approximation. The inexactness is controlled by the a-posteriori error estimator. The authors prove local convergence of the iterates to the solution of the non-linear optimal control problem. Thus, the convergence of the iterates — computed by the POD suboptimal control approach — to the solution of a nonlinear optimal control problem (due to the bilinear elliptic equation) is guaranteed.

Example 3.1 We demonstrate the efficiency of the POD a-posteriori error estimator for the nonlinear optimal control problem (1). The parameters for (1a) are chosen as in Example 2.4. For the cost we choose $y_d(t,\mathbf{x}) = b_1(\mathbf{x}) - b_3(\mathbf{x})$ for $(t,\mathbf{x}) \in Q$ and $\kappa = 0.001$ and we neglect the box constraints on the control. Then we apply the sequential quadratic programming (SQP) method in an infinite-dimensional framework (see, e.g., [22]) to solve (1). In each level of this optimization method a linear-quadratic subproblem has to be solved. Here, we apply a POD Galerkin projection and determine the number ℓ of POD basis functions in such a way that the POD solution to the linear-quadratic subproblem — using ℓ basis functions for the Galerkin projection — is sufficiently close the the (unknown) exact solution so that local superlinear or quadratic rate of convergence is ensured. For more details of this approach we refer to [29], where an optimal control problem governed by a bilinear elliptic equation is solved. The starting values for the SQP method are chosen as follows: the state y^0 is the solution to (1b) for $u_i(t) = 0$, $t \in [0,T]$, $1 \le i \le 4$, the control $u^0 = (u_1^0, \ldots, u_4^0)$ is chosen to be zero, and the dual variables are also set to zero. We stop the SQP method when the first-order necessary optimality condition is satisfied with a tolerance $\mathrm{tol} = 5 \cdot 10^{-5}$. The inexact SQP method stops after 8 iterations and the required CPU time is 26 seconds. The results are shown in Table 1.

Table 1 Example 3.1: Number ℓ of used POD basis functions, norm of the a-posteriori error estimator ζ^ℓ, first-order optimality residuum res^k and stopping tolerance ensuring superlinear convergence ε^k for each SQP iteration k.

SQP iteration	ℓ	$\|\zeta^\ell\|_{L^2(0,T;\mathbb{R}^4)}/\kappa$	res^k	ε^k
1	20	7.47e-04	5.42e-00	1.08e-03
2	30	4.09e-04	3.65e-00	1.08e-03
3	20	3.83e-05	7.51e-01	9.01e-04
4	30	8.40e-05	1.56e-01	1.88e-04
5	20	1.27e-08	1.39e-03	1.93e-05
6	20	4.88e-06	1.39e-03	1.67e-06
7	30	1.22e-07	4.49e-05	5.39e-08
8	20	6.35e-12	2.40e-06	2.88e-09

Note that $\|\zeta^\ell\|_{L^2(0,T;\mathbb{R}^4)}/\kappa \le \varepsilon^k$ for each SQP iteration. In Figure 2 (right plot) the optimal controls are plotted. We compare the result with the inexact SQP method using a standard finite-difference (FD) scheme for the discretization of the spatial variable and the implicit Euler for the time integration. This FD variant stops after 5 iterations and 91 seconds. The numerical FD solution is denoted by $(y^{h,*}, u^{h,*})$. For the relative error we obtained for

the state and control variables

$$\frac{\|y^{h,*} - y^{\ell,*}\|_{L^2(Q)}}{\|y^{h,*}\|_{L^2(Q)}} \approx 7 \cdot 10^{-6} \quad \text{and} \quad \frac{\|u^{h,*} - u^{\ell,*}\|_{L^2(0,T;\mathbb{R}^4)}}{\|u^{h,*}\|_{L^2(0,T;\mathbb{R}^4)}} \approx 9 \cdot 10^{-12},$$

respectively. Thus, the POS based solutions nearly coincide with the solutions computed by the high-dimensional FD discretization method. $\Diamond$

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