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Abstract Proper orthogonal decomposition (POD) is a powerful technique for model reduction of linear and non-linear systems. It is based on a Galerkin type discretization with basis elements created from the system itself. In this work POD is applied to estimate scalar parameters in a scalar non-linear Ginzburg-Landau equation. The parameter estimation is formulated in terms of an optimal control problem that is solved by an augmented Lagrangian method combined with a sequential quadratic programming algorithm. A numerical example illustrates the efficiency of the proposed solution method.

1 Introduction

Proper orthogonal decomposition (POD) is a method to derive low order models for systems of differential equations. It is based on projecting the 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. It is successfully used in different fields including signal analysis and pattern recognition (see, e.g., [4]), fluid dynamics and coherent structures (see, e.g., [7, 17]) and more recently in control theory (see, e.g., [13]). The relationship between POD and balancing is considered in [12, 16, 20]. In contrast to POD approximations, reduced-basis element methods for parameter dependent elliptic are investigated in [1, 14, 15], for instance.

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In this work we continue our research in [10] and apply a POD Galerkin approximation to estimate diffusion coefficients in a scalar, non-linear Ginzburg-Landau equation. The corresponding parameter identification problem is formulated as an optimal control problem with inequality constraints for the parameters. To solve this optimization problem with a scalar inequality constraint we apply an augmented Lagrangian method (see, e.g., [2, 3]) combined with a globalized sequential quadratic programming (SQP) algorithm as described in [6]. In [9] error estimates for POD Galerkin schemes for linear and certain semi-linear elliptic, parameter dependent systems are proved. The resulting error bounds depend on the number of POD basis functions and on the parameter grid that is used to generate the snapshots and to compute the POD basis.

The paper is organized in the following manner: In Section 2 we introduce the parameter identification problem and review some pre-requisites. The POD approximation is explained shortly in Section 3 and numerical examples are carried out in Section 4.

2 Identification problem

Let $\Omega \subset \mathbb{R}^r$, $r = 2$ or 3, be a bounded open domain and let $\Gamma = \partial\Omega$ denote the boundary of Ω. We suppose that Ω is split into m measurable disjunct subdomains Ω_i, i.e.,

$$\Omega = \bigcup_{i=1}^{m} \Omega_i \quad \text{and} \quad \Omega_i \cap \Omega_j = \emptyset \text{ for } i \neq j.$$

We consider a *scalar Ginzburg-Landau equation*

$$-\nabla \cdot \big(c\nabla u\big) + qu + u^3 = f \qquad \text{in } \Omega, \tag{1a}$$

$$c\,\frac{\partial u}{\partial n} + \sigma u = g \qquad \text{on } \Gamma, \tag{1b}$$

where $q \in L^\infty(\Omega)$ with $q(\mathbf{x}) \geq q_a > 0$ for almost all (f.a.a.) $\mathbf{x} \in \Omega$, $f \in L^2(\Omega)$, $\sigma \in L^\infty(\Gamma)$ with $\sigma(\mathbf{s}) \geq 0$ f.a.a. $\mathbf{s} \in \Gamma$ and $g \in L^2(\Gamma)$. Furthermore, c is supposed to be constant on the subdomains Ω_i:

$$c(\mathbf{x}) = c^i \quad \text{f.a.a. } \mathbf{x} \in \Omega_i \cup \big(\overline{\Omega}_i \cap \Gamma\big),\ 1 \leq i \leq m,$$

with positive c_i's. Problem (1) is a simplified model of the full Ginzburg-Landau equations of superconductivity valid in the absence of internal fields [18].

A function $u \in H^1(\Omega)$ is called a *weak solution* to (1) if

$$\sum_{i=1}^{m} \int_{\Omega_i} c^i \nabla u \cdot \nabla \varphi + \big(qu + u^3 - f\big)\varphi \,\mathrm{d}\mathbf{x} + \int_\Gamma \big(\sigma u - g\big)\varphi \,\mathrm{d}\mathbf{s} = 0 \quad \forall \varphi \in H^1(\Omega). \tag{2}$$

By standard Galerkin procedure it follows that (2) admits a unique solution $u \in H^1(\Omega)$. If Ω is convex with a Lipschitz-continuous boundary or if Ω has a boundary of class C^2 we derive $u \in H^2(\Omega)$ from regularity results for elliptic equations.

Remark 1. Note that for $c \equiv 1$, $q \equiv -1$, $f \equiv 0$, $g \equiv 0$, $\sigma \equiv 0$ problem (1) has the form

$$-\Delta u - u + u^3 = 0 \text{ in } \Omega \quad \text{and} \quad \frac{\partial u}{\partial n} = 0 \text{ on } \Gamma. \tag{3}$$

Then, the constant functions $u \equiv 0$, $u \equiv -1$, and $u \equiv 1$ solve (3). Hence, the assumption $q \geq q_a > 0$ almost everywhere in Ω is essential to prove uniqueness. $\Diamond$

The goal of the identification problem is to identify the diffusion coefficient c, i.e., the c_i's, from (perturbed) measurement u_d for the solution u to (1) on Γ. Therefore, we introduce the quadratic cost functional $J : H^1(\Omega) \times \mathbb{R}^m \to [0,\infty)$ by

$$J(u,c) = \frac{\alpha}{2} \int_\Gamma \left|u - u_d\right|^2 \mathrm{d}\mathbf{x} + \frac{1}{2} \sum_{i=1}^m \kappa_i \left|c^i\right|^2 \tag{4}$$

for $u \in H^1(\Omega)$ and $c = (c^1, \ldots, c^m) \in \mathbb{R}^m$. The optimal control problem is of the form

$$\min J(u,c) \quad \text{subject to (s.t.)} \quad (u,c) \in H^1(\Omega) \times C_{ad} \text{ solves (2)}, \tag{P}$$

where the set of admissible diffusion coefficients is given by

$$C_{ad} = \left\{ c = (c^1, \ldots, c^m) \in \mathbb{R}^m \,|\, c^i \geq c_a \text{ for } i = 1, \ldots, m \right\}$$

with a positive scalar c_a.

Using standard arguments it can be proven that (**P**) possesses a (local) solution $x_* = (u_*, c_*) \in H^1(\Omega) \times C_{ad}$. To characterize an optimal solution of (**P**) we introduce the Lagrange function $L : H^1(\Omega) \times \mathbb{R}^m \times H^1(\Omega) \to \mathbb{R}$ by

$$L(u,c,p) = J(u,c) + \sum_{i=1}^m \int_{\Omega_i} c^i \nabla u \cdot \nabla p + \left(qu + u^3 - f\right) p \,\mathrm{d}\mathbf{x} + \int_\Gamma \left(\sigma u - g\right) p \,\mathrm{d}\mathbf{s}$$

for $(u,c,p) \in H^1(\Omega) \times \mathbb{R}^m \times H^1(\Omega)$. Existence of a *Lagrange multiplier* (or *dual state*) p_* associated with $x_* = (u_*, c_*)$ is shown in [5, Theorem 3.3], where p_* satisfies the *dual system* (here written in its strong form)

$$-\nabla \cdot \left(c_* \nabla p_*\right) + q p_* + 3(u_*)^2 p_* = 0 \text{ in } \Omega, \quad c \frac{\partial p_*}{\partial n} + \sigma p_* = u_d - u_* \text{ on } \Gamma$$

and the *variational inequality*

$$\sum_{i=1}^m \left(\kappa_i c_*^i + \int_{\Omega_i} \nabla u_* \cdot \nabla p_* \,\mathrm{d}\mathbf{x} \right) \left(c^i - c_*^i\right) \geq 0 \quad \text{for all } c = (c^1, \ldots, c^m) \in C_{ad}.$$

To solve (3) we continue our earlier work [9, 10] and apply an augmented Lagrangian method combined with an globalized SQP algorithm. The discretization

of the state and the dual equations is carried out by a POD Galerkin approximation. We refer the reader to [8, 10], where a scalar potential parameter is identified in a linear elliptic partial differential equation.

3 POD approximation

In this section we introduce briefly the POD method. Suppose that for points $c_j = (c_j^1, \dots, c_j^m) \in C_{ad}$, $j = 1, \dots, n$, we know (at least approximately) the solution u_j to (1), e.g., by utilizing a finite element or finite difference discretization. We set

$$\mathcal{V} = \operatorname{span}\{u_1, \dots, u_n\} \subset H^1(\Omega)$$

with $d = \dim \mathcal{V} \leq n$. Then the *POD basis of rank* $\ell \leq d$ is given by the solution to

$$\min_{\psi_1,\dots,\psi_\ell} \sum_{j=1}^{n} \Big\| u_j - \sum_{i=1}^{\ell} \langle u_j, \psi_i \rangle_{H^1(\Omega)} \psi_i \Big\|^2_{H^1(\Omega)} \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle_{H^1(\Omega)} = \delta_{ij}. \tag{5}$$

The solution to (5) is characterized by the eigenvalue problem

$$\mathscr{R}\psi_i = \lambda_i \psi_i, \quad 1 \leq i \leq \ell,$$

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_\ell \geq \ldots \geq \lambda_d > 0$ denote the eigenvalues of the linear, bounded, self-adjoint, and non-negative operator $\mathscr{R} : H^1(\Omega) \to \mathcal{V}$ defined by

$$\mathscr{R}z = \sum_{j=1}^{n} \langle u_j, z \rangle_{H^1(\Omega)} u_j \quad \text{for } z \in H^1(\Omega);$$

see [7, 11, 19]. Suppose that we have determined a POD basis $\{\psi_i\}_{i=1}^{\ell}$. We set

$$V^\ell = \operatorname{span}\{\psi_1, \dots, \psi_\ell\} \subset \mathcal{V} \subset H^1(\Omega).$$

Then the following relation holds

$$\sum_{j=1}^{n} \Big\| u_j - \sum_{i=1}^{\ell} \langle u_j, \psi_i \rangle_{H^1(\Omega)} \psi_i \Big\|^2_{H^1(\Omega)} = \sum_{i=\ell+1}^{d} \lambda_i.$$

Next we introduce the *POD Galerkin scheme for* (2). The function $u^\ell = \sum_{i=1}^{\ell} u_i^\ell \psi_i \in V^\ell$ solves

$$\begin{aligned} \sum_{j=1}^{m} \int_{\Omega_j} c_j \nabla u^\ell \cdot \nabla \psi \, d\mathbf{x} + \int_\Omega \big(q u^\ell + (u^\ell)^3 \big) \psi \, d\mathbf{x} + \int_\Gamma \sigma u^\ell \psi \, d\mathbf{s} \\ = \int_\Omega f \psi \, d\mathbf{x} + \int_\Gamma g \psi \, d\mathbf{s} \quad \forall \psi \in V^\ell. \end{aligned} \tag{6}$$

Problem (6) is a non-linear system for the ℓ unknown modal coefficients $u_1^\ell, \ldots, u_\ell^\ell \in \mathbb{R}$. If

$$\mathscr{E}(\ell) = \frac{\sum_{i=1}^{\ell} \lambda_i}{\sum_{i=1}^{d} \lambda_i} \approx 1 \quad \text{for } \ell \ll d,$$

holds, (6) is called a *low-dimensional model* for (2).

4 Numerical example

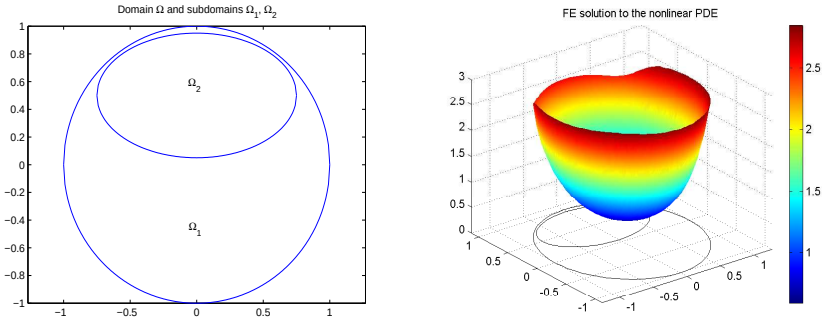
In this section we present a numerical example for the identification problem. The numerical test is executed on a standard 3.0 GHz desktop PC. We are using the MATLAB 7.1 package together with FEMLAB 3.1.

Run 1 Let $\Omega = \{\mathbf{x} = (x_1, x_2) \,|\, x_1^2 + x_2^2 < 1\}$ be the open unit cirle in $\mathbb{R}^2$ and the subdomains Ω_1, Ω_2 be given as

$$\Omega_1 = \Omega \setminus \Omega_2, \quad \Omega_2 = \left\{\mathbf{x} = (x_1, x_2) \in \Omega \,|\, \frac{x_1^2}{a^2} + \frac{(x_2 - 0.5)^2}{b^2} < 1\right\}$$

with $a = 0.75$ and $b = 0.45$; see Figure 1 (left plot). Thus, the diffusion coeffi-

Fig. 1 Domain Ω and subdomains Ω_1, Ω_2 (left plot); FE solution (right plot).



cient is given by $c = (c_1, c_2)$. In (1) we choose $q \equiv 10$, $f \equiv 3$, $\sigma \equiv 2$, $g(\mathbf{x}) = 10 + \cos(\pi x_1/2) \cdot \cos(\pi x_2/2)$ for $\mathbf{x} = (x_1, x_2) \in \Gamma$. For $\bar{c} = (0.7, 1.4)$ we calculate a finite element (FE) solution $\bar{u}^h = \bar{u}^h(\bar{c}) \in H^1(\Omega)$ using standard piecewise linear FE ansatz functions on a triangular mesh with 1147 degrees of freedom. The CPU time for the FE solve is 13.5 seconds. The FE solution is plotted in Figure 1 (right plot). To derive a POD basis we choose the diffusion values $c_j = (\eta_k, \eta_l) \in \mathbb{R}^2_+$, $1 \le j \le n$, with

$$j = 5(k-1) + l \text{ for } 1 \le k, l \le 5, \quad \eta_k = 0.5 + \frac{k-1}{4} \text{ for } k = 1, \ldots, 5$$

and compute the corresponding FE solutions $u_j^h = u^h(c_j) \in H^1(\Omega)$ to (1), i.e., we have $n = 25$ snapshots $\{u_j^h\}_{j=1}^n$. The computation of the snapshots requires 341 seconds. Next we compute the POD basis of rank ℓ as described in Section 3. The decay of the largest normalized eigenvalues $\lambda_i / \sum_{j=1}^d \lambda_j$, $1 \le i \le 9$, is plotted in Figure 2.

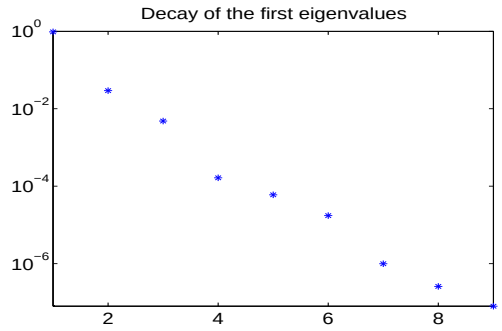


Fig. 2 Decay of the largest 9 normalized eigenvalues $\lambda_i / \sum_{j=1}^d \lambda_j$.

For the POD Galerkin approximation we choose $\ell = 7$ POD basis functions. The computation of the POD solution $\bar{u}^\ell = \bar{u}^\ell(\bar{c})$ for the diffusion parameter $\bar{c}$ requires 0.1 second. The relative error in the H^1-norm between the FE state $\bar{u}^h$ and the POD state $u^\ell(\bar{c})$ is 0.25%. Furthermore, the relative errors between the FE state and the POD state decreases with increasing number ℓ of POD basis functions (see Table 1). Let us mention that in [9] error estimates for POD Galerkin schemes are derived.

Table 1 Relative errors between the FE state and the POD state for different numbers ℓ of POD basis functions applying in the POD Galerkin approximation for (1).

	$\ell = 4$	$\ell = 5$	$\ell = 6$	$\ell = 7$	$\ell = 8$
$\frac{\|\bar{u}^h - \bar{u}^\ell\|_{H^1(\Omega)}}{\|\bar{u}^h\|_{H^1(\Omega)}}$	0.01160	0.00291	0.00289	0.00247	0.00246

Next turn to the identification problem. We set $c_a = 0.01$ in the definition of the admissible set C_{ad} of diffusion coefficients. Moreover, we choose the weights $\alpha = 100$ and $\kappa = 10^{-5}$ for the cost functional. For $\bar{c}$ we have already computed the FE solution $\bar{u}^h$ to (1). Let for any $\mathbf{x} \in \overline{\Omega}$ the term $\varepsilon(\mathbf{x}) \in [-1, 1]$ denote a random variable and let $\delta \ge 0$ be a given perturbation. In (4) we set $u_d = u_d^h|_\Gamma$ for the desired state, where $u_d^h = (1 + \delta\varepsilon)\bar{u}^h$. The goal of the identification problem is to recover $c_{\text{ideal}} = \bar{c}$ from the perturbed measurement u_d for $u_{\text{ideal}}^h = \bar{u}^h$ on the boundary Γ. We choose the perturbation $\delta = 0.05$ (i.e., 5% noise) and apply the augmented Lagrangian method

combined with a globalized SQP method to determine a numerical solution (u_*^ℓ, c_*^ℓ) with $c_*^\ell = (0.7041, 1.4018)$. This gives the relative error

$$\frac{|c_*^\ell - c_{\text{ideal}}|_2}{|c_{\text{ideal}}|_2} \approx 0.0029 = 0.29\%,$$

in the diffusion parameter, where $|\cdot|_2$ denotes the Euclidean norm in $\mathbb{R}^2$. Moreover, the relative errors in the state variable to the ideal data u_{ideal} and to the noisy data $(1+\delta\varepsilon)\vec{u}^h$ are presented in Table 2.

Table 2 Relative errors of the POD state u_*^ℓ compared to the ideal data u_{ideal} and to the noisy data u_d with 5% noise.

	$\frac{\|u_*^\ell - u\|_{H^1(\Omega)}}{\|u\|_{H^1(\Omega)}}$	$\frac{\|u_*^\ell - u\|_{L^2(\Omega)}}{\|u\|_{L^2(\Omega)}}$	$\frac{\|u_*^\ell - u\|_{L^2(\Gamma)}}{\|u\|_{L^2(\Gamma)}}$
$u = u_{\text{ideal}}^h$	0.0061	0.0018	0.0014
$u = u_d$	0.3406	0.0215	0.0235

Notice that the optimization algorithm only needs 1.6 seconds CPU time, whereas the FE based augmented Lagrangian method combined with a globalized SQP solver stops after 286 seconds. However, the CPU time for the computation of the snapshots is larger that the CPU time for the FE optimization method. The advantage of POD regarding computing times appears significantly when the identification problem has to be solved several times (e.g., for different data u_d) so that the already computed POD basis can be utilized again. For instance, if we take the perturbation $\delta = 0.03$ for the measurement data u_d and solve the optimal control prolem again we obtain an optimal solution after 2.2 seconds with $c_*^\ell = (0.7019, 1.3996)$ that leads to the relative error

$$\frac{|c_*^\ell - c_{\text{ideal}}|_2}{|c_{\text{ideal}}|_2} \approx 0.0012 = 0.12\%.$$

The relative errors in the state variable are presented in Table 3.

Table 3 Relative errors of the POD state u_*^ℓ compared to the ideal data u_{ideal} and to the noisy data u_d with 3% noise.

	$\frac{\|u_*^\ell - u\|_{H^1(\Omega)}}{\|u\|_{H^1(\Omega)}}$	$\frac{\|u_*^\ell - u\|_{L^2(\Omega)}}{\|u\|_{L^2(\Omega)}}$	$\frac{\|u_*^\ell - u\|_{L^2(\Gamma)}}{\|u\|_{L^2(\Gamma)}}$
$u = u_{\text{ideal}}^h$	0.0041	0.0014	0.0007
$u = u_d$	0.2122	0.0129	0.0141

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