Proper Orthogonal Decomposition Surrogate Models for Nonlinear Dynamical Systems: Error Estimates and Suboptimal Control

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1 Motivation

Optimal control problems for nonlinear partial differential equations are often hard to tackle numerically so that the need for developing novel techniques emerges. One such technique is given by reduced order methods. Recently the application of reduced-order models to optimal control problems for partial differential equations 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 elements of the subspaces are uncorrelated to the physical properties of the system that they approximate. The reduced basis method as developed, e.g., in [IR98] is one such reduced-order method with the basis elements corresponding to the dynamics of expected control regimes.

Proper orthogonal decomposition (POD) provides a method for deriving low order models of dynamical systems. It was successfully used in a variety of fields including signal analysis and pattern recognition (see [Fuk90]), fluid dynamics and coherent structures (see [AHLS88, HLB96, NAMTT03, RF94, Sir87]) and more recently in control theory (see [AH01, AFS00, LT01, SK98, TGP99]) and inverse problems (see [BJWW00]). Moreover, in [ABK01] POD was successfully utilized to compute reduced-order controllers. The relationship between POD and balancing was considered in [LMG, Row04, WP01]. Error analysis for nonlinear dynamical systems in finite dimensions were carried out in [RP02].

In our application we apply POD to derive a Galerkin approximation in the spatial variable, with basis functions corresponding to the solution of the physical system at pre-specified time instances. These are called the snapshots. Due to possible linear dependence or almost linear dependence, the snapshots themselves are not appropriate as a basis. Rather a singular value decomposition (SVD) is carried out and the leading generalized eigenfunctions are chosen as a basis, referred to as the POD basis.

The paper is organized as follows. In Section 2 the POD method and its relation to SVD is described. Furthermore, the snapshot form of POD for abstract parabolic equations is illustrated. Section 3 deals with reduced order modeling of nonlinear dynamical systems. Among other things, error estimates for reduced order models of a general equation in fluid mechanics obtained by the snapshot POD method are presented. Section 4 deals with suboptimal control strategies based on POD. For optimal open-loop control problems an adaptive optimization algorithm is presented which in every iteration uses a surrogate model obtained by the POD method instead of the full dynamics. In particular, in Section 4.2 first steps towards error estimation for optimal control problems are presented whose discretization is based on POD. The practical behavior of the proposed adaptive optimization algorithm is illustrated for two applications involving the time-dependent Navier-Stokes system in Section 5. For closed-loop control we refer the reader to [Gom02, KV99, KVX04, LV03], for instance. Finally, we draw some conclusions and discuss future research perspectives in Section 6.

2 The POD method

In this section we propose the POD method and its numerical realization. In particular, we consider both POD in $\mathbb{C}^n$ (finite-dimensional case) and POD in Hilbert spaces; see Sections 2.1 and 2.2, respectively. For more details we refer to, e.g., [HLB96, KV99, Vol01a].

2.1 Finite-dimensional POD

In this subsection we concentrate on POD in the finite dimensional setting and emphasize the close connection between POD and the singular value decomposition (SVD) of rectangular matrices; see [KV99]. Furthermore, the numerical realization of POD is explained.

POD and SVD

Let Y be a possibly complex valued $n \times m$ matrix of rank d. In the context of POD it will be useful to think of the columns $\{Y_{\cdot,j}\}_{j=1}^m$ of Y as the spatial coordinate vector of a dynamical system at time t_j. Similarly we consider the rows $\{Y_{i,\cdot}\}_{i=1}^n$ of Y as the time-trajectories of the dynamical system evaluated at the locations x_i.

From SVD (see, e.g., [Nob69]) the existence of real numbers $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_d > 0$ and unitary matrices $U \in \mathbb{C}^{n \times n}$ with columns $\{u_i\}_{i=1}^n$ and $V \in \mathbb{C}^{m \times m}$ with columns $\{v_i\}_{i=1}^m$ such that

$$U^H Y V = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} =: \Sigma \in \mathbb{C}^{n\times m}, \tag{1}$$

where $D = \mathrm{diag}\,(\sigma_1, \ldots, \sigma_d) \in \mathbb{R}^{d\times d}$, the zeros in (1) denote matrices of appropriate dimensions, and the superindex H stands for complex conjugation. Moreover, the vectors $\{u_i\}_{i=1}^d$ and $\{v_i\}_{i=1}^d$ satisfy

$$Y v_i = \sigma_i u_i \quad \text{and} \quad Y^H u_i = \sigma_i v_i \quad \text{for } i = 1, \ldots, d. \tag{2}$$

They are eigenvectors of YY^H and $Y^H Y$ with eigenvalues σ_i^2, $i = 1, \ldots, d$. The vectors $\{u_i\}_{i=d+1}^m$ and $\{v_i\}_{i=d+1}^m$ (if $d < n$ respectively $d < m$) are eigenvectors of YY^H and $Y^H Y$, respectively, with eigenvalue 0. If $Y \in \mathbb{R}^{n\times m}$ then U and V can be chosen to be real-valued.

From (2) we deduce that $Y = U\Sigma V^H$. It follows that Y can also be expressed as

$$Y = U^d D (V^d)^H, \tag{3}$$

where $U^d \in \mathbb{C}^{n\times d}$ and $V^d \in \mathbb{C}^{m\times d}$ are given by

$$\begin{aligned} U^d_{i,j} &= U_{i,j} \quad \text{for } 1 \le i \le n, 1 \le j \le d, \\ V^d_{i,j} &= V_{i,j} \quad \text{for } 1 \le i \le m, 1 \le j \le d. \end{aligned}$$

It will be convenient to express (3) as

$$Y = U^d B \quad \text{with } B = D(V^d)^H \in \mathbb{C}^{d\times m}.$$

Thus the column space of Y can be represented in terms of the d linearly independent columns of U^d. The coefficients in the expansion for the columns $Y_{\cdot,j}$, $j = 1, \ldots, m$, in the basis $\{U^d_{\cdot,i}\}_{i=1}^d$ are given by the $B_{\cdot,j}$. Since U is Hermitian we easily find that

$$Y_{\cdot,j} = \sum_{i=1}^d B_{i,j} U^d_{\cdot,i} = \sum_{i=1}^d \langle U_{\cdot,i}, Y_{\cdot,j} \rangle_{\mathbb{C}^n} U^d_{\cdot,i},$$

where $\langle \cdot\,, \cdot \rangle_{\mathbb{C}^n}$ denotes the canonical inner product in $\mathbb{C}^n$. In terms of the columns y_j of Y we express the last equality as

$$y_j = \sum_{i=1}^d B_{i,j} u_i = \sum_{i=1}^d \langle u_i, y_j \rangle_{\mathbb{C}^n} u_i, \quad j = 1, \ldots, m.$$

Let us now interpret singular value decomposition in terms of POD. One of the central issues of POD is the reduction of data expressing their "essential information" by means of a few basis vectors. The problem of approximating all spatial coordinate vectors y_j of Y simultaneously by a single, normalized vector as well as possible can be expressed as

$$\max \sum_{j=1}^{m} \left|\langle y_j, u\rangle_{\mathbb{C}^n}\right|^2 \text{ subject to (s.t.) } |u|_{\mathbb{C}^n} = 1. \tag{P}$$

Here, $|\cdot|_{\mathbb{C}^n}$ denotes the Euclidean norm in $\mathbb{C}^n$. Utilizing a Lagrangian framework a necessary optimality condition for (P) is given by the eigenvalue problem

$$YY^H u = \sigma^2 u. \tag{4}$$

Due to singular value analysis u_1 solves (P) and argmax (P) $= \sigma_1^2$. If we were to determine a second vector, orthogonal to u_1 that again describes the data set $\{y_i\}_{i=1}^m$ as well as possible then we need to solve

$$\max \sum_{j=1}^{m} \left|\langle y_j, u\rangle_{\mathbb{C}^n}\right|^2 \quad \text{s.t.} \quad |u|_{\mathbb{C}^n} = 1 \text{ and } \langle u, u_1\rangle_{\mathbb{C}^n} = 0. \tag{P$_2$}$$

Rayleigh's principle and singular value decomposition imply that u_2 is a solution to (P$_2$) and argmax (P$_2$) $= \sigma_2^2$. Clearly this procedure can be continued by finite induction so that u_k, $1 \le k \le d$, solves

$$\max \sum_{j=1}^{m} \left|\langle y_j, u\rangle_{\mathbb{C}^n}\right|^2 \quad \text{s.t.} \quad |u|_{\mathbb{C}^n} = 1 \text{ and } \langle u, u_i\rangle_{\mathbb{C}^n} = 0,\ 1 \le i \le k-1. \tag{P$_k$}$$

The following result which states that for every $\ell \le k$ the approximation of the columns of Y by the first ℓ singular vectors $\{u_i\}_{i=1}^{\ell}$ is optimal in the mean among all rank ℓ approximations to the columns of Y is now quite natural. More precisely, let $\hat{U} \in \mathbb{C}^{n\times d}$ denote a matrix with pairwise orthonormal vectors $\hat{u}_i$ and let the expansion of the columns of Y in the basis $\{\hat{u}_i\}_{i=1}^d$ be given by

$$Y = \hat{U}\hat{B}, \text{ where } \hat{B}_{i,j} = \langle \hat{u}_i, y_j\rangle_{\mathbb{C}^n} \quad \text{for } 1 \le i \le d, 1 \le j \le m.$$

Then for every $\ell \le k$ we have

$$\|Y - \hat{U}^\ell \hat{B}^\ell\|_F \ge \|Y - U^\ell B^\ell\|_F. \tag{5}$$

Here, $\|\cdot\|_F$ denotes the Frobenius norm, U^ℓ denotes the first ℓ columns of U, B^ℓ the first ℓ rows of B and similarly for $\hat{U}^\ell$ and $\hat{B}^\ell$. Note that the j-th column of $U^\ell B^\ell$ represents the Fourier expansion of order ℓ of the j-th column y_j of Y in the orthonormal basis $\{u_i\}_{i=1}^{\ell}$. Utilizing the fact that $\hat{U}\hat{B}^\ell$ has rank ℓ and recalling that $B^\ell = (D(V^k)^H)^\ell$ estimate (5) follows directly from singular value analysis [Nob69]. We refer to U^ℓ as the POD-basis of rank ℓ. Then we have

$$\sum_{i=\ell+1}^{d} \sigma_i^2 = \sum_{i=\ell+1}^{d} \left(\sum_{j=1}^{m} |B_{i,j}|^2\right) \le \sum_{i=\ell+1}^{d} \left(\sum_{j=1}^{m} |\hat{B}_{i,j}|^2\right). \tag{6}$$

and

$$\sum_{i=1}^{\ell} \sigma_i^2 = \sum_{i=1}^{\ell} \left(\sum_{j=1}^{m} |B_{i,j}|^2 \right) \geq \sum_{i=1}^{\ell} \left(\sum_{j=1}^{m} |\hat{B}_{i,j}|^2 \right). \tag{7}$$

Inequalities (6) and (7) establish that for every $1 \leq \ell \leq d$ the POD-basis of rank ℓ is optimal in the sense of representing in the mean the columns of Y as a linear combination by a basis of rank ℓ. Adopting the interpretation of the $Y_{i,j}$ as the velocity of a fluid at location x_i and at time t_j, inequality (7) expresses the fact that the first ℓ POD-basis functions capture more energy on average than the first ℓ functions of any other basis.

The POD-expansion Y^ℓ of rank ℓ is given by

$$Y^\ell = U^\ell B^\ell = U^\ell \left(D (V^d)^H \right)^\ell ,$$

and hence the "t-average" of the coefficients satisfies

$$\langle B^\ell_{i,\cdot}, B^\ell_{j,\cdot} \rangle_{\mathbb{C}^m} = \sigma_i^2 \delta_{ij} \quad \text{for } 1 \leq i, j \leq \ell.$$

This property is referred to as the fact that the POD-coefficients are uncorrelated.

Computational issues

Concerning the practical computation of a POD-basis of rank ℓ let us note that if $m < n$ then one can choose to determine m eigenvectors v_i corresponding to the largest eigenvalues of $Y^H Y \in \mathbb{C}^{m \times m}$ and by (2) determine the POD-basis from

$$u_i = \frac{1}{\sigma_i} Y v_i, \quad i = 1, \dots, \ell. \tag{8}$$

Note that the square matrix $Y^H Y$ has the dimension of number of "time-instances" t_j. For historical reasons [Sir87] this method of determine the POD-basis is sometimes called the method of snapshots.

For the application of POD to concrete problems the choice of ℓ is certainly of central importance, as is also the number and location of snapshots. It appears that no general a-priori rules are available. Rather the choice of ℓ is based on heuristic considerations combined with observing the ratio of the modeled to the total information content contained in the system Y, which is expressed by

$$\mathcal{E}(\ell) = \frac{\sum_{i=1}^{\ell} \sigma_i^2}{\sum_{i=1}^{d} \sigma_i^2} \quad \text{for } \ell \in \{1, \dots, d\}. \tag{9}$$

For a further discussion, also of adaptive strategies based e.g. on this term we refer to [MM03] and the literature cited there.

Application to discrete solutions to dynamical systems

Let us now assume that $Y \in \mathbb{R}^{n\times m}$, $n \geq m$, arises from discretization of a dynamical system, where a finite element approach has been utilized to discretize the state variable $y = y(x,t)$, i.e.,

$$y_h(x,t_j) = \sum_{i=1}^{n} Y_{i,j}\varphi_i(x) \quad \text{for } x \in \Omega,$$

with φ_i, $1 \leq i \leq n$, denoting the finite element functions and Ω being a bounded domain in $\mathbb{R}^2$ or $\mathbb{R}^3$. The goal is to describe the ensemble $\{y_h(\cdot\,,t_j)\}_{j=1}^m$ of L^2-functions simultaneously by a single normalized L^2-function ψ as well as possible:

$$\max \sum_{j=1}^{m} \left|\langle y_h(\cdot,t_j),\psi\rangle_{L^2(\Omega)}\right|^2 \quad \text{s.t.} \quad \|\psi\|_{L^2(\Omega)} = 1, \tag{$\tilde{\mathsf{P}}$}$$

where $\langle\cdot\,,\cdot\rangle_{L^2(\Omega)}$ is the canonical inner product in $L^2(\Omega)$. Since $y_h(\cdot\,,t_j) \in \operatorname{span}\{\varphi_1,\dots,\varphi_n\}$ holds for $1 \leq j \leq n$, we have $\psi \in \operatorname{span}\{\varphi_1,\dots,\varphi_n\}$. Let v be the vector containing the components v_i such that

$$\psi(x) = \sum_{i=1}^{n} v_i\varphi_i(x)$$

and let $S \in \mathbb{R}^{n\times n}$ denote the positive definite mass matrix with the elements $\langle\varphi_i,\varphi_j\rangle_{L^2(\Omega)}$. Instead of (4) we obtain that

$$YY^TSv = \sigma^2 v. \tag{10}$$

The eigenvalue problem (10) can be solved by utilizing singular value analysis. Multiplying (10) by the positive square root $S^{1/2}$ of S from the left and setting $u = S^{1/2}v$ we obtain the $n\times n$ eigenvalue problem

$$\tilde{Y}\tilde{Y}^Tu = \sigma^2 u, \tag{11}$$

where $\tilde{Y} = S^{1/2}Y \in \mathbb{R}^{n\times m}$. We mention that (11) coincides with (4) when $\{\varphi_i\}_{i=1}^n$ is an orthonormal set in $L^2(\Omega)$. Note that if Y has rank k the matrix $\tilde{Y}$ has also rank d. Applying the singular value decomposition to the rectangular matrix $\tilde{Y}$ we have

$$\tilde{Y} = U\Sigma V^T$$

(see (1)). Analogous to (3) it follows that

$$\tilde{Y} = U^dD(V^d)^T, \tag{12}$$

where again U^d and V^d contain the first k columns of the matrices U and V, respectively. Using (12) we determine the coefficient matrix $\Psi = S^{-1/2}U^d \in \mathbb{R}^{n\times d}$, so that the first k POD-basis functions are given by

$$\psi_j(x) = \sum_{i=1}^{n} \Psi_{i,j}\varphi_i(x), \quad j = 1, \ldots, d.$$

Due to (11) and $\Psi_{\cdot,j} = S^{-1/2}U^d_{\cdot,j}$, $1 \le j \le d$, the vectors $\Psi_{\cdot,j}$ are eigenvectors of problem (10) with corresponding eigenvalues σ_j^2:

$$YY^TS\Psi_{\cdot,j} = YY^TSS^{-1/2}U^k_{\cdot,j} = S^{-1/2}\tilde{Y}\tilde{Y}^TU^k_{\cdot,j} = \sigma_j^2S^{-1/2}U^k_{\cdot,j} = \sigma_j^2\Psi_{\cdot,j}.$$

Therefore, the function ψ_1 solves $(\tilde{\mathsf{P}})$ with argmax $(\tilde{\mathsf{P}}) = \sigma_1^2$ and, by finite induction, the function ψ_k, $k \in \{2, \ldots, d\}$, solves

$$\max \sum_{j=1}^{m} \left|\langle y_h(\cdot,t_j), \psi\rangle_{L^2(\Omega)}\right|^2 \text{ s.t. } \|\psi\|_{L^2(\Omega)} = 1,\ \langle \psi, \psi_i\rangle_{L^2(\Omega)} = 0, i < d, \quad (\tilde{\mathsf{P}}_k)$$

with argmax $(\tilde{\mathsf{P}}_k) = \sigma_k^2$. Since we have $\Psi_{\cdot,j} = S^{-1/2}U^d_{\cdot,j}$, the functions $\psi_1, \ldots, \psi_d$ are orthonormal with respect to the L^2-inner product:

$$\langle \psi_i, \psi_j\rangle_{L^2(\Omega)} = \langle \Psi_{\cdot,i}, S\Psi_{\cdot,j}\rangle_{\mathbb{C}^n} = \langle u_i, u_j\rangle_{\mathbb{C}^n} = \delta_{ij}, \quad 1 \le i,j \le d.$$

Note that the coefficient matrix Ψ can also be computed by using generalized singular value analysis. If we multiply (10) with S from the left we obtain the generalized eigenvalue problem

$$SYY^TSu = \sigma^2Su.$$

From generalized SVD [GL89] there exist orthogonal $V \in \mathbb{R}^{m\times m}$ and $U \in \mathbb{R}^{n\times n}$ and an invertible $R \in \mathbb{R}^{n\times n}$ such that

$$V(Y^TS)R = \begin{pmatrix} E & 0 \\ 0 & 0 \end{pmatrix} =: \Sigma_1 \in \mathbb{R}^{m\times n}, \tag{13a}$$

$$US^{1/2}R = \Sigma_2 \in \mathbb{R}^{n\times n}, \tag{13b}$$

where $E = \operatorname{diag}(e_1, \ldots, e_d)$ with $e_i > 0$ and $\Sigma_2 = \operatorname{diag}(s_1, \ldots, s_n)$ with $s_i > 0$. From (13b) we infer that

$$R = S^{-1/2}U^T\Sigma_2. \tag{14}$$

Inserting (14) into (13a) we obtain that

$$\Sigma_2^{-1}\Sigma_1^T = \Sigma_2^{-1}R^TSYV^T = US^{1/2}YV^T,$$

which is the singular value decomposition of the matrix $S^{1/2}Y$ with $\sigma_i = e_i/s_i > 0$ for $i = 1, \ldots, d$. Hence, Ψ is again equal to the first k columns of $S^{1/2}U$.

If $m \le n$ we proceed to determine the matrix Ψ as follows. From $u_j = (1/\sigma_j)\,S^{1/2}Yv_j$ for $1 \le j \le d$ we infer that

$$\Psi_{\cdot,j} = \frac{1}{\sigma_j} Y v_j,$$

where v_j solves the $m \times m$ eigenvalue problem

$$Y^T S Y v_j = \sigma_i^2 v_j, \quad 1 \le j \le d.$$

Note that the elements of the matrix $Y^T SY$ are given by the integrals

$$\langle y(\cdot, t_i), y(\cdot, t_j)\rangle_{L^2(\Omega)}, \quad 1 \le i, j \le n, \tag{15}$$

so that the matrix $Y^T SY$ is often called a *correlation matrix*.

2.2 POD for parabolic systems

Whereas in the last subsection POD has been motivated by rectangular matrices and SVD, we concentrate on POD for dynamical (non-linear) systems in this subsection.

Abstract nonlinear dynamical system

Let V and H be real separable Hilbert spaces and suppose that V is dense in H with compact embedding. By $\langle \cdot\,, \cdot\rangle_H$ we denote the inner product in H. The inner product in V is given by a symmetric bounded, coercive, bilinear form $a : V \times V \to \mathbb{R}$:

$$\langle \varphi, \psi\rangle_V = a(\varphi, \psi) \quad \text{for all } \varphi, \psi \in V \tag{16}$$

with associated norm given by $\|\cdot\|_V = \sqrt{a(\cdot\,,\cdot)}$. Since V is continuously injected into H, there exists a constant $c_V > 0$ such that

$$\|\varphi\|_H \le c_V \, \|\varphi\|_V \quad \text{for all } \varphi \in V. \tag{17}$$

We associate with a the linear operator A:

$$\langle A\varphi, \psi\rangle_{V',V} = a(\varphi, \psi) \quad \text{for all } \varphi, \psi \in V,$$

where $\langle \cdot\,, \cdot\rangle_{V',V}$ denotes the duality pairing between V and its dual. Then, by the Lax-Milgram lemma, A is an isomorphism from V onto V'. Alternatively, A can be considered as a linear unbounded self-adjoint operator in H with domain

$$D(A) = \{\varphi \in V : A\varphi \in H\}.$$

By identifying H and its dual H' it follows that

$$D(A) \hookrightarrow V \hookrightarrow H = H' \hookrightarrow V',$$

each embedding being continuous and dense, when $D(A)$ is endowed with the graph norm of A.

Moreover, let $F : V \times V \to V'$ be a bilinear continuous operator mapping $D(A) \times D(A)$ into H. To simplify the notation we set $F(\varphi) = F(\varphi, \varphi)$ for $\varphi \in V$. For given $f \in C([0,T]; H)$ and $y_0 \in V$ we consider the nonlinear evolution problem

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle y(t), \varphi \rangle_H + a(y(t), \varphi) + \langle F(y(t)), \varphi \rangle_{V',V} = \langle f(t), \varphi \rangle_H \tag{18a}$$

for all $\varphi \in V$ and $t \in (0,T]$ a.e. and

$$y(0) = y_0 \quad \text{in } H. \tag{18b}$$

Assumption (A1). *For every $f \in C([0,T]; H)$ and $y_0 \in V$ there exists a unique solution of* (18) *satisfying*

$$y \in C([0,T]; V) \cap L^2(0,T; D(A)) \cap H^1(0,T; H). \tag{19}$$

Computation of the POD basis

Throughout we assume that Assumption **(A1)** holds and we denote by y the unique solution to (18) satisfying (19). For given $n \in \mathbb{N}$ let

$$0 = t_0 < t_1 < \ldots < t_n \le T \tag{20}$$

denote a grid in the interval $[0,T]$ and set $\delta t_j = t_j - t_{j-1}$, $j = 1, \ldots, n$. Define

$$\Delta t = \max\ (\delta t_1, \ldots, \delta t_n) \quad \text{and} \quad \delta t = \min\ (\delta t_1, \ldots, \delta t_n). \tag{21}$$

Suppose that the *snapshots* $y(t_j)$ of (18) at the given time instances t_j, $j = 0, \ldots, n$, are known. We set

$$\mathcal{V} = \operatorname{span}\{y_0, \ldots, y_{2n}\},$$

where $y_j = y(t_j)$ for $j = 0, \ldots, n$, $y_j = \overline{\partial}_t y(t_{j-n})$ for $j = n+1, \ldots, 2n$ with $\overline{\partial}_t y(t_j) = (y(t_j) - y(t_{j-1}))/\delta t_j$, and refer to $\mathcal{V}$ as the ensemble consisting of the snapshots $\{y_j\}_{j=0}^{2n}$, at least one of which is assumed to be nonzero. Furthermore, we call $\{t_j\}_{j=0}^{n}$ the snapshot grid. Notice that $\mathcal{V} \subset V$ by construction. Throughout the remainder of this section we let X denote either the space V or H.

*Remark 1 (*compare [KV01, Remark 1]). It may come as a surprise at first that the finite difference quotients $\overline{\partial}_t y(t_j)$ are included into the set $\mathcal{V}$ of snapshots. To motivate this choice let us point out that while the finite difference quotients are contained in the span of $\{y_j\}_{j=0}^{2n}$, the POD bases differ depending on whether $\{\overline{\partial}_t y(t_j)\}_{j=1}^{n}$ are included or not. The linear dependence does not constitute a difficulty for the singular value decomposition which is required to compute the POD basis. In fact, the snapshots themselves can be linearly dependent. The resulting POD basis is, in any case, maximally linearly independent in the sense expressed in ($\mathbf{P}_\ell$) and Proposition 1. Secondly, in anticipation of the rate of convergence results that will be presented in Section 3.3 we note that the time derivative of y in (18) must be approximated by the Galerkin POD based scheme. In case the terms $\{\overline{\partial}_t y(t_j)\}_{j=1}^n$ are included in the snapshot ensemble, we are able to utilize the estimate

$$\sum_{j=1}^n \alpha_j \left\| \overline{\partial}_t y(t_j) - \sum_{i=1}^\ell \langle \overline{\partial}_t y(t_j), \psi_i \rangle_X \psi_i \right\|_X^2 \leq \sum_{i=\ell+1}^d \lambda_i. \tag{22}$$

Otherwise, if only the snapshots $y_j = y(t_j)$ for $j = 0, \ldots, n$, are used, we obtain instead of (37) the error formula

$$\sum_{j=0}^n \alpha_j \left\| y(t_j) - \sum_{i=1}^\ell \langle y(t_j), \psi_i \rangle_X \psi_i \right\|_X^2 = \sum_{i=\ell+1}^d \lambda_i,$$

and (22) must be replaced by

$$\sum_{j=1}^n \alpha_j \left\| \overline{\partial}_t y(t_j) - \sum_{i=1}^\ell \langle \overline{\partial}_t y(t_j), \psi_i \rangle_X \psi_i \right\|_X^2 \leq \frac{2}{(\delta t)^2} \sum_{i=\ell+1}^d \lambda_i, \tag{23}$$

which in contrast to (22) contains the factor $(\delta t)^{-2}$ on the right-hand side. In [HV03] this fact was observed numerically. Moreover, in [LV03] it turns out that the inclusion of the difference quotients improves the stability properties of the computed feedback control laws. Let us mention the article [AG03], where the time derivatives were also included in the snapshot ensemble to get a better approximation of the dynamical system. $\diamondsuit$

Let $\{\psi_i\}_{i=1}^d$ denote an orthonormal basis for $\mathcal{V}$ with $d = \dim \mathcal{V}$. Then each member of the ensemble can be expressed as

$$y_j = \sum_{i=1}^d \langle y_j, \psi_i \rangle_X \psi_i \quad \text{for } j = 0, \ldots, 2n. \tag{24}$$

The method of POD consists in choosing an orthonormal basis such that for every $\ell \in \{1, \ldots, d\}$ the mean square error between the elements y_j, $0 \leq j \leq 2n$, and the corresponding ℓ-th partial sum of (24) is minimized on average:

$$\begin{aligned} &\min J(\psi_1, \ldots, \psi_\ell) = \sum_{j=0}^{2n} \alpha_j \left\| y_j - \sum_{i=1}^\ell \langle y_j, \psi_i \rangle_X \psi_i \right\|_X^2 \\ &\text{s.t. } \langle \psi_i, \psi_j \rangle_X = \delta_{ij} \quad \text{for } 1 \leq i \leq \ell, 1 \leq j \leq i. \end{aligned} \tag{$\mathbf{P}_\ell$}$$

Here $\{\alpha_j\}_{j=0}^{2n}$ are positive weights, which for our purposes are chosen to be

$$\alpha_0 = \frac{\delta t_1}{2}, \quad \alpha_j = \frac{\delta t_j + \delta t_{j+1}}{2} \text{ for } j = 1, \ldots, n-1, \quad \alpha_n = \frac{\delta t_n}{2}$$

and $\alpha_j = \alpha_{j-n}$ for $j = n+1, \ldots, 2n$.

Remark 2. 1) Note that

$$\mathcal{I}_n(y) = J(\psi_1, \ldots, \psi_\ell)$$

can be interpreted as a trapezoidal approximation for the integral

$$\mathcal{I}(y) = \int_0^T \Big\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i \rangle_X \psi_i \Big\|_X^2 + \Big\| y_t(t) - \sum_{i=1}^{\ell} \langle y_t(t), \psi_i \rangle_X \psi_i \Big\|_X^2 \, \mathrm{d}t.$$

For all $y \in C^1([0,T]; X)$ it follows that $\lim_{n\to\infty} \mathcal{I}_n(y) = \mathcal{I}(y)$. In Section 4.2 we will address the continuous version of POD (see, in particular, Theorem 4).

2) Notice that $(\mathbf{P}_\ell)$ is equivalent with

$$\max \sum_{i=1}^{\ell} \sum_{j=0}^{2n} \alpha_j \big| \langle y_j, \psi_i \rangle_X \big|^2 \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle_X = \delta_{ij}, \; 1 \le j \le i \le \ell. \quad (25)$$

For $X = \mathbb{C}^n$, $\ell = 1$ and $\alpha_j = 1$ for $1 \le j \le n$ and $\alpha_j = 0$ otherwise, (25) is equivalent with (P). $\Diamond$

A solution $\{\psi_i\}_{i=1}^{\ell}$ to $(\mathbf{P}_\ell)$ is called *POD basis of rank* ℓ. The subspace spanned by the first ℓ POD basis functions is denoted by V^ℓ, i.e.,

$$V^\ell = \operatorname{span}\{\psi_1, \ldots, \psi_\ell\}. \quad (26)$$

The solution of $(\mathbf{P}_\ell)$ is characterized by necessary optimality conditions, which can be written as an eigenvalue problem; compare Section 2.1. For that purpose we endow $\mathbb{R}^{2n+1}$ with the weighted inner product

$$\langle v, w \rangle_\alpha = \sum_{j=0}^{2n} \alpha_j v_j w_j \quad (27)$$

for $v = (v_0, \ldots, v_{2n})^T, w = (w_0, \ldots, w_{2n})^T \in \mathbb{R}^{2n+1}$ and the induced norm.

Remark 3. Due to the choices for the weights α_j's the weighted inner product $\langle \cdot\,, \cdot \rangle_\alpha$ can be interpreted as the trapezoidal approximation for the H^1-inner product

$$\langle v, w \rangle_{H^1(0,T)} = \int_0^T vw + v_t w_t \, \mathrm{d}t \quad \text{for } v, w \in H^1(0,T)$$

so that (27) is a discrete H^1-inner product (compare Section 4.2). $\Diamond$

Let us introduce the bounded linear operator $\mathcal{Y}_n : \mathbb{R}^{2n+1} \to X$ by

$$\mathcal{Y}_n v = \sum_{j=0}^{2n} \alpha_j v_j y_j \quad \text{for } v \in \mathbb{R}^{2n+1}. \tag{28}$$

Then the adjoint $\mathcal{Y}_n^* : X \to \mathbb{R}^{2n+1}$ is given by

$$\mathcal{Y}_n^* z = \big(\langle z, y_0 \rangle_X, \ldots, \langle z, y_{2n} \rangle_X \big)^T \quad \text{for } z \in X. \tag{29}$$

It follows that $\mathcal{R}_n = \mathcal{Y}_n \mathcal{Y}_n^* \in \mathcal{L}(X)$ and $\mathcal{K}_n = \mathcal{Y}_n^* \mathcal{Y}_n \in \mathbb{R}^{(2n+1)\times(2n+1)}$ are given by

$$\mathcal{R}_n z = \sum_{j=0}^{2n} \alpha_j \langle z, y_j \rangle_X y_j \quad \text{for } z \in X \quad \text{and} \quad \big(\mathcal{K}_n\big)_{ij} = \alpha_j \, \langle y_j, y_i \rangle_X \tag{30}$$

respectively. By $\mathcal{L}(X)$ we denote the Banach space of all linear and bounded operators from X into itself and the matrix $\mathcal{K}_n$ is again called a *correlation matrix*; compare (15).

Using a Lagrangian framework we derive the following optimality conditions for the optimization problem $(\mathbf{P}_\ell)$:

$$\mathcal{R}_n \psi = \lambda \psi, \tag{31}$$

compare e.g. [HLB96, pp. 88-91] and [Vol01a, Section 2]. Thus, it turns out that analogous to finite-dimensional POD, we obtain an eigenvalue problem; see (4).

Note that $\mathcal{R}_n$ is a bounded, self-adjoint and nonnegative operator. Moreover, since the image of $\mathcal{R}_n$ has finite dimension, $\mathcal{R}_n$ is also compact. By Hilbert-Schmidt theory (see e.g. [RS80, p. 203]) there exist an orthonormal basis $\{\psi_i\}_{i\in\mathbb{N}}$ for X and a sequence $\{\lambda_i\}_{i\in\mathbb{N}}$ of nonnegative real numbers so that

$$\mathcal{R}_n \psi_i = \lambda_i \psi_i, \quad \lambda_1 \geq \ldots \geq \lambda_d > 0 \quad \text{and } \lambda_i = 0 \quad \text{for} \quad i > d. \tag{32}$$

Moreover, $\mathcal{V} = \operatorname{span}\{\psi_i\}_{i=1}^d$. Note that $\{\lambda_i\}_{i\in\mathbb{N}}$ as well as $\{\psi_i\}_{i\in\mathbb{N}}$ depend on n.

Remark 4. a) Setting $\sigma_i = \sqrt{\lambda_i}$, $i = 1, \ldots, d$, and

$$v_i = \frac{1}{\sigma_i} \, \mathcal{Y}_n^* \psi_i \quad \text{for } i = 1, \ldots, d \tag{33}$$

we find

$$\mathcal{K}_n v_i = \lambda_i v_i \quad \text{and} \quad \langle v_i, v_j \rangle_\alpha = \delta_{ij}, \ 1 \leq i, j \leq d. \tag{34}$$

Thus, $\{v_i\}_{i=1}^d$ is an orthonormal basis of eigenvectors of $\mathcal{K}_n$ for the image of $\mathcal{K}_n$. Conversely, if $\{v_i\}_{i=1}^d$ is a given orthonormal basis for the image of

$\mathcal{K}_n$, then it follows that the first d eigenfunctions of $\mathcal{R}_n$ can be determined by

$$\psi_i = \frac{1}{\sigma_i}\, \mathcal{Y}_n v_i \quad \text{for } i = 1, \ldots, d, \tag{35}$$

see (8). Hence, we can determine the POD basis by solving either the eigenvalue problem for $\mathcal{R}_n$ or the one for $\mathcal{K}_n$. The relationship between the eigenfunctions of $\mathcal{R}_n$ and the eigenvectors for $\mathcal{K}_n$ is given by (33) and (35), which corresponds to SVD for the finite-dimensional POD.

b) Let us introduce the matrices

$$D = \operatorname{diag}(\alpha_0, \ldots, \alpha_{2n}) \in \mathbb{R}^{(2n+1)\times(2n+1)},$$
$$\widetilde{\mathcal{K}}_n = \big((\langle y_j, y_i\rangle_X)\big)_{0\le i,j\le 2n} \in \mathbb{R}^{(2n+1)\times(2n+1)}.$$

Note that the matrix $\widetilde{\mathcal{K}}_n$ is symmetric and positive semi-definite with $\operatorname{rank}\widetilde{\mathcal{K}}_n = d$. Then the eigenvalue problem (34) can be written in matrix-vector-notation as follows:

$$\widetilde{\mathcal{K}}_n D v_i = \lambda_i v_i \quad \text{and} \quad v_i^T D v_j = \delta_{ij},\ 1 \le i, j \le d. \tag{36}$$

Multiplying the first equation in (36) with $D^{1/2}$ from the left and setting $w_i = D^{1/2} v_i$, $1 \le i \le d$, we derive

$$D^{1/2}\widetilde{\mathcal{K}}_n D^{1/2} w_i = \lambda_i w_i \quad \text{and} \quad w_i^T w_j = \delta_{ij},\ 1 \le i, j \le d.$$

where the matrix $\widehat{\mathcal{K}}_n = D^{1/2}\widetilde{\mathcal{K}}_n D^{1/2}$ is symmetric and positive semi-definite with $\operatorname{rank}\widehat{\mathcal{K}}_n = d$. Therefore, it turns out that (34) can be expressed as a symmetric eigenvalue problem. ♢

The sequence $\{\psi_i\}_{i=1}^{\ell}$ solves the optimization problem $(\mathbf{P}_\ell)$. This fact as well as the error formula below were proved in [HLB96, Section 3], for example.

Proposition 1. *Let $\lambda_1 \ge \ldots \ge \lambda_d > 0$ denote the positive eigenvalues of $\mathcal{R}_n$ with the associated eigenvectors $\psi_1, \ldots, \psi_d \in X$. Then, $\{\psi_i^n\}_{i=1}^{\ell}$ is a POD basis of rank $\ell \le d$, and we have the error formula*

$$J(\psi_1, \ldots, \psi_\ell) = \sum_{j=0}^{2n} \alpha_j \left\| y_j - \sum_{i=1}^{\ell} \langle y_j, \psi_i\rangle_X \psi_i \right\|_X^2 = \sum_{i=\ell+1}^{d} \lambda_i. \tag{37}$$

3 Reduced-order modeling for dynamical systems

In the previous section we have described how to compute a POD basis. In this section we focus on the Galerkin projection of dynamical systems utilizing the POD basis functions. We obtain reduced-order models and present error estimates for the POD solution compared to the solution of the dynamical system.

3.1 A general equation in fluid dynamics

In this subsection we specify the abstract nonlinear evolution problem that will be considered in this section and present an existence and uniqueness result, which ensures Assumption **(A1)** introduced in Section 2.2.

We introduce the continuous operator $R : V \to V'$, which maps $D(A)$ into H and satisfies

$$\begin{aligned} \|R\varphi\|_H &\le c_R \, \|\varphi\|_V^{1-\delta_1} \|A\varphi\|_H^{\delta_1} && \text{for all } \varphi \in D(A), \\ |\langle R\varphi, \varphi\rangle_{V',V}| &\le c_R \, \|\varphi\|_V^{1+\delta_2} \|\varphi\|_H^{1-\delta_2} && \text{for all } \varphi \in V \end{aligned}$$

for a constant $c_R > 0$ and for $\delta_1, \delta_2 \in [0, 1)$. We also assume that $A + R$ is coercive on V, i.e., there exists a constant $\eta > 0$ such that

$$a(\varphi, \varphi) + \langle R\varphi, \varphi\rangle_{V',V} \ge \eta \, \|\varphi\|_V^2 \quad \text{for all } \varphi \in V. \tag{38}$$

Moreover, let $B : V \times V \to V'$ be a bilinear continuous operator mapping $D(A) \times D(A)$ into H such that there exist constants $c_B > 0$ and $\delta_3, \delta_4, \delta_5 \in [0, 1)$ satisfying

$$\begin{aligned} \langle B(\varphi, \psi), \psi\rangle_{V',V} &= 0, \\ \left|\langle B(\varphi, \psi), \phi\rangle_{V',V}\right| &\le c_B \, \|\varphi\|_H^{\delta_3} \|\varphi\|_V^{1-\delta_3} \|\psi\|_V \|\phi\|_V^{\delta_3} \|\phi\|_H^{1-\delta_3}, \\ \|B(\varphi, \chi)\|_H + \|B(\chi, \varphi)\|_H &\le c_B \, \|\varphi\|_V \|\chi\|_V^{1-\delta_4} \|A\chi\|_H^{\delta_4}, \\ \|B(\varphi, \chi)\|_H &\le c_B \, \|\varphi\|_H^{\delta_5} \|\varphi\|_V^{1-\delta_5} \|\chi\|_V^{1-\delta_5} \|A\chi\|_H^{\delta_5}, \end{aligned}$$

for all $\varphi, \psi, \phi \in V$, for all $\chi \in D(A)$.

In the context of Section 2.2 we set $F = B + R$. Thus, for given $f \in C(0, T; H)$ and $y_0 \in V$ we consider the nonlinear evolution problem

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle y(t), \varphi\rangle_H + a(y(t), \varphi) + \big\langle F(y(t)), \varphi\big\rangle_{V',V} = \langle f(t), \varphi\rangle_H \tag{39a}$$

for all $\varphi \in V$ and almost all $t \in (0, T]$ and

$$y(0) = y_0 \quad \text{in } H. \tag{39b}$$

The following theorem guarantees **(A1)**.

Theorem 1. *Suppose that the operators R and B satisfy the assumptions stated above. Then, for every $f \in C(0, T; H)$ and $y_0 \in V$ there exists a unique solution of* (39) *satisfying*

$$y \in C([0, T]; V) \cap L^2(0, T; D(A)) \cap H^1(0, T; H). \tag{40}$$

Proof. The proof is analogous to that of Theorem 2.1 in [Tem88, p. 111], where the case with time-independent f was treated. $\square$

Example 1. Let Ω denote a bounded domain in $\mathbb{R}^2$ with boundary Γ and let $T > 0$. The *two-dimensional Navier-Stokes equations* are given by

$$\varrho\,\big(u_t + (u\cdot\nabla)u\big) - \nu\Delta u + \nabla p = f \quad \text{in } Q = (0,T)\times\Omega, \tag{41a}$$

$$\operatorname{div} u = 0 \quad \text{in } Q, \tag{41b}$$

where $\varrho > 0$ is the density of the fluid, $\nu > 0$ is the kinematic viscosity, f represents volume forces and

$$(u\cdot\nabla)u = \Big(u_1\frac{\partial u_1}{\partial x_1} + u_2\frac{\partial u_1}{\partial x_2}, u_1\frac{\partial u_2}{\partial x_1} + u_2\frac{\partial u_2}{\partial x_2}\Big)^T.$$

The unknowns are the velocity field $u = (u_1, u_2)$ and the pressure p. Together with (41) we consider nonslip boundary conditions

$$u = u_d \quad \text{on } \Sigma = (0,T)\times\Gamma \tag{41c}$$

and the initial condition

$$u(0,\cdot) = u_0 \quad \text{in } \Omega. \tag{41d}$$

In [Tem88, pp. 104-107, 116-117] it was proved that (41) can be written in the form (18) and that **(A1)** holds provided the boundary Γ is sufficiently smooth. ◇

3.2 POD Galerkin projection of dynamical systems

Given a snapshot grid $\{t_j\}_{j=0}^n$ and associated snapshots $y_0, \ldots, y_n$ the space V^ℓ is constructed as described in Section 2.2. We obtain the POD-Galerkin surrogate of (39) by replacing the space of test functions V by $V^\ell = \operatorname{span}\{\psi_1, \ldots, \psi_\ell\}$, and by using the ansatz

$$Y(t) = \sum_{i=1}^{\ell} \alpha_i(t)\psi_i \tag{42}$$

for its solution. The result is a ℓ-dimensional nonlinear dynamical system of ordinary differential equations for the functions α_i $(i = 1, \ldots, \ell)$ of the form

$$M\dot\alpha + A\alpha + n(\alpha) = \mathcal{F}, \quad M\alpha(0) = (\langle y_0, \psi_j\rangle_H)_{j=1}^{\ell}, \tag{43}$$

where $M = (\langle\psi_i, \psi_j\rangle_H)_{i,j=1}^{\ell}$ denotes the POD mass matrix, $A = (a(\psi_i, \psi_j))_{i,j=1}^{\ell}$ the POD stiffness matrix, $n(\alpha) = (\langle F(Y), \psi_j\rangle_{V',V})_{j=1}^{\ell}$ the nonlinearity, and $\mathcal{F} = (\langle f, \psi_j\rangle_H)_{j=1}^{\ell}$. We note that M is the identity matrix if in $(\mathbf{P}_\ell)$ $X = H$ is chosen.

For the time discretization we choose $m \in \mathbb{N}$ and introduce the time grid

$$0 = \tau_0 < \tau_1 < \ldots < \tau_m = T, \quad \delta\tau_j = \tau_j - \tau_{j-1} \quad \text{for } j = 1, \ldots, m,$$

and set

$$\delta\tau = \min\{\delta\tau_j : 1 \le j \le m\} \quad \text{and} \quad \Delta\tau = \max\{\delta\tau_j : 1 \le j \le m\}.$$

Notice that the snapshot grid and the time grid usually does not coincide. Throughout we assume that $\Delta\tau/\delta\tau$ is bounded uniformly with respect to m. To relate the snapshot grid $\{t_j\}_{j=0}^n$ and the time grid $\{\tau_j\}_{j=0}^m$ we set for every τ_k, $0 \le k \le m$, an associated index $\bar{k} = \operatorname{argmin}\{|\tau_k - t_j| : 0 \le j \le n\}$ and define $\sigma_n \in \{1, \ldots, n\}$ as the maximum of the occurrence of the same value $t_{\bar{k}}$ as k ranges over $0 \le k \le m$.

The problem consists in finding a sequence $\{Y_k\}_{k=0}^m$ in V^ℓ satisfying

$$\langle Y_0, \psi\rangle_H = \langle y_0, \psi\rangle_H \quad \text{for all } \psi \in V^\ell \tag{44a}$$

and

$$\langle \overline{\partial}_\tau Y_k, \psi\rangle_H + a(Y_k, \psi) + \langle F(Y_k), \psi\rangle_{V',V} = \langle f(\tau_k), \psi\rangle_H \tag{44b}$$

for all $\psi \in V^\ell$ and $k = 1, \ldots, m$, where we have set $\overline{\partial}_\tau Y_k = (Y_k - Y_{k-1})/\delta\tau_k$. Note that (44) is a backward Euler scheme for (39).

For every $k = 1, \ldots, m$ there exists at least one solution Y_k of (44). If $\Delta\tau$ is sufficiently small, the sequence $\{Y_k\}_{k=1}^m$ is uniquely determined. A proof was given in [KV02, Theorem 4.2].

3.3 Error estimates

Our next goal is to present an error estimate for the expression

$$\sum_{k=0}^m \beta_k \, \|Y_k - y(\tau_k)\|_H^2,$$

where $y(\tau_k)$ is the solution of (39) at the time instances $t = \tau_k$, $k = 1, \ldots, m$, and the positive weights β_j are given by

$$\beta_0 = \frac{\delta\tau_1}{2}, \quad \beta_j = \frac{\delta\tau_j + \delta\tau_{j+1}}{2} \text{ for } j = 1, \ldots, m-1, \quad \text{and} \quad \beta_m = \frac{\delta\tau_m}{2}.$$

Let us introduce the orthogonal projection $\mathcal{P}_n^\ell$ of X onto V^ℓ by

$$\mathcal{P}_n^\ell \varphi = \sum_{i=1}^\ell \langle \varphi, \psi_i\rangle_X \psi_i \quad \text{for } \varphi \in X. \tag{45}$$

In the context of finite element discretizations, $\mathcal{P}_n^\ell$ is called the *Ritz projection*.

Estimate for the choice $X = V$

Let us choose $X = V$ in the context of Section 2.2. Since the Hilbert space V is endowed with the inner product (16), the Ritz-projection $\mathcal{P}_n^\ell$ is the orthogonal projection of V on V^ℓ.

We make use of the following assumptions:

(H1) *$y \in W^{2,2}(0,T;V)$, where $W^{2,2}(0,T;V) = \{\varphi \in L^2(0,T;V) \ : \ \varphi_t, \varphi_{tt} \in L^2(0,T;V)\}$ is a Hilbert space endowed with its canonical inner product.*

(H2) *There exists a normed linear space W continuously embedded in V and a constant $c_a > 0$ such that $y \in C([0,T];W)$ and*

$$a(\varphi, \psi) \le c_a \ \|\varphi\|_H \|\psi\|_W \quad \text{for all } \varphi \in V \text{ and } \psi \in W. \tag{46}$$

Example 2. For $V = H_0^1(\Omega)$, $H = L^2(\Omega)$, with Ω a bounded domain in $\mathbb{R}^l$ and

$$a(\varphi, \psi) = \int_\Omega \nabla\varphi \cdot \nabla\psi \, \mathrm{d}x \text{ for all } \varphi, \psi \in H_0^1(\Omega),$$

choosing $W = H^2(\Omega) \cap H_0^1(\Omega)$ implies $a(\varphi, \psi) \le \|\varphi\|_W \|\psi\|_H$ for all $\varphi \in W$, $\psi \in V$, and (46) holds with $c_a = 1$. ◇

Remark 5. In the case $X = V$ we infer from (16) that

$$a(\mathcal{P}_n^\ell \varphi, \psi) = a(\varphi, \psi) \quad \text{for all } \psi \in V^\ell,$$

where $\varphi \in V$. In particular, we have $\|\mathcal{P}_n^\ell\|_{L(V)} = 1$. Moreover, **(H2)** yields

$$\|\mathcal{P}_n^\ell\|_{\mathcal{L}(H)} \le c_P \quad \text{for all } 1 \le \ell \le d$$

where $c_P = c\ell/\lambda_\ell$ (see [KV02, Remark 4.4]) and $c > 0$ depends on y, c_a, and T, but is independent of ℓ and of the eigenvalues λ_i. ◊

The next theorem was proved in [KV02, Theorem 4.7 and Corollary 4.11].

Theorem 2. *Assume that* **(H1)**, **(H2)** *hold and that $\Delta\tau$ is sufficiently small. Then there exists a constant C depending on T, but independent of the grids $\{t_j\}_{j=0}^n$ and $\{\tau_j\}_{j=0}^m$, such that*

$$\begin{aligned} \sum_{k=0}^m \beta_k \ \|Y_k - y(\tau_k)\|_H^2 &\le C\sigma_n \Delta\tau(\Delta\tau + \Delta t)\|y_{tt}\|_{L^2(0,T;V)}^2 \\ &+ C\Big(\sum_{i=\ell+1}^d \Big(\big|\langle \psi_i, y_0\rangle_V\big|^2 + \frac{\sigma_n \Delta\tau}{\delta t}\lambda_i \Big) + \sigma_n \Delta\tau \Delta t \|y_t\|_{L^2(0,T;V)}^2 \Big). \end{aligned} \tag{47}$$

Remark 6. a) If we take the snapshot set

$$\tilde{\mathcal{V}} = \operatorname{span}\{y(t_0), \dots, y(t_n)\}$$

instead of $\mathcal{V}$, we obtain instead of (47) the following estimate:

$$\begin{aligned}
&\sum_{k=0}^{m} \beta_k \, \|Y_k - y(\tau_k)\|_H^2 \\
&\leq C \sum_{i=\ell+1}^{d} \Big(\big|\langle \psi_i, y_0 \rangle_V\big|^2 + \frac{\sigma_n}{\delta t}\Big(\frac{1}{\delta\tau} + \Delta\tau\Big)\lambda_i \Big) + C\sigma_n \Delta\tau\Delta t \, \|y_t\|^2_{L^2(0,T;V)} \\
&\quad + C\sigma_n \Delta\tau(\Delta\tau + \Delta t)\|y_{tt}\|^2_{L^2(0,T;H)}
\end{aligned}$$

(compare [KV02, Theorem 4.7]). As we mentioned in Remark 1 the factor $(\delta t \; \delta\tau)^{-1}$ arises on the right-hand of the estimate. While computations for many concrete situations show that $\sum_{i=\ell+1}^{d} \lambda_i$ is small compared to $\Delta\tau$, the question nevertheless arises whether the term $1/(\delta\tau\delta t)$ can be avoided in the estimates. However, we refer the reader to [HV03, Section 4], where significantly better numerical results were obtained using the snapshot set $\mathcal{V}$ instead of $\tilde{\mathcal{V}}$. We refer also to [LV04], where the computed feedback gain was more stabilizing providing information about the time derivatives was included.

b) If the number of POD elements for the Galerkin scheme coincides with the dimension of $\mathcal{V}$ then the first additive term on the right-hand side disappears. $\Diamond$

Asymptotic estimate

Note that the terms $\{\lambda_i\}_{i=1}^d$, $\{\psi_i\}_{i=1}^d$ and σ_n depend on the time discretization of $[0,T]$ for the snapshots as well as the numerical integration. We address this dependence next. To obtain an estimate that is independent of the spectral values of a specific snapshot set $\{y(t_j)\}_{j=0}^n$ we assume that $y \in W^{2,2}(0,T;V)$, so that in particular **(H1)** holds, and introduce the operator $\mathcal{R} \in \mathcal{L}(V)$ by

$$\mathcal{R}z = \int_0^T \langle z, y(t)\rangle_V y(t) + \langle z, y_t(t)\rangle_V y_t(t) \,\mathrm{d}t \quad \text{for } z \in V. \tag{48}$$

Since $y \in W^{2,2}(0,T;V)$ holds, it follows that $\mathcal{R}$ is compact, see, e.g., [KV02, Section 4]. From the Hilbert-Schmidt theorem it follows that there exists a complete orthonormal basis $\{\psi_i^\infty\}_{i\in\mathbb{N}}$ for X and a sequence $\{\lambda_i^\infty\}_{i\in\mathbb{N}}$ of nonnegative real numbers so that

$$\mathcal{R}\psi_i^\infty = \lambda_i^\infty \psi_i^\infty, \quad \lambda_1^\infty \geq \lambda_2^\infty \geq \ldots, \quad \text{and } \lambda_i^\infty \to 0 \text{ as } i \to \infty.$$

The spectrum of $\mathcal{R}$ is a pure point spectra except for possibly 0. Each non-zero eigenvalue of $\mathcal{R}$ has finite multiplicity and 0 is the only possible accumulation point of the spectrum of $\mathcal{R}$, see [Kat80, p. 185]. Let us note that

$$\int_0^T \|y(t)\|_X^2 \,\mathrm{d}t = \sum_{i=1}^{\infty} \lambda_i \quad \text{and} \quad \|y_\circ\|_X^2 = \sum_{i=1}^{\infty} \big|\langle y_\circ, \psi_i\rangle_X\big|^2.$$

Due to the assumption $y \in W^{2,2}(0,T;V)$ we have

$$\lim_{\Delta t \to 0} \|\mathcal{R}_n - \mathcal{R}\|_{\mathcal{L}(V)} = 0,$$

where the operator $\mathcal{R}_n$ was introduced in (30). The following theorem was proved in [KV02, Corollary 4.12].

Theorem 3. *Let all hypothesis of Theorem* 2 *be satisfied. Let us choose and fix ℓ such that $\lambda_\ell^\infty \neq \lambda_{\ell+1}^\infty$. If $\Delta t = O(\delta\tau)$ and $\Delta\tau = O(\delta t)$ hold, then there exists a constant $C > 0$, independent of ℓ and the grids $\{t_j\}_{j=0}^n$ and $\{\tau_j\}_{j=0}^m$, and a $\overline{\Delta t} > 0$, depending on ℓ, such that*

$$\begin{aligned} \sum_{k=0}^{m} \beta_k \, \|Y_k - y(\tau_k)\|_H^2 &\le C \sum_{i=\ell+1}^{\infty} \Big(\left|\langle y_0, \psi_i^\infty \rangle_V\right|^2 + \lambda_i^\infty \Big) \\ &+ C \Big(\Delta\tau\Delta t \, \|y_t\|^2_{L^2(0,T;V)} + \Delta\tau(\Delta\tau + \Delta t) \, \|y_{tt}\|^2_{L^2(0,T;V)} \Big) \end{aligned} \tag{49}$$

for all $\Delta t \le \overline{\Delta t}$.

Remark 7. In case of $X = H$ the spectral norm of the POD stiffness matrix with the elements $\langle \psi_j, \psi_i \rangle_V$, $1 \le i, j, \le d$, arises on the right-hand side of the estimate (47); see [KV02, Theorem 4.16]. For this reason, no asymptotic analysis can be done for $X = H$. ♢

4 Suboptimal control of evolution problems

In this section we propose a reduced-order approach based on POD for optimal control problems governed by evolution problems. For linear-quadratic optimal control problems we among other things present error estimates for the suboptimal POD solutions.

4.1 The abstract optimal control problem

For $T > 0$ the space $W(0,T)$ is defined as

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

which is a Hilbert space endowed with the common inner product (see, for example, in [DL92, p. 473]). It is well-known that $W(0,T)$ is continuously embedded into $C([0,T];H)$, the space of continuous functions from $[0,T]$ to H, i.e., there exists an embedding constant $c_e > 0$ such that

$$\|\varphi\|_{C([0;T];H)} \le c_e \, \|\varphi\|_{W(0,T)} \quad \text{for all } \varphi \in W(0,T). \tag{50}$$

We consider the abstract problem introduced in Section 2.2. Let $\mathcal{U}$ be a Hilbert space which we identify with its dual $\mathcal{U}'$, and let $\mathcal{U}_{\mathsf{ad}} \subset \mathcal{U}$ a closed and convex subset. For $y_0 \in H$ and $u \in \mathcal{U}_{\mathsf{ad}}$ we consider the nonlinear evolution problem on $[0,T]$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\langle y(t),\varphi\rangle_H + a(y(t),\varphi) + \langle F(y(t)),\varphi\rangle_{V',V} = \langle(\mathcal{B}u)(t)),\varphi\rangle_{V',V} \tag{51a}$$

for all $\varphi \in V$ and

$$y(0) = y_0 \quad \text{in } H, \tag{51b}$$

where $\mathcal{B} : \mathcal{U} \to L^2(0,T;V')$ is a continuous linear operator. We suppose that for every $u \in \mathcal{U}_{\mathsf{ad}}$ and $y_0 \in H$ there exists a unique solution y of (51) in $W(0,T)$. This is satisfied for many practical situations, including, e.g., the controlled viscous Burgers and two-dimensional incompressible Navier-Stokes equations, see, e.g., [Tem88, Vol01b].

Next we introduce the cost functional $J : W(0,T) \times \mathcal{U} \to \mathbb{R}$ by

$$J(y,u) = \frac{\alpha_1}{2}\,\|\mathcal{C}y - z_1\|^2_{W_1} + \frac{\alpha_2}{2}\,\|\mathcal{D}y(T) - z_2\|^2_{W_2} + \frac{\sigma}{2}\|u\|^2_{\mathcal{U}}, \tag{52}$$

where W_1, W_2 are Hilbert spaces and $\mathcal{C} : L^2(0,T;H) \to W_1$ and $\mathcal{D} : H \to W_2$ are bounded linear operators, $z_1 \in W_1$ and $z_2 \in W_2$ are given desired states and $\alpha_1, \alpha_2, \sigma > 0$.

The optimal control problem is given by

$$\min J(y,u) \quad \text{s.t.} \quad (y,u) \in W(0,T) \times \mathcal{U}_{\mathsf{ad}} \text{ solves (51).} \tag{\textbf{CP}}$$

In view of Example 1 a standard discretization (based on, e.g., finite elements) of (**CP**) may lead to a large-scale optimization problem which can not be solved with the currently available computer power. Here we propose a suboptimal solution approach that utilizes POD. The associated suboptimal control problem is obtained by replacing the dynamical system (51) in (**CP**) through the POD surrogate model (43), using the Ansatz (42) for the state. With $\mathcal{F}$ replaced by $(\langle(\mathcal{B}u)(t),\psi_j\rangle_H)_{j=1}^{l}$ it reads

$$\min J(\alpha,u) \quad \text{s.t.} \quad (\alpha,u) \in H^1(0,T)^\ell \times \mathcal{U}_{\mathsf{ad}} \text{ solves (43).} \tag{\textbf{SCP}}$$

At this stage the question arises which snapshots to use for the POD surrogate model, since it is by no means clear that the POD model computed with snapshots related to a control u_1 is also able to resolve the presumably completely different dynamics related to a control $u_2 \neq u_1$. To cope with this difficulty we present the following adaptive pseudo-optimization algorithm which is proposed in [AH00, AH01]. It successively updates the snapshot samples on which the the POD surrogate model is to be based upon. Related ideas are presented in [AFS00, Rav00].

Choose a sequence of increasing numbers N_j.

Algorithm 4.1 (POD-based adaptive control)

1. Let a set of snapshots $y_i^0, i = 1, \ldots, N_0$ be given and set j=0.

2. Set (or determine) l, and compute the POD modes and the space V^l.
3. Solve the reduced optimization problem (**SCP**) for u^j.
4. Compute the state y^j corresponding to the current control u^j and add the snapshots $y_i^{j+1}, i = N_j+1, \ldots, N_{j+1}$ to the snapshot set $y_i^j, i = 1, \ldots, N_j$.
5. If $|u^{j+1} - u^j|$ is not sufficiently small, set j = j+1 and goto 2.

We note that the term snapshot here may also refer to difference quotients of snapshots, compare Remark 1. We note further that it is also possible to replace its step 4. by

4.' Compute the state y^j corresponding to the current control u^j and store the snapshots $y_i^{j+1}, i = N_j + 1, \ldots, N_{j+1}$ while the snapshot set $y_i^j, i = 1, \ldots, N_j$ is neglected.

Many numerical investigations on the basis of Algorithm 4.1 with step 4' can be found in [Afa02]. This reference also contains a numerical comparison of POD to other model reduction techniques, including their applications to optimal open-loop control.

To anticipate discussion we note that the number N_j of snapshots to be taken in the j-th iteration ideally should be determined during the adaptive optimization process. We further note that the choice of ℓ in step 2 might be based on the information content $\mathcal{E}$ defined in (9), compare Section 5.2. We will pick up these items again in Section 6.

Remark 8. It is numerically infeasible to compute an optimal closed-loop feedback control strategy based on a finite element discretization of (51), since the resulting nonlinear dynamical system in general has large dimension and numerical solution of the related Hamilton-Jacobi-Bellman (HJB) equation is infeasible. In [KVX04] model reduction techniques involving POD are used to numerically construct suboptimal closed-loop controllers using the HJB equations of the reduced order model, which in this case only is low dimensional. $\Diamond$

4.2 Error estimates for linear-quadratic optimal control problems

It is still an open problem to estimate the error between solutions of (**CP**) and the related suboptimal control problem (**SCP**), and also to prove convergence of Algorithm 4.1. As a first step towards we now present error estimates for discrete solutions of linear-quadratic optimal control problems with a POD model as surrogate. For this purpose we combine techniques of [KV01, KV02] and [DH02, DH04, Hin04].

We consider the abstract control problem (**CP**) with $F \equiv 0$ and $\mathcal{U}_{\mathsf{ad}} \equiv \mathcal{U}$. We note that J from (52) is twice continuously Fréchet-differentiable. In particular, the second Fréchet-derivative of J at a given point $x = (y, u) \in W(0,T) \times \mathcal{U}$ in a direction $\delta x = (\delta y, \delta u) \in W(0,T) \times \mathcal{U}$ is given by

$$\nabla^2 J(x)(\delta x, \delta x) = \alpha_1 \|\mathcal{C}\delta y\|^2_{W_1} + \alpha_2 \|\mathcal{D}\delta y(T)\|^2_{W_2} + \sigma \|\delta u\|^2_{\mathcal{U}} \geq 0.$$

Thus, $\nabla^2 J(x)$ is a non-negative operator.

The goal is to minimize the cost J subject to (y, u) solves the linear evolution problem

$$\langle y_t(t), \varphi \rangle_H + a(y(t), \varphi) = \langle (\mathcal{B}u)(t), \varphi \rangle_H \tag{53a}$$

for all $\varphi \in V$ and almost all $t \in (0, T)$ and

$$y(0) = y_0 \quad \text{in } H. \tag{53b}$$

Here, $y_0 \in H$ is a given initial condition. It is well-known that for every $u \in \mathcal{U}$ problem (53) admits a unique solution $y \in W(0, T)$ satisfying

$$\|y\|_{W(0,T)} \leq C \left(\|y_0\|_H + \|u\|_{\mathcal{U}} \right)$$

for a constant $C > 0$; see, e.g., [DL92, pp. 512-520]. If, in addition, $y_0 \in V$ and if there exist two constants $c_1, c_2 > 0$ with

$$\langle A\varphi, -\Delta\varphi \rangle_H \geq c_1 \, \|\varphi\|^2_{D(A)} - c_2 \, \|\varphi\|^2_H \quad \text{for all } \varphi \in D(A) \cap V,$$

then we have

$$y \in L^2(0, T; D(A) \cap V) \cap H^1(0, T; H), \tag{54}$$

compare [DL92, p. 532]. From (54) we infer that y is almost everywhere equal to an element of $C([0, T]; V)$.

The minimization problem, which is under consideration, can be written as a linear-quadratic optimal control problem

$$\min J(y, u) \quad \text{s.t.} \quad (y, u) \in W(0, T) \times \mathcal{U} \text{ solves (53).} \tag{\textbf{LQ}}$$

Applying standard arguments one can prove that there exists a unique optimal solution $\bar{x} = (\bar{y}, \bar{u})$ to (**LQ**).

There exists a unique Lagrange-multiplier $\bar{p} \in W(0, T)$ satisfying together with $\bar{x} = (\bar{y}, \bar{u})$ the first-order necessary optimality conditions, which consist in the *state equations* (53), in the *adjoint equations*

$$-\langle \bar{p}_t(t), \varphi \rangle_H + a(\bar{p}(t), \varphi) = -\alpha_1 \, \langle \mathcal{C}^*(\mathcal{C}\bar{y}(t) - z_1(t)), \varphi \rangle_H \tag{55a}$$

for all $\varphi \in V$ and almost all $t \in (0, T)$ and

$$\bar{p}(T) = -\alpha_2 \mathcal{D}^*(\mathcal{D}\bar{y}(T) - z_2) \quad \text{in } H, \tag{55b}$$

and in the *optimality condition*

$$\sigma \bar{u} - \mathcal{B}^* \bar{p} = 0 \quad \text{in } \mathcal{U}. \tag{56}$$

Here, the linear and bounded operators $\mathcal{C}^* : W_1 \to L^2(0, T; H)$, $\mathcal{D}^* : W_2 \to H$, and $\mathcal{B}^* : L^2(0, T; H) \to \mathcal{U}$ stand for the Hilbert space adjoints of $\mathcal{C}$, $\mathcal{D}$, and $\mathcal{B}$, respectively.

Introducing the reduced cost functional

$$\hat{J}(u) = J(y(u), u),$$

where $y(u)$ solves (53) for the control $u \in \mathcal{U}$, we can express (**LQ**) as the reduced problem

$$\min \hat{J}(u) \quad \text{s.t.} \quad u \in \mathcal{U}. \tag{$\hat{\mathbf{P}}$}$$

From (56) it follows that the gradient of $\hat{J}$ at $\bar{u}$ is given by

$$\hat{J}'(\bar{u}) = \sigma \bar{u} - \mathcal{B}^* \bar{p}. \tag{57}$$

Let us define the operator $G : \mathcal{U} \to \mathcal{U}$ by

$$G(u) = \sigma u - \mathcal{B}^* p, \tag{58}$$

where $y = y(u)$ solves the state equations with the control $u \in \mathcal{U}$ and $p = p(y(u))$ satisfies the adjoint equations for the state y. As a consequence of (56) it follows that the first-order necessary optimality conditions for ($\hat{\mathbf{P}}$) are

$$G(u) = 0 \quad \text{in } \mathcal{U}. \tag{59}$$

In the POD context the operator G will be replaced by an operator $G_\ell : \mathcal{U} \to \mathcal{U}$ which then represents the optimality condition of the optimal control problem (**SCP**). The construction of G_ℓ is described in the following.

Computation of the POD basis

Let $u \in \mathcal{U}$ be a given control for (**LQ**) and $y = y(u)$ the associated state satisfying $y \in C^1([0,T]; V)$. To keep the notation simple we apply only a spatial discretization with POD basis functions, but no time integration by, e.g., an implicit Euler method. Therefore, we apply a continuous POD, where we choose $X = V$ in the context of Section 2.2. Let us mention the work [HY02], where estimates for POD Galerkin approximations were derived utilizing also a continuous version of POD.

We define the bounded linear $\mathcal{Y} : H^1(0,T;\mathbb{R}) \to V$ by

$$\mathcal{Y}\varphi = \int_0^T \varphi(t)y(t) + \varphi_t(t)y_t(t)\,\mathrm{d}t \quad \text{for } \varphi \in H^1(0,T;\mathbb{R}).$$

Notice that the operator $\mathcal{Y}$ is the continuous variant of the discrete operator $\mathcal{Y}_n$ introduced in (28). The adjoint $\mathcal{Y}^* : V \to H^1(0,T;\mathbb{R})$ is given by

$$\big(\mathcal{Y}^* z\big)(t) = \langle z, y(t) + y_t(t)\rangle_V \quad \text{for } z \in V.$$

(compare (29)). The operator $\mathcal{R} = \mathcal{Y}\mathcal{Y}^* \in \mathcal{L}(V)$ is already introduced in (48).

Remark 9. Analogous to the theory of singular value decomposition for matrices, we find that the operator $\mathcal{K} = \mathcal{Y}^*\mathcal{Y} \in \mathcal{L}(H^1(0,T;\mathrm{I\!R}))$ given by

$$\big(\mathcal{K}\varphi\big)(t) = \int_0^T \langle y(s), y(t)\rangle_V \varphi(s) + \langle y_t(s), y_t(t)\rangle_V \varphi_t(s)\,\mathrm{d}s \quad \text{for } \varphi \in H^1(0,T;\mathrm{I\!R})$$

has the eigenvalues $\{\lambda_i^\infty\}_{i=1}^\infty$ and the eigenfunctions

$$v_i^\infty(t) = \frac{1}{\sqrt{\lambda_i^\infty}}\,\big(\mathcal{Y}^*\psi_i^\infty\big)(t) = \frac{1}{\sqrt{\lambda_i^\infty}}\,\langle \psi_i^\infty, y(t) + y_t(t)\rangle_V$$

for $i \in \{j \in \mathrm{I\!N} : \lambda_j^\infty > 0\}$ and almost all $t \in [0,T]$. $\Diamond$

In the following theorem we formulate properties of the eigenvalues and eigenfunctions of $\mathcal{R}$. For a proof we refer to [HLB96], for instance.

Theorem 4. *For every $\ell \in \mathbb{N}$ the eigenfunctions $\psi_1^\infty, \dots, \psi_\ell^\infty \in V$ solve the minimization problem*

$$\min \mathfrak{J}(\psi_1, \dots, \psi_\ell) \quad \text{s.t.} \quad \langle \psi_j, \psi_i\rangle_X = \delta_{ij} \quad \text{for } 1 \le i, j \le \ell, \tag{60}$$

where the cost functional $\mathfrak{J}$ is given by

$$\mathfrak{J}(\psi, \dots, \psi_\ell) = \int_0^T \Big\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i\rangle_V \psi_i \Big\|_X^2 + \Big\| y_t(t) - \sum_{i=1}^{\ell} \langle y_t(t), \psi_i\rangle_V \psi_i \Big\|_V^2 \,\mathrm{d}t.$$

Moreover, the eigenfunctions $\{\lambda_i^\infty\}_{i\in\mathrm{I\!N}}$ and eigenfunctions $\{\psi_i^\infty\}_{i\in\mathrm{I\!N}}$ of $\mathcal{R}$ satisfy the formula

$$\mathfrak{J}(\psi_1^\infty, \dots, \psi_\ell^\infty) = \sum_{i=\ell+1}^{\infty} \lambda_i^\infty. \tag{61}$$

Proof. The proof of the theorem relies on the fact that the eigenvalue problem

$$\mathcal{R}\psi_i^\infty = \lambda_i^\infty \psi_i^\infty \quad \text{for } i = 1, \dots, \ell$$

is the first-order necessary optimality condition for (60). For more details we refer the reader to [HLB96].

Galerkin POD approximation

Let us introduce the set $V^\ell = \text{span}\,\{\psi_1^\infty, \dots, \psi_\ell^\infty\} \subset V$. To study the POD approximation of the operator G we introduce the orthogonal projection $\mathcal{P}^\ell$ of V onto V^ℓ by

$$\mathcal{P}^\ell \varphi = \sum_{i=1}^{\ell} \langle \varphi, \psi_i^\infty\rangle_V \psi_i^\infty \quad \text{for } \varphi \in V. \tag{62}$$

(compare (45)). Note that

$$\begin{aligned}\mathfrak{J}(\psi,\dots,\psi_\ell)\\ = \int_0^T \left\|y(t)-\mathcal{P}^\ell y(t)\right\|_V^2 + \left\|y_t(t)-\mathcal{P}^\ell y_t(t)\right\|_V^2 \,\mathrm{d}t = \sum_{i=\ell+1}^{\infty}\lambda_i^\infty .\end{aligned} \tag{63}$$

From (16) it follows directly that

$$a(\mathcal{P}^\ell\varphi,\psi) = a(\varphi,\psi) \quad \text{for all } \psi\in V^\ell,$$

where $\varphi\in V$. Clearly, we have $\|\mathcal{P}^\ell\|_{\mathcal{L}(V)}=1$.

Next we define the approximation $G_\ell:\mathcal{U}\to\mathcal{U}$ of the operator G by

$$G_\ell(u) = \sigma u - \mathcal{B}^* p^\ell, \tag{64}$$

where $p^\ell\in W(0,T)$ is the solution to

$$-\langle p_t^\ell(t),\psi\rangle_H + a(p^\ell(t),\psi) = -\alpha_1\,\langle \mathcal{C}^*(\mathcal{C}y^\ell - z_1),\psi\rangle_H \tag{65a}$$

for all $\psi\in V^\ell$ and $t\in(0,T)$ a.e. and

$$p^\ell(T) = -\alpha_2\,\mathcal{P}^\ell\big(\mathcal{D}^*(\mathcal{D}y^\ell(T)-z_2)\big) \tag{65b}$$

and $y^\ell\in W(0,T)$, which solves

$$\langle y_t^\ell(t),\psi\rangle_H + a(y^\ell(t),\psi) = \langle(\mathcal{B}u)(t),\psi\rangle_H \tag{66a}$$

for all $\psi\in V^\ell$ and almost all $t\in(0,T)$ and

$$y^\ell(0) = \mathcal{P}^\ell y_0 \tag{66b}$$

Notice that $G_\ell(u)=0$ are the first-order optimality conditions for the optimal control problem

$$\min \hat{J}^\ell(u) \quad \text{s.t.} \quad u\in\mathcal{U},$$

where $\hat{J}^\ell(u)=J(y^\ell(u),u)$ and $y^\ell(u)$ denotes the solution to (66).

It follows from standard arguments (Lax-Milgram lemma) that the operator G_ℓ is well-defined. Furthermore we have

Theorem 5. *The equation*

$$G_\ell(u) = 0 \quad \textit{in } \mathcal{U} \tag{67}$$

admits a unique solution $u^\ell\in\mathcal{U}$ which together with the unique solution u of (59) *satisfies the estimate*

$$\|u-u^\ell\|_{\mathcal{U}} \le \frac{1}{\sigma}\Big(\|\mathcal{B}^*(P-P^\ell)\mathcal{B}u\|_{\mathcal{U}} + \|\mathcal{B}^*(S^*-S_\ell^*)\mathcal{C}^*z_1\|_{\mathcal{U}}\Big). \tag{68}$$

Here, $P:=S^*\mathcal{C}^*\mathcal{C}S$, $P^\ell:=S_\ell^*\mathcal{C}^*\mathcal{C}S_\ell$, with S,S_l denoting the solution operators in (53) *and* (66)*, respectively.*

A proof of this theorem immediately follows from the fact, that u^l is a admissible test function in (59), and u in (67). Details will be given in [HV05].

Remark 10. We note, that Theorem 5 remains also valid in the situation where admissible controls are taken from a closed convex subset $\mathcal{U}_{\mathsf{ad}} \subset \mathcal{U}$. The solutions u, u^l in this case satisfy the variational inequalities

$$\langle G(u), v - u \rangle_{\mathcal{U}} \geq 0 \quad \text{for all } v \in \mathcal{U}_{\mathsf{ad}},$$

and

$$\langle G_\ell(u^\ell), v - u^\ell \rangle_{\mathcal{U}} \geq 0 \quad \text{for all } v \in \mathcal{U}_{\mathsf{ad}},$$

so that adding the first inequality with $v = u^\ell$ and the second with $v = u$ and straightforward estimation finally give (68) also in the present case. The crucial point here is that the set of admissible controls is not discretized a-priori. The discretization of the optimal control u^ℓ is determined by that of the corresponding Lagrange multiplier p^ℓ. For details of this discrete concept we refer to [Hin04].

It follows from the structure of estimate (68), that error estimates for $y - y^\ell$ and $p - p^l$ directly lead to an error estimate for $u - u^\ell$.

Proposition 2. *Let $\ell \in \mathbb{N}$ with $\lambda_\ell^\infty > 0$ be fixed, $u \in \mathcal{U}$ and $y = y(u)$ and $p = p(y(u))$ the corresponding solutions of the state equations* (53) *and adjoint equations* (55) *respectively. Suppose that the POD basis of rank ℓ is computed by using the snapshots $\{y(t_j)\}_{j=0}^n$ and its difference quotients. Then there exist constants $c_y, c_p > 0$ such that*

$$\|y^\ell - y\|^2_{L^\infty(0,T;H)} + \|y^\ell - y\|^2_{L^2(0,T;V)} \leq c_y \sum_{i=\ell+1}^{\infty} \lambda_i^\infty \tag{69}$$

and

$$\begin{aligned} &\|p^\ell - p\|^2_{L^2(0,T;V)} \\ &\qquad \leq c_p \Big(\sum_{i=\ell+1}^{\infty} \lambda_i^\infty + \|\mathcal{P}^\ell p - p\|^2_{L^2(0,T;V)} + \|\mathcal{P}^\ell p_t - p_t\|^2_{L^2(0,T;V)} \Big), \end{aligned} \tag{70}$$

where y^ℓ and p^ℓ solve (66) *and* (65)*, respectively, for the chosen u inserted in* (66a).

Proof. Let

$$y^\ell(t) - y(t) = y^\ell(t) - \mathcal{P}^\ell y(t) + \mathcal{P}^\ell y(t) - y(t) = \vartheta(t) + \varrho(t),$$

where $\vartheta = y^\ell - \mathcal{P}^\ell y$ and $\varrho = \mathcal{P}^\ell y - y$. From (16), (62), (63) and the continuous embedding $H^1(0,T;V) \hookrightarrow L^\infty(0,T;H)$ we find

$$\|\varrho\|^2_{L^\infty(0,T;H)} + \|\varrho\|^2_{L^2(0,T;V)} \le c_E \sum_{i=\ell+1}^{\infty} \lambda_i^\infty \tag{71}$$

with an embedding constant $c_E > 0$. Utilizing (53) and (66) we obtain

$$\langle \vartheta_t(t), \psi \rangle_H + a(\vartheta(t), \psi) = \langle y_t(t) - \mathcal{P}^\ell y_t(t), \psi \rangle_H$$

for all $\psi \in V^\ell$ and almost all $t \in (0,T)$. From (16), (17) and Young's inequality it follows that

$$\frac{\mathrm{d}}{\mathrm{d}t} \|\vartheta(t)\|^2_H + \|\vartheta(t)\|^2_V \le c_V^2 \, \|y_t(t) - \mathcal{P}^\ell y_t(t)\|^2_V. \tag{72}$$

Due to (66b) we have $\vartheta(0) = 0$. Integrating (72) over the interval $(0,t)$, $t \in (0,T]$, and utilizing (37), (45) and (63) we arrive at

$$\|\vartheta(t)\|^2_H + \int_0^t \|\vartheta(s)\|^2_V \,\mathrm{d}s \le c_V^2 \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$$

for almost all $t \in (0,T)$. Thus,

$$\operatorname*{ess\,sup}_{t\in[0,T]} \|\vartheta(t)\|^2_H + \int_0^T \|\vartheta(s)\|^2_V \,\mathrm{d}s \le c_V^2 \sum_{i=\ell+1}^{\infty} \lambda_i^\infty. \tag{73}$$

Estimates (71) and (73) imply the existence of a constant $c_y > 0$ such that (69) holds. We proceed by estimating the error arising from the discretization of the adjoint equations and write

$$p^\ell(t) - p(t) = p^\ell(t) - \mathcal{P}^\ell p(t) + \mathcal{P}^\ell p(t) - p(t) = \theta(t) + \rho(t),$$

where $\theta = p^\ell - \mathcal{P}^\ell p$ and $\rho = \mathcal{P}^\ell p - p$. From (16), (50), and (65b) we get

$$\begin{aligned} \|\theta(T)\|^2_H &\le \alpha_2^2 \, \|\mathcal{D}\|^2_{\mathcal{L}(H,W_1)} \, \|y^\ell(T) - y(T)\|^2_H \\ &\le \alpha_2^2 \, \|\mathcal{D}\|^2_{\mathcal{L}(H,W_1)} \|y^\ell - y\|^2_{C([0,T];H)}. \end{aligned}$$

Thus, applying (50), (69) and the techniques used above for the state equations, we obtain

$$\begin{aligned} &\operatorname*{ess\,sup}_{t\in[0,T]} \|\theta(t)\|^2_H + \int_0^T \|\theta(s)\|^2_V \,\mathrm{d}s \\ &\qquad \le 2c_V^2 \Big(c_V^2 c_e^2 c_y \, \|\mathcal{D}\|^4_{\mathcal{L}(H,W_1)} \sum_{i=\ell+1}^{\infty} \lambda_i^\infty + \|p_t - \mathcal{P}^\ell p_t\|^2_{L^2(0,T;V)} \Big). \end{aligned}$$

Hence, there exists a constant $c_p > 0$ satisfying (70).

Remark 11.

a) The error in the discretization of the state variable is only bounded by the sum over the not modeled eigenvalues λ_i^∞ for $i > \ell$. Since the POD basis is not computed utilizing adjoint information, the term $\mathcal{P}^\ell p - p$ in the $H^1(0,T;V)$-norm arises in the error estimate for the adjoint variables. For POD based approximation of partial differential equations one cannot rely on results clarifying the approximation properties of the POD-subspaces to elements in function spaces as e.g. L^p or C. Such results are an essential building block for e.g. finite element approximations to partial differential equations.
b) If we have already computed a second POD basis of rank $\tilde{\ell} \in \mathbb{N}$ for the adjoint variable, then we can express the term involving the difference $\mathcal{P}^{\tilde{\ell}} p - p$ by the sum over the eigenvalues corresponding to eigenfunctions, which are not used as POD basis functions in the discretization.
c) Recall that $\{\psi_i^\infty\}_{i \in \mathbb{N}}$ is a basis of V. Thus we have

$$\int_0^T \|p(t) - \mathcal{P}^\ell p(t)\|_V^2 \, \mathrm{d}t \le \int_0^T \sum_{i=\ell+1}^\infty |a(p(t), \psi_i^\infty)|^2 \, \mathrm{d}t.$$

The sum on the right-hand side converges to zero as ℓ tends to ∞. However, usually we do not have a rate of convergence result available. In numerical applications we can evaluate $\|p - \mathcal{P}^\ell p\|_{L^2(0,T;V)}$. If the term is large then we should increase ℓ and include more eigenfunctions in our POD basis.
d) For the choice $X = H$ we have instead of (71) the estimate

$$\|\varrho\|_{L^\infty(0,T;H)}^2 + \|\varrho\|_{L^2(0,T;V)}^2 \le C \, \|S\|_2 \sum_{i=\ell+1}^\infty \lambda_i^\infty,$$

where C is a positive constant, S denotes the stiffness matrix with the elements $S_{ij} = \langle \psi_j^\infty, \psi_i^\infty \rangle_V$, $1 \le i, j \le \ell$, and $\|\cdot\|_2$ stands the spectral norm for symmetric matrices, see [KV02, Lemma 4.15]. ◊

Applying (58), (64), and Proposition 2 we obtain for every $u \in \mathcal{U}$

$$\|G_\ell(u) - G(u)\|_{\mathcal{U}}^2 \le c_G \Big(\sum_{i=\ell+1}^\infty \lambda_i^\infty + \|\mathcal{P}^\ell p - p\|_{L^2(0,T;H)}^2 + \|\mathcal{P}^\ell p_t - p_t\|_{L^2(0,T;H)}^2 \Big) \tag{74}$$

for a constant $c_G > 0$ depending on c_λ and $\mathcal{B}$.

Suppose that $u_1, u_2 \in \mathcal{U}$ are given and that $y_1^\ell = y_1^\ell(u_1)$ and $y_2^\ell = y_2^\ell(u_2)$ are the corresponding solutions of (66). Utilizing Young's inequality it follows that there exists a constant $c_V > 0$ such that

$$
\begin{aligned}
&\|y_1^\ell - y_2^\ell\|^2_{L^\infty(0,T;H)} + \|y_1^\ell - y_2^\ell\|^2_{L^2(0,T;V)} \\
&\qquad \le c_V^2 \ \|\mathcal{B}\|^2_{\mathcal{L}(\mathcal{U},L^2(0,T;H))} \ \|u_1 - u_2\|^2_{\mathcal{U}}.
\end{aligned} \tag{75}
$$

Hence, we conclude from (65) and (75) that

$$
\begin{aligned}
&\|p_1^\ell - p_2^\ell\|^2_{L^\infty(0,T;H)} + \|p_1^\ell - p_2^\ell\|^2_{L^2(0,T;V)} \\
&\quad \le \max\left(\alpha_1 c_V^2 \ \|\mathcal{C}\|^2_{\mathcal{L}(L^2(0,T;H),W_1)}, \alpha_2 \|\mathcal{D}\|^2_{\mathcal{L}(H,W_2)}\right) \cdot \\
&\quad \cdot \Big(\|y_1^\ell - y_2^\ell\|^2_{L^\infty(0,T;H)} + \|y_1^\ell - y_2^\ell\|^2_{L^2(0,T;V)}\Big) \\
&\quad \le C \ \|u_1 - u_2\|^2_{\mathcal{U}}.
\end{aligned} \tag{76}
$$

where

$$
C = \frac{c_V^4}{2} \ \|\mathcal{B}\|^2_{\mathcal{L}(\mathcal{U},L^2(0,T;H))} \max\left(\alpha_1^2 c_V^2 \ \|\mathcal{C}\|^2_{\mathcal{L}(L^2(0,T;H),W_1)}, \alpha_2 \|\mathcal{D}\|^2_{\mathcal{L}(H,W_2)}\right).
$$

If the POD basis of rank ℓ is computed for the control u_1, then (64), (74) and (76) lead to the existence of a constant $\hat{C} > 0$ satisfying

$$
\begin{aligned}
&\|G_\ell(u_2) - G(u_1)\|^2_{\mathcal{U}} \le 2 \ \|G_\ell(u_2) - G_\ell(u_1)\|^2_{\mathcal{U}} + 2 \ \|G_\ell(u_1) - G(u_1)\|^2_{\mathcal{U}} \\
&\le \hat{C} \ \|u_2 - u_1\|^2_{\mathcal{U}} \\
&\quad + \hat{C} \left(\sum_{i=\ell+1}^{\infty} \lambda_i^\infty + \|\mathcal{P}^\ell p_1 - p_1\|^2_{L^2(0,T;V)} + \|\mathcal{P}^\ell (p_1)_t - (p_1)_t\|^2_{L^2(0,T;V)} \right).
\end{aligned}
$$

Hence, $G_\ell(u_2)$ is close to $G(u_1)$ in the $\mathcal{U}$-norm provided the terms $\|u_1 - u_2\|_{\mathcal{U}}$ and $\sum_{i=\ell+1}^{\infty} \lambda_i^\infty$ are small and provided the ℓ POD basis functions $\psi_1^\infty, \dots, \psi_\ell^\infty$ leads to a good approximation of the adjoint variable p_1 in the $H^1(0,T;V)$-norm. In particular, $G_\ell(u)$ in this case is small, if u denotes the unique optimal control of the continuous control problem, i.e., the solution of $G(u) = 0$.

We further have that both, G and G_ℓ are Fréchet differentiable with constant derivatives $G' \equiv \sigma Id - \mathcal{B}^* p'$ and $G'_\ell \equiv \sigma Id - \mathcal{B}^* (p^\ell)'$. Moreover, since $-\mathcal{B}^* p'$ and $-\mathcal{B}^* p'$ are selfadjoint positive operators, G' and G'_ℓ are invertible, satisfying

$$
\|(G')^{-1}\|_{\mathcal{L}(U)}, \|(G'_\ell)^{-1}\|_{\mathcal{L}(\mathcal{U})} \le \frac{1}{\sigma}.
$$

Since G_l also is Lipschitz continuous with some positive constant K we now may argue with a Newton-Kantorovich argument [D85, Theorem 15.6] that the equation

$$
G_\ell(v) = 0 \quad \text{in } \mathcal{U}
$$

admits a unique solution in $u^\ell \in B_{2\epsilon}(u)$, provided

$$
\|(G'_\ell)^{-1} G_\ell(u)\|_{\mathcal{U}} \le \epsilon \quad \text{and} \quad \frac{2K\epsilon}{\sigma} < 1.
$$

Thus, we in a different fashion again proved existence of a unique solution u^l of (67), compare Theorem 5, and also provided an error estimate for $u - u^l$ in terms of $\sum_{i=\ell+1}^{\infty} \lambda_i^{\infty} + \|\mathcal{P}^\ell p_1 - p_1\|^2_{L^2(0,T;V)} + \|\mathcal{P}^\ell (p_1)_t - (p_1)_t\|^2_{L^2(0,T;V)}$.

We close this section with noting that existence and local uniqueness of discrete solutions u^ℓ may be proved following the lines above also in the non-linear case , i.e., in the case $F \neq 0$ in (51).

5 Navier-Stokes control using POD surrogate models

In the present section we demonstrate the potential of the POD method applied as suboptimal open-loop control method for the example of the Navier-Stokes system in (41a)-(41d) as subsidiary condition in control problem (**CP**).

5.1 Setting

We present two numerical examples. The flow configuration is taken as flow around a circular cylinder in 2 spatial dimensions and is depicted in Fig. 1 for Example 5.2, compare the benchmark of Schäfer and Turek in [ST96], and in Fig. 8 for Example 5.3. At the inlet and at the upper and lower boundaries

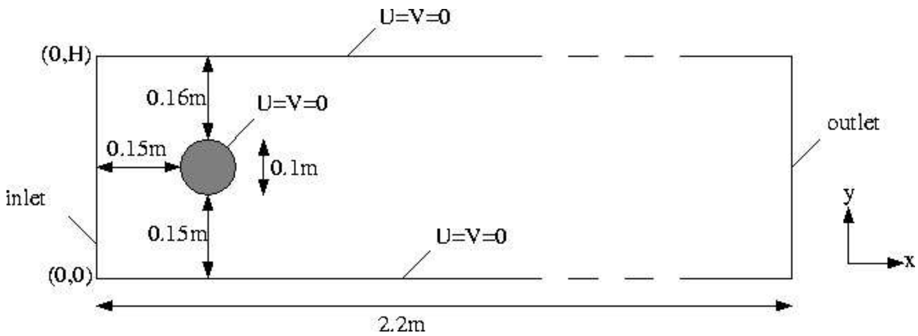

Fig. 1. Flow configuration for Example 5.2

inhomogeneous Dirichlet conditions are prescribed, and at the outlet the so called 'do-nothing' boundary conditions are used [HRT96]. As a consequence the boundary conditions for the Navier-Stokes equations have to be suitably modified. The control objective is to track the Navier Stokes flow to some pre-specified flow field z, which in our numerical experiments is either taken as Stokes flow or mean of snapshots. As control we take distributed forces in the spatial domain. Thus, the optimal control problem in the primitive setting is given by

$$
\left.\begin{array}{l}
\min\limits_{(y,u)\in W\times\mathcal{U}} \ J(y,u) := \dfrac{1}{2}\displaystyle\int_0^T \int_\Omega |y-z|^2 \,\mathrm{d}x\mathrm{d}t + \dfrac{\alpha}{2}\displaystyle\int_0^T \int_\Omega |u|^2 \,\mathrm{d}x\mathrm{d}t \\
\text{subject to} \\
\begin{array}{ll}
y_t + (y\cdot\nabla)y - \nu\Delta y + \nabla p = \mathcal{B}u & \text{in } \ Q = (0,T)\times\Omega, \\
\operatorname{div} y = 0 & \text{in } \ Q, \\
y(t,\cdot) = y_d & \text{on } \ (0,T)\times\Gamma_d, \\
\nu\partial_\eta y(t,\cdot) = p\eta & \text{on } \ (0,T)\times\Gamma_{out}, \\
y(0,\cdot) = y_0 & \text{in } \ \Omega,
\end{array}
\end{array}\right\} \tag{77}
$$

where $Q := \Omega\times(0,T)$ denotes the time-space cylinder, Γ_d the Dirichlet boundary at the inlet and Γ_{out} the outflow boundary. In this example the volume for the flow measurements and the control volume for the application of the volume forces each cover the whole spatial domain, i.e. $\mathcal{B}$ denotes the injection from $L^2(Q)$ into $L^2(0,T;V')$, $W_1 := L^2(Q)$ and $\mathcal{C}\equiv Id$. Further we have $\mathcal{U}_{ad} = \mathcal{U} = L^2(Q)$, $\alpha_1 = \frac{1}{2}$, $\alpha_2 = 0$, and $\sigma = \alpha$. Since we are interested in open-loop control strategies it is certainly feasible to use the whole of Q as observation domain (use as much information as attainable). Furthermore, from the practical point of view distributed control in the whole domain may be realized by Lorentz forces if the fluid is a electro-magnetically conductive, say [BGGBW97]. From the numerical standpoint this case can present difficulties, since the inhomogeneities in the primal and adjoint equations are large.

We note that it is an open problem to prove existence of global smooth solutions in two space dimensions for the instationary Navier-Stokes equations with do-nothing boundary conditions [Ran00].

The weak formulation of the Navier-Stokes system in (77) in primitive variables reads: Given $u\in\mathcal{U}$ and $y_0\in H$, find $p(t)\in L^2(\Omega)$, $y(t)\in H^1(\Omega)^2$ such that $y(0)=y_0$, and

$$
\begin{aligned}
\nu\langle\nabla y,\nabla\phi\rangle_H + \langle y_t + y\cdot\nabla y,\phi\rangle_H - \langle p,\operatorname{div}\phi\rangle = \langle\mathcal{B}u,\phi\rangle_H \text{ for all } \phi\in V, \\
\langle\chi,\operatorname{div} y\rangle_H = 0 \text{ for all } \chi\in L^2(\Omega),
\end{aligned} \tag{78}
$$

holds a.e. in $(0,T)$, where $V := \{\phi\in H^1(\Omega)^2, \phi_{\Gamma_D}=0\}$, compare [HRT96].

The Reynolds number Re$=1/\nu$ for the configurations used in our numerical studies is determined by

$$
\mathrm{Re} = \frac{\bar{U}d}{\mu},
$$

with $\bar{U}$ denoting the bulk velocity at the inlet, d the diameter of the cylinder, μ the molecular viscosity of the fluid and $\rho = 1$.

We now present two numerical examples. The first example presents a detailed description of the POD method as suboptimal control strategy in flow control. In the first step, the POD model for a particular control is validated against the full Navier-Stokes dynamics, and in the second step Algorithm 4.1 successfully is applied to compute suboptimal open-loop controls. The flow configuration is taken from [ST96]. The second example presents optimization results of Algorithm 4.1 for an open flow.

5.2 Example 1

In the first numerical experiment to be presented we choose a parabolic inflow profile at the inlet, homogeneous Dirichlet boundary conditions at upper and lower boundary, $d = 1$, Re=100 and the channel length is $l = 20d$. For the spatial discretization the Taylor-Hood finite elements on a grid with 7808 triangles, 16000 velocity and 4096 pressure nodes are used. As time interval in (77) we use $[0, T]$ with $T = 3.4$ which coincides with the length of one period of the wake flow. The time discretization is carried out by a fractional step Θ-scheme [Bän91] or a semi-implicit Euler-scheme on a grid containing $n = 500$ points. This corresponds to a time step size of $\delta t = 0.0068$. The total number of variables in the optimization problem (77) therefore is of order 5.4×10^7 (primal, adjoint and control variables). Subsequently we present a suboptimal approach based on POD in order to obtain suboptimal solutions to (77).

Construction and validation of the POD model

The reduced-order approach to optimal control problems such as (**CP**) or, in particular, (77) is based on approximating the nonlinear dynamics by a Galerkin technique utilizing basis functions that contain characteristics of the controlled dynamics. Since the optimal control is unknown, we apply a heuristic (see [AH01, AFS00]), which is well tested for optimal control problems, in particular for nonlinear boundary control of the heat equation, see [DV01].

Here we use the snapshot variant of POD introduced by Sirovich in [Sir87] to obtain a low-dimensional approximation of the Navier-Stokes equations. To describe the model reduction let $y^1, \ldots, y^m$ denote an ensemble of snapshots of the flow corresponding to different time instances which for simplicity are taken on an equidistant snapshot grid over the time horizon $[0, T]$. For the approximated flow we make the ansatz

$$y = \bar{y} + \sum_{i=1}^{m} \alpha_i \Phi_i \tag{79}$$

with modes Φ_i that are obtained as follows (compare Section 2.2):

1. Compute the mean $\bar{y} = \frac{1}{m} \sum\limits_{i=1}^{m} y^i$.
2. Build the correlation matrix $K = k_{ij}$, $k_{ij} = \int_\Omega (y^i - \bar{y})(y^j - \bar{y}) \,\mathrm{d}x$.
3. Compute the eigenvalues $\lambda_1, \ldots, \lambda_m$ and eigenvectors $v^1, \ldots, v^m$ of K.
4. Set $\Phi_i := \sum\limits_{j=1}^{m} v_j^i (y^j - \bar{y})$, $1 \le i \le d$.

5. Normalize $\Phi_i = \frac{\Phi_i}{\|\Phi_i\|_{L^2(\Omega)}}$, $1 \le i \le d$.

The modes Φ_i are pairwise orthonormal and are optimal with respect to the L^2 inner product in the sense that no other basis of $D := \text{span}\{y_1 - \bar{y}, \ldots, y_m - \bar{y}\}$ can contain more energy in fewer elements, compare Proposition 1 with $X = H$. We note that the term energy is meaningful in this context, since the vectors y are related to flow velocities. If one would be interested in modes which are optimal w.r.t. enstrophy, say, the H^1-norm should be used instead of the L^2-norm in step 2 above.

The Ansatz (79) is commonly used for model reduction in fluid dynamics. The theory of Sections 2,3 also applies to this situation.

In order to obtain a low-dimensional basis for the Galerkin Ansatz modes corresponding to small eigenvalues are neglected. To make this idea more precise let $D^M := \text{span}\{\Phi_1, \ldots, \Phi_M\}$ $(1 \le M \le N := \text{dim}D)$ and define the relative information content of this basis by

$$\mathrm{I}(M) \; := \; \sum_{k=1}^{M} \lambda_k \,/\, \sum_{k=1}^{N} \lambda_k,$$

compare (9). If the basis is required to describe $\gamma\%$ of the total information contained in the space D, then the dimension M of the subspace D^M is determined by

$$M = \text{argmin} \left\{ \mathrm{I}(M) : \mathrm{I}(M) \ge \frac{\gamma}{100} \right\}. \tag{80}$$

The reduced dynamical system is obtained by inserting (79) into the Navier-Stokes system and using a subspace D^M containing sufficient information as test space. Since all functions Φ_i are solenoidal by construction this results in

$$\langle y_t, \Phi_j \rangle_H + \nu \, \langle \nabla y, \nabla \Phi_j \rangle_H + \langle (y \cdot \nabla) y, \Phi_j \rangle_H = \langle \mathcal{B}u, \Phi_j \rangle \quad (1 \le j \le M),$$

which may be rewritten as

$$\dot{\alpha} + A\alpha = n(\alpha) + \beta + r, \quad \alpha(0) = a_0, \tag{81}$$

compare (43). Here, $\langle \cdot \, , \cdot \rangle$ denotes the $L^2 \times L^2$ inner product. The components of a_0 are computed from $\bar{y} + \sum_{k=1}^{M} (y_0 - \bar{y}, \Phi_k) \Phi_k$. The matrix A is the POD stiffness matrix and the inhomogeneity r results from the contribution of the mean $\bar{y}$ to the ansatz in (79). For the entries of β we obtain

$$\beta_j = \langle \mathcal{B}u, \Phi_j \rangle,$$

i.e. the control variable is not discretized. However, we note that it is also feasible to make an Ansatz for the control.

To validate the model in (81) we set $u \equiv 0$ and take as initial condition y_0 the uncontrolled wake flow at Re=100. In Fig. 2 a comparison of the full Navier-Stokes dynamics and the reduced order model based on 50 (left) as well

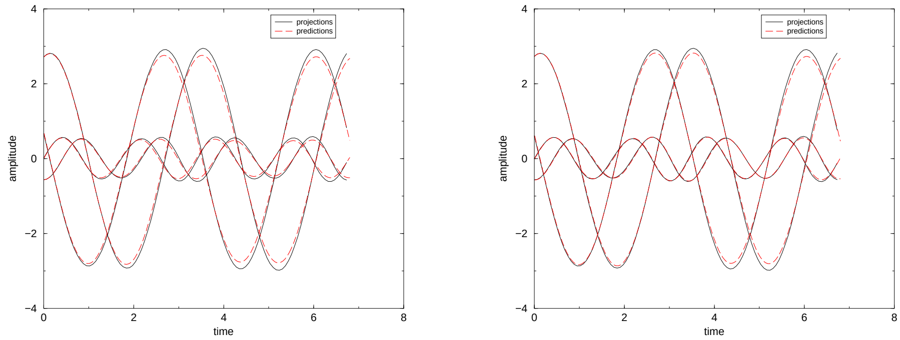

Fig. 2. Evolution of $\alpha_i(t)$ compared to that of $(y(t) - \bar{y}, \Phi_i)$ for $i = 1, \ldots, 4$. Left 50 snapshots, right 100 snapshots

as on 100 snapshots (right) is presented. As one can see the reduced order model based on 50 snapshots already provides a very good approximation of the full Navier-Stokes dynamics. In Fig. 3 the long-term behavior of the reduced order model based on 100 snapshots for different dimensions of the reduced order model are presented. Graphically the dynamics are already recovered utilizing eight modes. Note, that the time horizon shown in this figure is $[34, 44]$ while the snapshots are taken only in the interval $[0, 3.4]$. Finally, in Fig. 4 the vorticities of the first ten modes generated from the

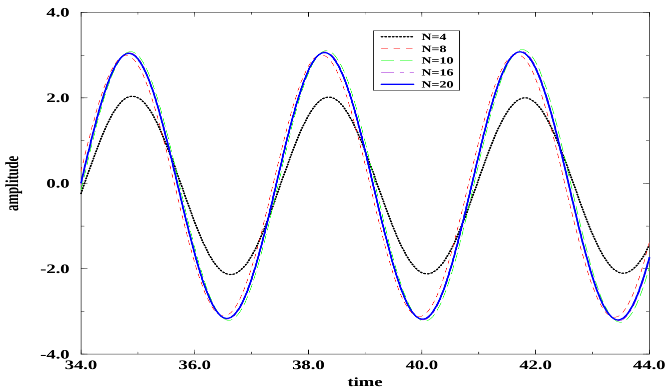

Fig. 3. Development of amplitude $\alpha_1(t)$ for varying number N of snapshots

uncontrolled snapshots are presented. Thus, the reduced order model obtained

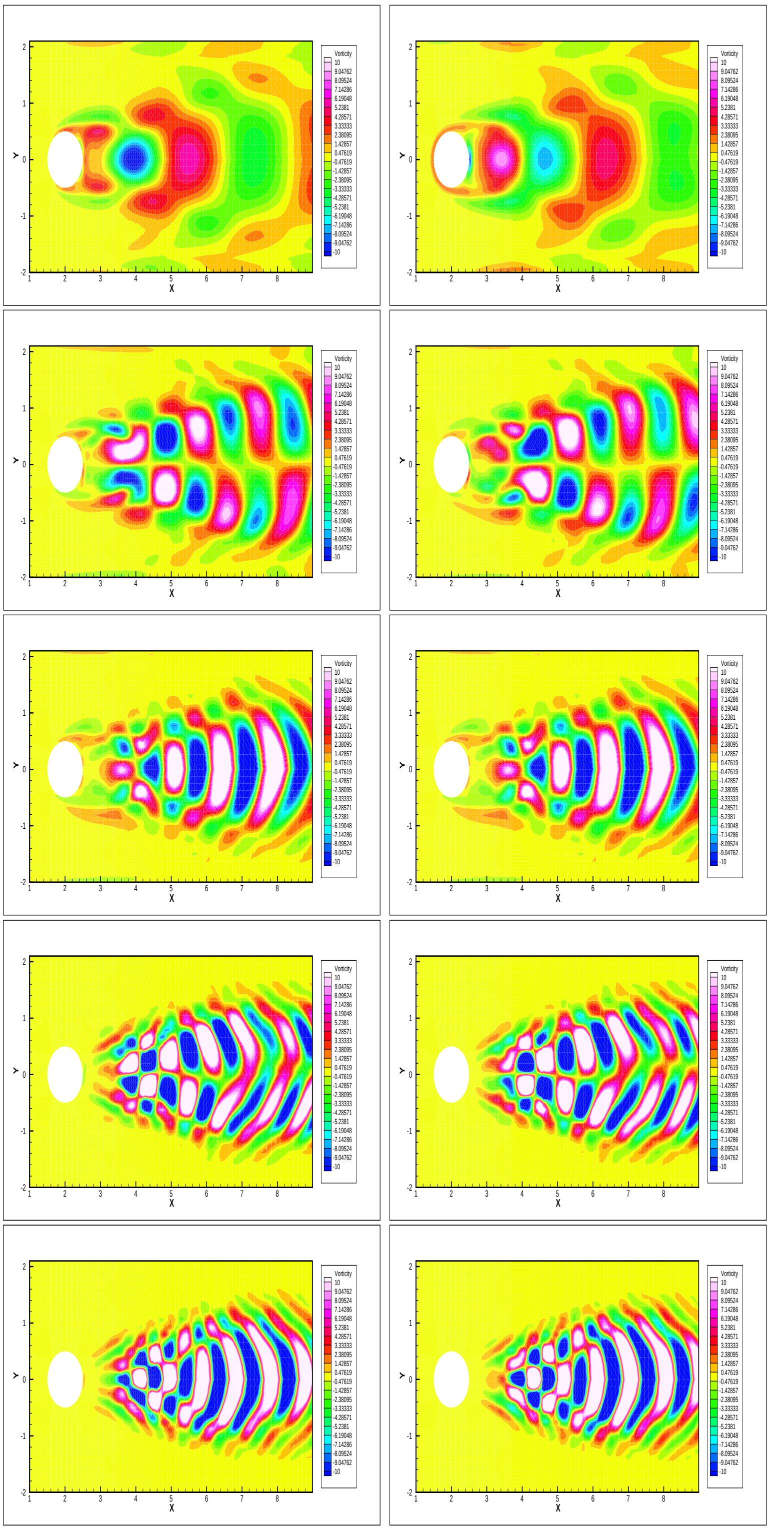

Fig. 4. First 10 modes generated from uncontrolled snapshots, vorticity

by snapshot POD captures the essential features of the full Navier-Stokes system, and in a next step may serve as surrogate of the full Navier-Stokes system in the optimization problem (77).

Optimization with the POD model

The reduced optimization problem corresponding to (77) is obtained by plugging (79) into the cost functional and utilizing the reduced dynamical system (81) as constraint in the optimization process. Altogether we obtain

$$\text{(ROM)} \begin{cases} \min \tilde{J}(\alpha, u) = J(y, u) \\ \text{s.t.} \\ \dot{\alpha} + A\alpha = n(\alpha) + \beta + r, \quad \alpha(0) = a_0. \end{cases} \tag{82}$$

At this stage we recall that the flow dynamics strongly depends on the control u, and it is not clear at all from which kind of dynamics snapshots should be taken in order to compute an approximation of a solution u^* of (77). For the present examples we apply Algorithms 4.1 with a sequence of increasing numbers N_j, where in step 2 the dimension of the space D^M, i.e. the value of M, for a given value $\gamma \in (0, 1]$ is chosen according to (80).

In the present application the value for α in the cost functional is chosen to be $\alpha = 2.10^{-2}$. For the POD method we add 100 snapshots to the snapshot set in every iteration of Algorithm 4.1. The relative information content of the basis formed by the modes is required to be larger than 99.99%, i.e. $\gamma = 99.99$. We note that within this procedure a storage problem pops up with increasing iteration number of Algorithm 4.1. However, in practice it is sufficient to keep only the modes of the previous iteration while adding to this set the snapshots of the current iteration. An application of Algorithm 4.1 with step 4' instead of step 4 is presented in Example 5.3 below.

The suboptimal control u is sought in the space of deviations from the mean, i.e we make the ansatz

$$u = \sum_{i=1}^{M} \beta_i \Phi_i, \tag{83}$$

and the control target is tracking of the Stokes flow whose streamlines are depicted in Fig. 5 (bottom). The same figure also shows the vorticity and the streamlines of the uncontrolled flow (top). For the numerical solution of the reduced optimization problems the Schur-complement SQP-algorithm is used, in the optimization literature frequently referred to as dual or range-space approach [NW99].
We first present a comparison between the optimal open-loop control strategy computed by Newton's method, and Algorithm 4.1. For details of the the implementation of Newton's method and further numerical results we refer the reader to [Hin99, HK00, HK01]. In Fig. 6 selected iterates of the evolution

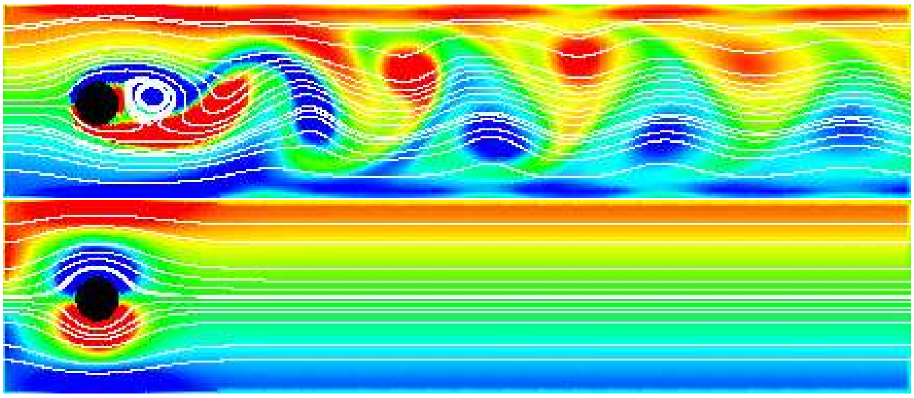

Fig. 5. Uncontrolled flow (top) and Stokes flow (bottom)

of the cost in $[0, T]$ for both approaches are given. The adaptive algorithm 4.1 terminates after 5 iterations to obtain the suboptimal control $\tilde{u}^*$. The termination criterium of step 5 in Algorithm 4.1 here is replaced by

$$\frac{|\hat{J}(u^{i+1}) - \hat{J}(u^i)|}{\hat{J}(u^i)} \leq 10^{-2}, \tag{84}$$

where

$$\hat{J}(u) = J(y(u), u)$$

denotes the so-called reduced cost functional and $y(u)$ stands for the solution to the Navier-Stokes equations for given control u. The algorithm achieves a remarkable cost reduction decreasing the value of the cost functional for the uncontrolled flow $\hat{J}(u^0) = 22.658437$ to $\hat{J}(\tilde{u}^*) = 6.440180$. It is also worth recording that to recover 99.99% of the energy stored in the snapshots in the first iteration 10 modes have to be taken, 20 in the second iteration, 26 in the third, 30 in the fourth, and 36 in the final iteration.

The computation of the optimal control with the Newton method takes approximately 17 times more cpu than the suboptimal approach. This includes an initialization process with a step-size controlled gradient algorithm. To obtain a relative error $|\nabla\hat{J}(u^n)|/|\nabla\hat{J}(u^0)|$ lower than 10^{-2}, 32 gradient iterations are needed with $\hat{J}(u^{32}) = 1.138325$. As initial control $u^0 = 0$ is taken. Note that every gradient step amounts to solving the non-linear Navier-Stokes equations in (77), the the corresponding adjoint equations, and a further Navier-Stokes system for the computation of the step-size in the gradient algorithm, compare [HK01]. Newton's algorithm then is initialized with u^{32} and 3 Newton steps further reduce the value of the cost functional to $\hat{J}(u^*) = 1.090321$. The controlled flow based on the Newton method is graphically almost indistinguishable from the Stokes flow in Fig.5. Fig. 7 shows the streamlines and the vorticity of the flow controlled by the adaptive approach at $t = 3.4$

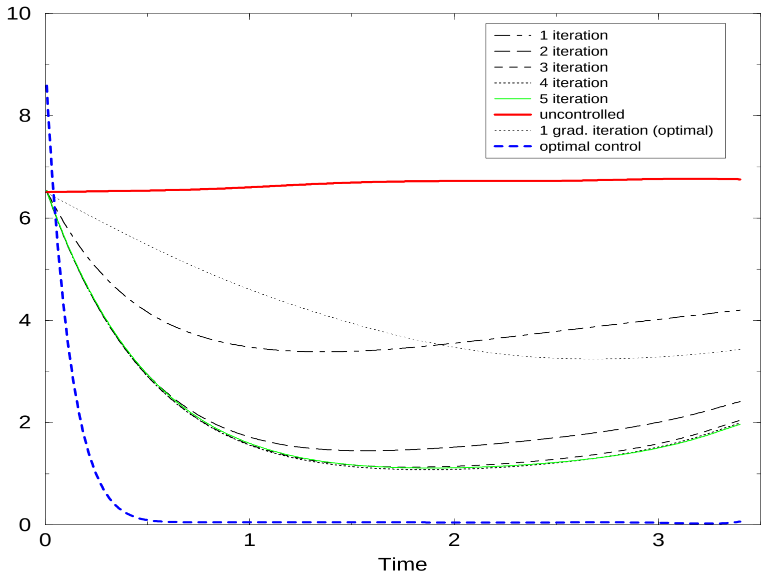

Fig. 6. Evolution of cost

(top) and the mean flow $\bar{y}$ (bottom), the latter formed with the snapshots of all 5 iterations. The controlled flow no longer contains vortex sheddings and is approximately stationary. Recall that the controls are sought in the space of deviations from the mean flow. This explains the remaining recirculations behind the cylinder. We expect that they can be reduced if the Ansatz for the controls in (83) is based on a POD of the snapshots themselves rather than on a POD of the deviation from their mean.

5.3 Example 2

The numerical results of the second application are taken from [AH00], compare also [Afa02]. The computational domain is given by $[-5, 15] \times [-5, 5]$ and is depicted in Fig. 8. At the inflow a block-profile is prescribed, at the outflow do-nothing boundary conditions are used, and at the top and bottom boundary the velocity of the block profile is prescribed, i.e. the flow is open. The Reynolds number is chosen to be Re=100, so that the period of the flow covers the time horizon $[0, T]$ with $T = 5.8$. The numerical simulations are performed on an equidistant grid over this time interval containing 500 gridpoints. The control target z is given by the mean of the uncontrolled flow simulation, the regularization parameter in the cost functional is taken as $\alpha = \frac{1}{10}$. The termination criterion in Algorithm 4.1 is chosen as in (84), the initial control is taken as $u^0 \equiv 0$. The iteration history for the value of

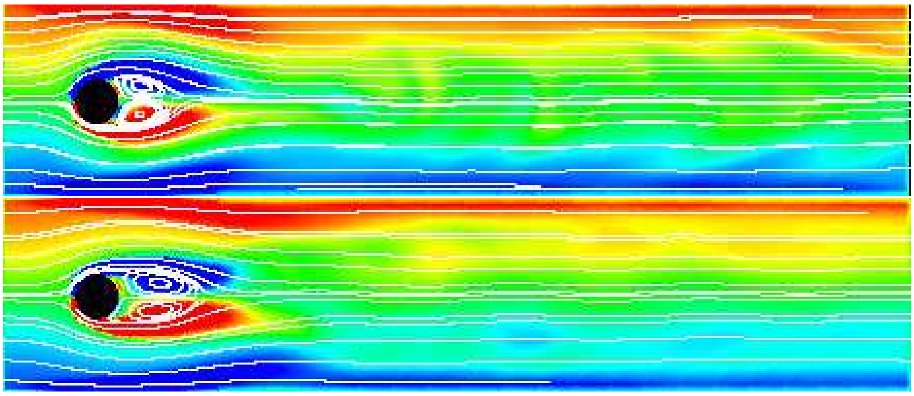

Fig. 7. Example 1: POD controlled flow (top) and mean flow $\bar{y}$ (bottom)

the cost functional is shown in Fig. 9, Fig. 10 contains the iteration history for the control cost.

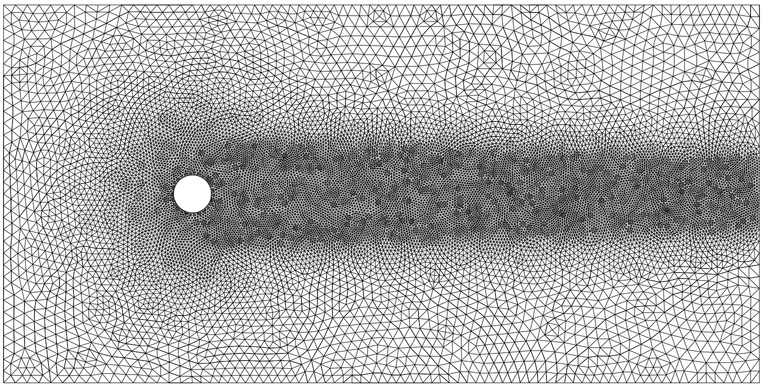

Fig. 8. Computational domain for the second application, 15838 velocity nodes.

The convergence criterium in Algorithm 4.1 is met after 7 iterations, where step 4 is replaced with step 4'. The value of the cost functional is $\hat{J}(\tilde{u}^*) = 0.941604$. Newton's method (without initialization by a gradient method) met the convergence criterium after 11 iterations with $\hat{J}(u_N^*) = 0.642832$, the gradient method needs 29 iterations with $\hat{J}(u_G^*) = 0.798193$. The total numerical

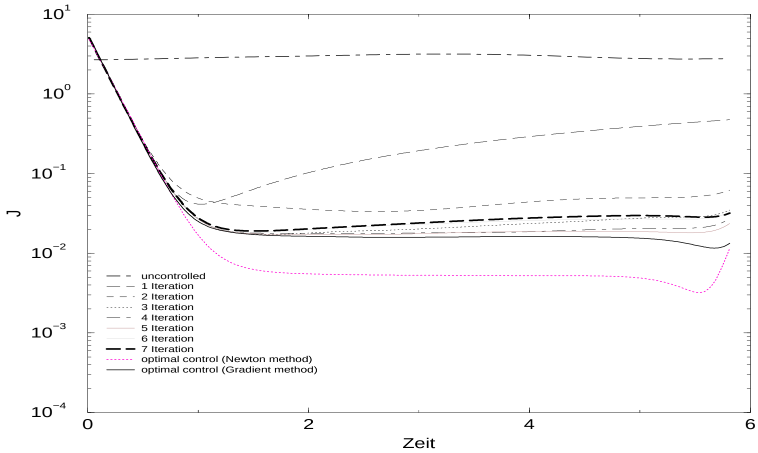

Fig. 9. Iteration history of functional values for Algorithm 4.1, second application

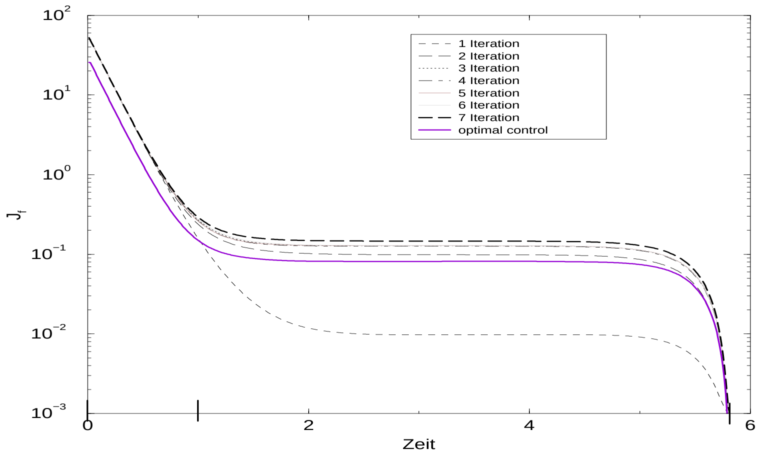

Fig. 10. Iteration history of control costs for Algorithm 4.1, second application

amount for the computation of the suboptimal control $\tilde{u}^*$ for this numerical example is approximately 25 times smaller than that for the computation of u_N^*. The resulting open-loop control strategies are visually nearly indistinguishable. For a further discussion of the approach presented in this section we refer the reader to [Afa02, AH01].

We close this section with noting that the basic numerical ingredient in Algorithm 4.1 is the flow solver. The optimization with the surrogate model can be performed with MATLAB. Therefore, it is not necessary to develop numerical integration techniques for adjoint systems, which are one of the major ingredients of Newton- and gradient-type algorithms when applied to the full optimization problem (77).

6 Future work and conclusions

6.1 Future research directions

To the authors knowledge it is an open problem in many applications

1) to estimate how many snapshots to take, and
2) where to take them.

In this context goal-oriented concepts should be a future research direction. For an overview of goal oriented concepts in a-posteriori error analysis for finite elements we refer the reader to [BR01].

To report on first attempts for 1) and 2) we now sketch the idea of the goal-oriented concept. Denoting by $J(y)$ the quantity of interest, frequently called the goal (for example the drag or lift of the wake flow) and by $J(y_h)$ the response of the discrete model, the difference $J(y) - J(y_h)$ can be expressed approximately in terms of the residual of the state equation ρ and an appropriate adjoint variable z, i.e.

$$J(y) - J(y_h) = \langle \rho(y), z \rangle, \tag{85}$$

where $\langle \cdot, \cdot \rangle$ denotes an appropriate pairing.

With regard to 1) above, it is proposed in [HH04] to substitute y, z in (85) by their discrete counterparts y_h, z_h obtained from the POD model, and, starting on a coarse snapshot grid, to refine the snapshot grid and forming new POD models as long as the difference $J(y) - J(y_h)$ is larger than a given tolerance.

With regard to 2) a goal-oriented concept for the choice of modes out of a given set is presented in [MM03]. In [HH05] a goal-oriented adaptive time-stepping method for time-dependent pdes is proposed which uses POD models to compute the adjoint variables. In view of optimization of complex time dependent systems based on POD models adaptive goal oriented time stepping here serves a dual purpose; it provides a time-discrete model of minimum complexity in the full spatial setting w.r.t. the goal, and the time grid suggested by the approach may be considered as ideal snapshot grid upon which the model reduction should be based.

Let us also refer to [AG03], where the authors presented a technique to choose a fixed number of snapshots from a fine snapshot grid.

A further research area is the development of robust and efficient suboptimal feedback strategies for nonlinear partial differential equations. Here, we refer to the [KV99, KVX04, LV03, LV04]. However, the development of feedback laws based on partial measurement information still remains a challenging research area.

6.2 Conclusions

In the first part of this paper we present a mathematical introduction to finite- and infinite dimensional POD. It is shown that POD is closely related to the singular value decomposition for rectangular matrices. Of particular interest is the case when the columns of such matrices are snapshots of dynamical systems, such as parabolic equations, or the Navier-Stokes system. In this case POD allows to compute coherent structures, frequently called modes, which cary the relevant information of the underlying dynamical process. It then is a short step to use these modes in a Galerkin method to construct low order surrogate models for the full dynamics. The major contribution in the first part consists in presenting error estimates for solutions of these surrogate models.

In the second part we work out how POD surrogate models might be used to compute suboptimal controls for optimal control problems involving complex, nonlinear dynamics. Since controls change the dynamics, POD surrogate models need to be adaptively modified during the optimization process. With Algorithm 4.1 we present a method to cope with this difficulty. This algorithm in combination with the snapshot form of POD then is successfully applied to compute suboptimal controls for the cylinder flow at Reynolds number 100. It is worth noting that the numerical ingredients for this suboptimal control concept are a forward solver for the Navier-Stokes system, and an optimization environment for low-dimensional dynamical systems, such as MATLAB. As a consequence coding of adjoints, say is not necessary. As a further consequence the number of functional evaluations to compute suboptimal controls in essence is given by the number of iterations needed by Algorithm 4.1. The suboptimal concept therefore is certainly a candidate to obey the rule

$$\frac{\text{effort of optimization}}{\text{effort of simulation}} \leq \text{constant},$$

with a constant of moderate size. We emphasize that obeying this rule should be regarded as one of the major goals for every algorithm developed for optimal control problems with PDE-constraints.

Finally, we present first steps towards error estimation of suboptimal controls obtained with POD surrogate models. For linear-quadratic control problems the size of the error in the controls can be estimated in terms of the error of the states, and of the adjoint states. We note that for satisfactory estimates also POD for the adjoint system needs to be performed.

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