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Error Bounds for POD expansions of parameterized transient temperatures.

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Abstract

We focus on the convergence analysis of the POD expansion for the parameterized solution of transient heat equations. The parameter of interest is the conductivity coefficient. We prove that this expansion converges with exponential accuracy, uniformly if the conductivity coefficient remains within a compact set of positive numbers. This convergence result is independent of the regularity of the temperature with respect to the space and time variables. We present some numerical experiments to show that a reduced number of modes allows to represent with high accuracy the family of solutions corresponding to parameters that lie in the compact set under study.

1 Introduction

Karhunen-Loève's expansion (KLE) provides a reliable procedure for computing a low dimensional representation of spatiotemporal signals (see [20, 10]) and is widely used in various communities. It is referred to as the principal components analysis (PCA) in statistics (see [22, 14, 15]), or called singular value decomposition (SVD) in linear algebra (see [11]). In computational mechanics where it is wide-spread, it bears the name of proper orthogonal decomposition (POD) (see [3, 13]). Since the last decades, it is fitted within the frame of reduced basis methods to perform the numerical simulations of parameter-depending dynamic systems, which allow substantial savings of computational costs and makes affordable the solution of problems that need a large amount of data. An important work may be found in the context of parameterized partial differential equations. We refer to (see [13, 9, 25, 26, 6, 5]) without being exhaustive

We focus our contribution on the accuracy of the truncated KLE or POD for the transient temperature functions T, when parameterized by the conduction coefficient γ. This is a continuation work of [2], where the time was taken as the parameter while the space was the central variable.

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The problem being bivariant, POD is strictly equivalent to decomposition by PGD and so the results obtained therefore apply for both cases

The study we undertake here aims a bound of the approximation error that decays exponentially fast, in the number of the retained modes. This convergence is uniform in the conductivity coefficient provided it remains bounded away from zero. Let us point out the important fact that the smoothness of the temperature with respect to the space-time variables has no impact on the final estimates. The main theoretical tool is to apply the Courant-Weyl Theorem [19] (also known as Courant-Fisher min-max principle) to the POD operator whose kernel is the temperature field $T = T(\gamma)$. An appropriate approximation of the temperature field by polynomials yields the desired bound on the truncating POD error approximation. The accuracy of such an approximation requires some smoothness results of the temperature $T = T(\gamma)$. In spite of their role, the way these results may be derived is not the heart of our work. Hence, the simplicity option is preferred here ; we call hence for the Fourier analysis to obtain the desired regularity. In case the Fourier basis is not accessible, alternatives for the investigation of the regularity of T upon γ may be available. The reader interested in is referred to the highly technical mathematics in [7, 17], where similar results can be found for elliptic value problems.
We present afterwards some numerical simulations to check out the theoretical convergence rate of the POD expansion of the solution to the heat equation. We also confirm the dependence of the convergence rate with respect to the range of thermal diffusivities.

The outlines are as follows. Section 2 recalls the POD or Karhunen-Loève expansion for biparametric functions. Section 3 analyzes the velocity of convergence of the POD expansion when applied to the solutions of the heat equation. Finally, in Section 4 we present the numerical investigation.

Notation — Let $X \subset \mathbb{R}^d$ be a given Lipschitz domain. We denote by $L^2(X)$ the space of measurable and square integrable functions on X. The Sobolev spaces $H^1(X)$ contain all the function that belong to $L^2(X)$ together with all its first derivatives (see [1]). Then let G be a measure space and H a Hilbert space. We denote by $L^2(G, H)$ the Bochner space of measurable and square integrable vector-valued functions from G on H (cf. [8]).

2 Karhunen-Loève decomposition

The Karhunen-Loève decomposition, also known as Proper Orthogonal decomposition (POD in the sequel) provides a technique to obtain low-dimensional approximations of parametric functions. For a rapid description of it, we consider $G \subset \mathbb{R}^d$ and $\mathcal{Q} \subset \mathbb{R}^n$ two bounded domains, d and n are integers ≥ 1. G will be the set of parameters and $\mathcal{Q}$ stands for the spatio-temporal domain. Let T be a given function in the Lebesgue space $L^2(G \times \mathcal{Q})$ that we want to approximate in a low-dimensional variety. Define then the integral operator with kernel T expressed as

$$\varphi \mapsto B\,\varphi, \qquad (B\,\varphi)(z) = \int_G T(\gamma, z)\varphi(\gamma)\, d\gamma. \tag{1}$$

B belongs to $\mathcal{L} = \mathcal{L}(L^2(G), L^2(\mathcal{Q}))$, the space of bounded linear operators mapping $L^2(G)$ into $L^2(\mathcal{Q})$ and we have

$$\|B\|_{\mathcal{L}} \leq \|T\|_{L^2(G\times\mathcal{Q})}.$$

The adjoint operator B^* is defined from $L^2(\mathcal{Q})$ into $L^2(G)$ as

$$v \mapsto B^*\, v, \qquad (B^*\, v)(\gamma) = \int_{\mathcal{Q}} T(\gamma, z)v(z)dz. \tag{2}$$

Let us then consider the POD operator $A = B^*B$, which is also an integral operator whose kernel $K \in L^2(G \times G)$ is expressed by

$$K(\gamma, \mu) = \int_{\mathcal{Q}} T(\gamma, z)\, T(\mu, z)\, dz. \tag{3}$$

The operator A is linear, bounded, self-adjoint and compact. This results from the fact that the operator B is compact by the Kolmogorov compactness criterion in $L^2(G)$ (cf. Muller [21], Chapter 2). Consequently, there exists a complete orthonormal basis of $L^2(G)$ formed by eigenvectors $(\varphi_m)_{m\geq 0}$ of A, associated to non-negative eigenvalues $(\lambda_m)_{m\geq 0}$, that we assume to be ordered in decreasing value, such that $\lim_{m\to\infty} \lambda_m = 0$. Each non-zero eigenvalue has a finite multiplicity, and 0 is the only possible accumulation point of the spectrum.
Moreover, setting $\sigma_m = (\lambda_m)^{1/2}$, the sequence $(v_m)_{m\geq 0}$ given by

$$v_m = \frac{1}{\sigma_m}\, B\varphi_m,$$

is an orthogonal basis of $L^2(\mathcal{Q})$, and

$$B^* v_m = \sigma_m \varphi_m. \tag{4}$$

The terms of the sequence $(\sigma_m)_{m\geq 0}$ are the singular values of B. The positivity of the operator A makes the kernel K be a Mercer kernel. Using Mercer's theorem yields the following decomposition (see [13, Chapter 3.8.2, Proposition 2])

$$K(\gamma, \mu) = \sum_{m\geq 0} \lambda_m\, \varphi_m(\gamma)\varphi_m(\mu), \qquad \text{in} \quad G \times G.$$

This statement comes from the Hilbert-Schmidt theorem on the spectral decomposition of self-adjoint compact operators.
This decomposition results in the POD expansion.

Lemma 2.1 *We have that*

$$T(\gamma, z) = \sum_{m \geq 0} \sigma_m \, \varphi_m(\gamma) \, v_m(z), \quad \text{in } G \times \mathcal{Q}, \tag{5}$$

where the series is convergent in $L^2(G \times \mathcal{Q})$.

The POD expansion is optimal in the L^2-norm (cf. [21], Chapter 2). Indeed, let us denote T_M the truncated POD expansion to the order $M \geq 1$. Then , let W_M be the subspace Span $(w_0, \cdots, w_M) \subset L^2(\mathcal{Q})$. The following holds,

Lemma 2.2 ([13]) *The following inequality holds*

$$\|T - T_M\|_{L^2(G\times\mathcal{Q})} \leq \inf_{S_M \in L^2(G, W_M)} \|T - S_M\|_{L^2(G\times\mathcal{Q})}.$$

3 Analysis of parameterized transient temperatures

We focus here on the homogeneous Dirichlet boundary value problem for the heat equation on a bounded domain $\Omega \subset \mathbb{R}^n$ and a time interval $[0, b]$,

$$\begin{aligned} \partial_t T - \gamma\, \Delta T &= f && \text{in } Q, \\ T &= 0 && \text{in } \partial\Omega \times (0, b), \\ T(x, 0) &= a(x) && \text{in } \Omega, \end{aligned} \tag{6}$$

where $\gamma > 0$ is the thermal conductivity, and we set $\mathcal{Q} = \Omega \times (0, b)$. If $f \in L^2(\mathcal{Q})$ and $a \in L^2(\Omega)$ then problem (6) admits a unique solution $T \in \mathscr{C}([0, b], L^2(\Omega)) \cap L^2(0, b; H^1_0(\Omega))$. In particular, the following stability holds (see [18])

$$\|T(t)\|_{L^2(\Omega)} \leq C(\|a\|_{L^2(\Omega)} + \|f\|_{L^2(Q)}), \qquad \forall t \in (0, b).$$

The constant C depends on b and is independent of γ.

We shall be concerned, in some places, with the thermal conductivity γ ranging in a finite interval G strongly contained in $]0, +\infty[$ that is $G \subset \overline{G} \subset]0, +\infty[$.

Let us consider the POD expansion (5) of the temperature $T = T(\gamma, z)$ as a function in γ and $z = (x, t)$. Then, we denote T_M, the function given the truncated expansion

$$T_M(\gamma, z) = \sum_{m=0}^{M} \sigma_m\, \varphi_m(\gamma) v_m(z). \tag{7}$$

Recall that the sequence T_M converges to T in $L^2(G \times Q)$ with a rate obviously connected with the asymptotics of the singular values. Our purpose is to prove that the rate of convergence is exponential. This requires some beforehand preparation.

Let $(e_\ell = e_\ell(x))_{\ell \geq 0}$ be the orthonormal Fourier basis of $L^2(\Omega)$, formed by eigenfunctions of the Laplace operator,

$$\begin{aligned} -\Delta e_\ell &= \lambda_\ell\, e_\ell && \text{in } \Omega, \\ e_\ell &= 0 && \text{on } \partial\Omega, \end{aligned}$$

where $\lambda_\ell > 0$ is the eigenvalue associated to e_ℓ. The sequence $(\lambda_\ell)_{\ell \geq 0}$ is ordered so that it is non-decreasing. We have that $\lim_{k \to \infty} \lambda_\ell = +\infty$.

For the calculation of the Fourier series of T, we need first the Fourier decompositions of $a(\cdot)$ and $f(\cdot, t)$,

$$a(x) = \sum_{\ell \geq 0} a_\ell\, e_\ell(x), \qquad f(x, t) = \sum_{\ell \geq 0} f_\ell(t)\, e_\ell(x).$$

Their Fourier coefficients are respectively given by

$$a_\ell = (a, e_\ell)_{L^2(\Omega)}, \qquad f_\ell(t) = (f(\cdot, t), e_\ell)_{L^2(\Omega)}.$$

The series are respectively convergent in $L^2(\Omega)$ and $L^2(\mathcal{Q})$, and

$$\|a\|^2_{L^2(\Omega)} = \sum_{\ell \geq 0} |a_\ell|^2, \qquad \|f\|^2_{L^2(\mathcal{Q})} = \sum_{\ell \geq 0} \|f_\ell\|^2_{L^2(0,b)}.$$

Now, based on these Fourier decompositions, the solution of problem (6) can be expressed as

$$T(\gamma, x, t) = \sum_{\ell \geq 0} \theta_\ell(\gamma, t)\, e_\ell(x),$$

where the coefficients $(\theta_k)_{k\geq 0}$ are determined by

$$\theta_\ell(\gamma, t) = a_\ell\, e^{-\gamma\,\lambda_\ell\, t} + \int_0^t f_\ell(s)\, e^{-\gamma\lambda_\ell(t-s)}\, ds. \tag{8}$$

This is set, we consider now the temperature field T as a function mapping the segment $G = [\gamma_m, \gamma_M]$ into $L^2(\mathcal{Q})$. We have that $0 < \gamma_m \leq \gamma_M$, and we denote $|G| = (\gamma_M - \gamma_m)$ the length of G. Finally we introduce

$$\rho_* = \frac{(\sqrt{\gamma_m} + \sqrt{\gamma_M})^2}{\gamma_M - \gamma_m} > 1.$$

The following important approximation result holds.

Theorem 3.1 *Assume that $f \in L^2(\mathcal{Q})$ and $a \in L^2(\Omega)$. The truncated POD series expansion T_M satisfies the error estimate*

$$\|T - T_M\|_{L^2(G\times Q)} \leq C_\rho\, \rho^{-M}, \qquad \forall \rho,\, 1 < \rho < \rho_*, \tag{9}$$

where $C_\rho > 0$ is a constant depending on ρ.

As indicated above, the clue of the proof is the asymptotics of the singular values of the integral operator B, with kernel T. Their decreasing rate is tightly related to the smoothness of the temperature T with respect to the conductivity γ. The proof is long and technical, we chose to expose it in several steps. We start by proving the preliminary statement

Lemma 3.2 Let $g \in L^2(0, b)$ and $\lambda > 0$ be given, the function

$$G : \gamma \mapsto \int_0^t g(s)\, e^{-\gamma\lambda(t-s)}\, ds,$$

mapping $]0, +\infty[$ into $L^2(0, b)$ is analytic.

Proof: To check it out, one could use results from the theory of parameter dependent integrals. We rather follow the direct procedure and show that $\gamma \mapsto G(\gamma)$ is locally expressed as a convergent entire or power series. Let $\gamma_0 > 0$ be fixed. On account of the analyticity of the exponential we derive that

$$G(\gamma, t) = \sum_{n\geq 0} \frac{(\gamma - \gamma_0)^n}{n!} \int_0^t g(s)[-\lambda(t-s)]^n e^{-\gamma_0\lambda(t-s)}\, ds := \sum_{n\geq 0} \frac{(\gamma - \gamma_0)^n}{n!} G_n(t),$$

This series is absolutely convergent in $L^2(0, b)$. Indeed, the integral term being a convolution, then Young's inequality can be used which implies that

$$\begin{aligned}\sum_{n\geq 0} \frac{(\gamma - \gamma_0)^n}{n!} \|G_n\|_{L^2(0,b)} &\leq \sum_{n\geq 0} \frac{(\gamma - \gamma_0)^n}{n!} \|g\|_{L^2(0,b)} \|[-\lambda t]^n e^{-\gamma_0\lambda t}\|_{L^1(0,\infty)} \\ &= \frac{1}{\lambda}\|g\|_{L^2(0,b)} \sum_{n\geq 0} \frac{(\gamma - \gamma_0)^n}{(\gamma_0)^n}.\end{aligned}$$

The geometrical series is convergent for γ such that $|\gamma-\gamma_0| < \eta$ provided that $\eta < \gamma_0$. The function $\gamma \mapsto G(\gamma)$ is then analytic in $]0, +\infty[$ with $L^2(0,b)$ as co-domain. The proof is complete. ∎

Then, we step forth towards the analyticity of the vector-valued function $\gamma \mapsto T(\gamma)$, subject of the following

Lemma 3.3 *The function $\gamma \mapsto T(\gamma)$, mapping $]0, +\infty[$ into $L^2(\mathcal{Q})$, is analytic.*

Proof: According to (8), the temperature field T is the sum of two contributions, one is due to the initial condition $a(\cdot)$ and the other is generated by the source $f(\cdot,\cdot)$. The analyticity is here checked out for each of them.

i. — Let us begin by the part generated by the initial condition

$$T(\gamma, x, t) = \sum_{\ell \geq 0} a_\ell \, e^{-\gamma\lambda_\ell t} \, e_\ell(x).$$

Obviously each of the terms in the series determines an analytic function from $]0, +\infty[$ into $L^2(\mathcal{Q})$. If the series converges uniformly on each interval $[\epsilon, +\infty[$, forall $\epsilon > 0$, then the limit will be analytic in $]0, +\infty[$ (see [16,]). To check this out, let us bound the residual

$$\begin{aligned}
\sup_{\gamma \geq \epsilon} \Big\| \sum_{\ell \geq L} a_\ell e^{-\gamma\lambda_\ell t} \, e_\ell \Big\|^2_{L^2(\mathcal{Q})} &= \sup_{\gamma \geq \epsilon} \sum_{\ell \geq L} (a_\ell)^2 \int_0^b e^{-2\gamma\lambda_\ell t} \, dt \\
&= \sup_{\gamma \geq \epsilon} \sum_{\ell \geq L} (a_\ell)^2 \frac{1 - e^{-2\gamma\lambda_\ell b}}{2\gamma\lambda_\ell} \leq \frac{1}{2\epsilon\lambda_0} \sum_{\ell \geq L} (a_\ell)^2,
\end{aligned}$$

for some $L > 0$. The series is hence uniformly convergent in $]0, +\infty[$ and the limit T determines thus an analytic function in γ.

ii. — The second and last step is to investigate the part arisen from the source f, provided by

$$T(\gamma, x, t) = \sum_{\ell \geq 0} \left(\int_0^t f_\ell(s) \, e^{-\gamma\lambda_\ell(t-s)} \, ds \right) e_\ell(x). \tag{10}$$

According Lemma 3.2, this is a series of analytical functions we shall cope its uniformly convergent in $[\epsilon, +\infty[$, forall $\epsilon > 0$. Before doing so, it is convenient to denote by $F_\ell(\gamma, t)$ the integral term in the infinite sum. Then, for a given L we have that

$$\begin{aligned}
\sup_{\gamma \geq \epsilon} \Big\| \sum_{\ell \geq L} F_\ell(\gamma, \cdot) e_\ell \Big\|^2_{L^2(\mathcal{Q})} &= \sup_{\gamma \geq \epsilon} \sum_{\ell \geq L} \|F_\ell(\gamma, \cdot)\|^2_{L^2(0,b)} \\
&\leq \sup_{\gamma \geq \epsilon} \sum_{\ell \geq L} \|f_\ell\|^2_{L^2(0,b)} \|e^{-\gamma\lambda_\ell t}\|^2_{L^1(0,\infty)} \leq \frac{1}{(\epsilon\lambda_0)^2} \sum_{\ell \geq L} \|f_\ell\|^2_{L^2(0,b)}.
\end{aligned}$$

The last infinite sum decays towards zero when L grows up to infinity. This indicates that the series (10) of analytic functions is uniformly convergent. As a result, the limit is also analytic. The proof is complete. ∎

Remark 3.1 *The analyticity is readily extended to γ belonging to the right half complex plan $(\Re\zeta > 0)$. No changes are required in the proof; it is identical.*

Another preliminary tool required in our study is related to the polynomial approximation of regular vector-valued functions. We shall adapt a result by S. Bernstein (in 1912), stated for complex-valued functions, and improved since then in many works (see for instance [19]). For some $\rho > 1$, let the set E_ρ in the complex plan be defined as

$$E_\rho = \{\zeta \in \mathbb{C}; \qquad |\zeta - 1| + |\zeta + 1| \leq \rho + \rho^{-1}\}.$$

Consider a function $F : E_\rho \to H$ where H is a Hilbert space. For a given integer number $M \geq 0$ let F_M be the truncated Chebyshev polynomial series expansion of F of degree M with coefficients in H. Although the shape of the polynomial F_M will be fixed later on, we do not detail the construction of F_M as we do not need it. Following the proof as exposed in [19], we come up with

Lemma 3.4 *Assume that F is analytic and bounded in E_ρ. There holds that*

$$\max_{\xi \in [-1,1]} \|F(\xi) - F_M(\xi)\|_H \leq C_\rho \, \rho^{-M}.$$

Remark 3.2 *The constant in the lemma may be fixed to*

$$C_\rho = \frac{2}{\rho - 1} \|F\|_{L^\infty(E_\rho)}.$$

It diverges as ρ close to unity.

We now need to derive similar approximation estimates for analytic vector valued functions defined from G into $L^2(G, L^2(\mathcal{Q}))$. Notice first that polynomials S_M with degree $\leq M$ may be written under the following form

$$S_M(\gamma) = \sum_{0 \leq m \leq M} U_m(\gamma) w_m, \qquad \forall \gamma \in G.$$

The symbol U_m is for the polynomial obtained, by transforming to the interval G, the Chebyshev polynomial of degree m, defined in $[-1, 1]$. The coefficients $(w_m)_{0 \leq m \leq M}$ belong of course to $L^2(\mathcal{Q})$. The following result holds

Lemma 3.5 *There exists a polynomial S_M ranging from G into $L^2(\mathcal{Q})$, with degree $\leq M$, such that: forall $\rho\,(1 < \rho < \rho_*)$,*

$$\max_{\gamma \in [\gamma_m, \gamma_M]} \|T(\gamma) - S_M(\gamma)\|_{L^2(\mathcal{Q})} \leq C_\rho \, \rho^{-M},$$

Proof: We only give a sketch of the proof. Following Lemma 3.3 complemented by Remark 3.1, the vector-valued function $\gamma \mapsto T$ is analytic in $]0, +\infty[$. This implies that provided that $\rho < \rho_*$, the ellipse

$$\mathcal{E}_\rho = \left\{\zeta \in \mathbb{C}; \qquad |\zeta - \gamma_M| + |\zeta - \gamma_m| \leq \frac{|G|}{2}(\rho + \rho^{-1})\right\},$$

is included in the analyticity set of T. Consider thus the coordinates transformation([1])

$$\zeta = \tau(\hat{\zeta}) := \frac{|G|}{2}\hat{\zeta} + m_G = \frac{\gamma_M - \gamma_m}{2}\hat{\zeta} + \frac{\gamma_M + \gamma_m}{2}, \qquad \hat{\zeta} \in E_\rho.$$

It is affine and bijective from E_ρ into $\mathcal{E}_\rho$ and transforms the reference interval $[-1, 1]$ into $G = [\gamma_m, \gamma_M]$. This transformation makes it possible to construct such a polynomial S_M. In fact, we start by constructing the truncated Chebyshev series expansion $\hat{S}_M(\hat{\zeta})$ of the (transformed) function $\hat{T}(\hat{\zeta}) = T(\zeta)$. Then, back to the interval G, we set $S_M(\zeta) = \hat{S}_M(\hat{\zeta})$. The error estimate is directly issued from Lemma 3.4. The proof is complete. ∎

Proof of Theorem 3.1: Let S_M be the vector-valued polynomial (in γ) constructed in Lemma 3.5. After applying Lemma 2.2, the following identity holds,

$$\|T - T_M\|_{L^2(G\times\mathcal{Q})} \le \|T - S_M\|_{L^2(G\times\mathcal{Q})} \le |G|^{1/2} \max_{\gamma\in G} \|T(\gamma) - S_M(\gamma)\|_{L^2(\mathcal{Q})}.$$

Applying the result stated in Lemma 3.5 it follows that

$$\|T - T_M\|_{L^2(G\times\mathcal{Q})} \le C_\rho\, \rho^{-M}.$$

The proof of the theorem is complete. ∎

Remark 3.3 *The smoothness of the solution T with respect to $z = (t, x)$ have no effect on the analaysis conducted here. The fact that $T \in L^2(\mathcal{Q})$ is enough to procede with the proof. The rate of the POD-error is only dependent on the regularity of T with repect to the conductivitry γ. Numerical experiences confirm this fact. Similar observations have been already made for elliptic problems* (see [23, 7]).

Bounds for the singular-values $(\sigma_m)_{m\ge 0}$ of the POD operator B may be obtained, as a by-product of the former result.

cor 3.6 *There holds that*

$$\sigma_{M+1} \le C_\rho\, \rho^{-M}, \qquad \forall \rho,\ 1 < \rho < \rho_*.$$

Proof: The proof is based on the Courant-Weyl theorem, deriving bounds of the singular values from the approximation of a compact linear operator by finite rank operators (see [19, Lemma 1]). The following bound holds

$$\sigma_{M+1} = \min_{B_M\in\mathcal{L},\ \mathrm{rank}\ B_M\le M} \|B - B_M\|_{\mathcal{L}}. \tag{11}$$

This result may be encountered under the terminology Schmidt's approximation theorem which is actually an extension to the infinite dimension of the widely known Eckart-Young approximation

[1] The notation m_G is for the middle point of G.

(see [24]).

Now, let $\tilde{B}_M$ be the integral operator associated to the kernel T_M, that is

$$(\tilde{B}_M\varphi)(z) = \int_G T_M(\gamma, z)\varphi(\gamma)\, d\gamma. \qquad \forall z \in \mathcal{Q} \tag{12}$$

It is easily seen that rank $\tilde{B}_M \leq M$. According to the estimate (11), we derive that

$$\sigma_{M+1} \leq \|B - \tilde{B}_M\|_{\mathcal{L}} \leq \|T - T_M\|_{L^2(G\times\mathcal{Q})}.$$

Calling for Theorem 3.1 yields the result and completes the proof. ∎

Remark 3.4 *A similar analysis applies to mixed homogeneous Neumann, Neumann-Dirichlet or Robin conditions. with the necessary modifications skipped over here. They are not difficult to understand and their realization seems straightforward.*

4 Numerical experiments

This section is devoted to determining the effective convergence rate of the POD approximation of some solutions to the transient heat equation when parameterized by the conductivity coefficient. We first assess the exponential convergence rate and then, we investigate the variation of this rate with respect to the interval $G = [\gamma_m, \gamma_M]$. We also study the approximation of the heat equation by the POD expansion in norms stronger than $L^2(G, L^2(\mathcal{Q}))$. We evaluate the convergence in the space $L^2(G, L^2(0, b; H^1(\Omega))$. As will be confirmed, we still recover an exponential convergence rate in all cases.

We consider the time-dependent heat equation in the domain $\mathcal{Q} = (0,1) \times (0,1)$ and we select three possible pairs of source terms and boundary conditions, given by

$$\begin{aligned}
&\textbf{Data 1:} \qquad f(t,x) = \sqrt{|x-t-0.3|}, \qquad T_0(x) = 0,\\
&\textbf{Data 2:} \qquad f(t,x) = 0, \qquad T_0(x) = |x-0.4|,\\
&\textbf{Data 3:} \qquad f(t,x) = \sqrt{|x-t-0.3|}, \qquad T_0(x) = |x-0.4|.
\end{aligned}$$

These data have singularities, so the temperature solutions of (6), have a low regularity with respect to x and t, in particular for $t = 0$ for the two last data. The heat problem is discretized by an Euler scheme/Gauss-Lobatto-Legendre spectral method see [4] (the time step is $\delta t = 10^{-2}$ and the polynomial degree is $N = 64$).
Calculation for the matrix representations of the POD operators B and A are realized by means of accurate quadrature formulas. Indeed, various integrals (with respect to either γ or (t,x)) are computed using Gauss-Lobatto quadrature formulas with high resolution in the corresponding intervals. The singular value decomposition is therefore achieved using the iterative PGD procedure (see [5]). Let us observe that the temperatures computed as solutions of the heat equation by the numerical procedures are used as the “exact” or “reference” solutions to compute for each case of the POD expansions.

Test 1: Exponential convergence rate.
To test the exponential convergence speed predicted by Theorem 3.1, we fix the thermal conductivities interval to $G = [1, 100]$. We display, in the left panel of Figure 1, the convergence history of the POD expansion in terms of the number of modes in the expansion, for the three solutions of the heat equation (7). Here and in the subsequent, all the curves are drawn in a semi-logarithmic scale. We observe that the POD error, the norm of $(T - T_M)$ in $L^2(G \times \mathcal{Q})$, decays exponentially fast according to the theoretical findings. In the right panel we draw the singular values. They are decreasing exponentially fast. Moreover, we aim to illustrate the POD-error for a cut-off M is equivalent to the singular-value σ_{M+1} as predicted

$$\|T - T_M\|_{L^2(G\times\mathcal{Q})} = C_\rho\, \rho^{-M}, \qquad \sigma_{M+1} = \|T - T_M\|_{L^2(G\times\mathcal{Q})}.$$

Then, in Figure 2 , are depicted the curves representing the variations of $\|T - T_M\|_{L^2(G\times\mathcal{Q})}$ and σ_{M+1} with respect to M. In the range of $M(2 \leq M \leq 15)$, they almost coincide. Recall that the truncation is the sum of $(\sigma_m)_{m\geq M+1}$. The fact that it is close to σ_{M+1} is in agreement with the exponential convergecne rate.

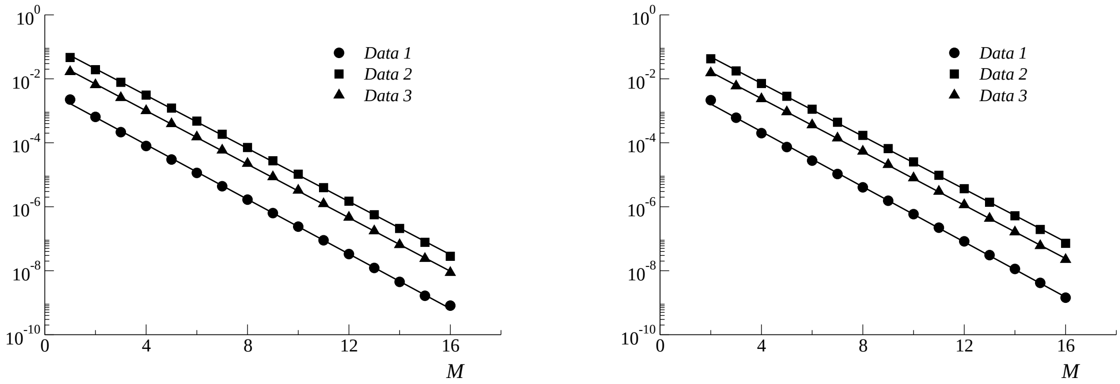

Figure 1: History for the POD-error (left). Largest singular values (σ_M) (right).

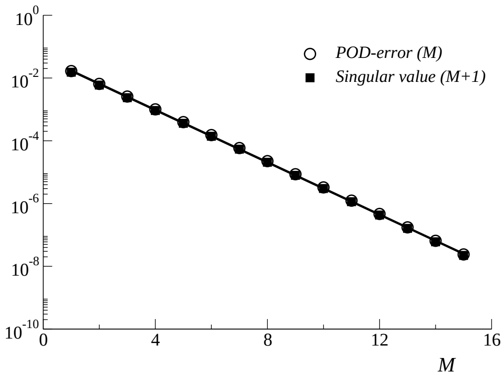

Figure 2: POD-error $\|T - T_M\|_{L^2}$ and the singular value σ_{M+1} (for Data 1).

Test 2: Dependence of the convergence rate with respect to the conductivities range.
The dependence with respect to the interval G of the exponential convergence rate, stated by Theorem 3.1, is illustrated in Figure 3. We depict the convergence history for Data 3, computed for three different ranges $G = [\gamma_m, \gamma_M]$ of thermal conductivities, that is $|G| = (\gamma_M - \gamma_m) = 1, 3$ and 10. The origin of the interval G is located at three possible positions, $\gamma_m = 1, 5$ or 10. Two facts can be immediately pointed out. First, the convergence rate degrades for longer intervals, when γ_M increases. This is in accordance with the fact that

$$\rho_* = \frac{(\sqrt{\gamma_m} + \sqrt{\gamma_M})^2}{\gamma_M - \gamma_m},$$

decrease when γ_M increases up. The second is that the truncated POD converges faster for greater

γ_m. This fact is also predicted since the analyticity domain of T becomes larger and so does ρ_*. In Table 1, we present the computed exponential rates $\rho = \rho_c$ (by calculating the exponential regression) and the theoretical ones given by $\rho = \rho_*$. We observe that the computed convergence rate increases as the theoretical one increases. Notice that ratio of both convergence rates suggests that the effective convergence is two times faster than the theoretical one. A possible explanation is that the truncated POD expansion gives an approximation more accurate than the truncated Chebyshev series expansion, on which the result of Theorem 3.1 relies. The convergence is *twice* faster for the POD-approximation.

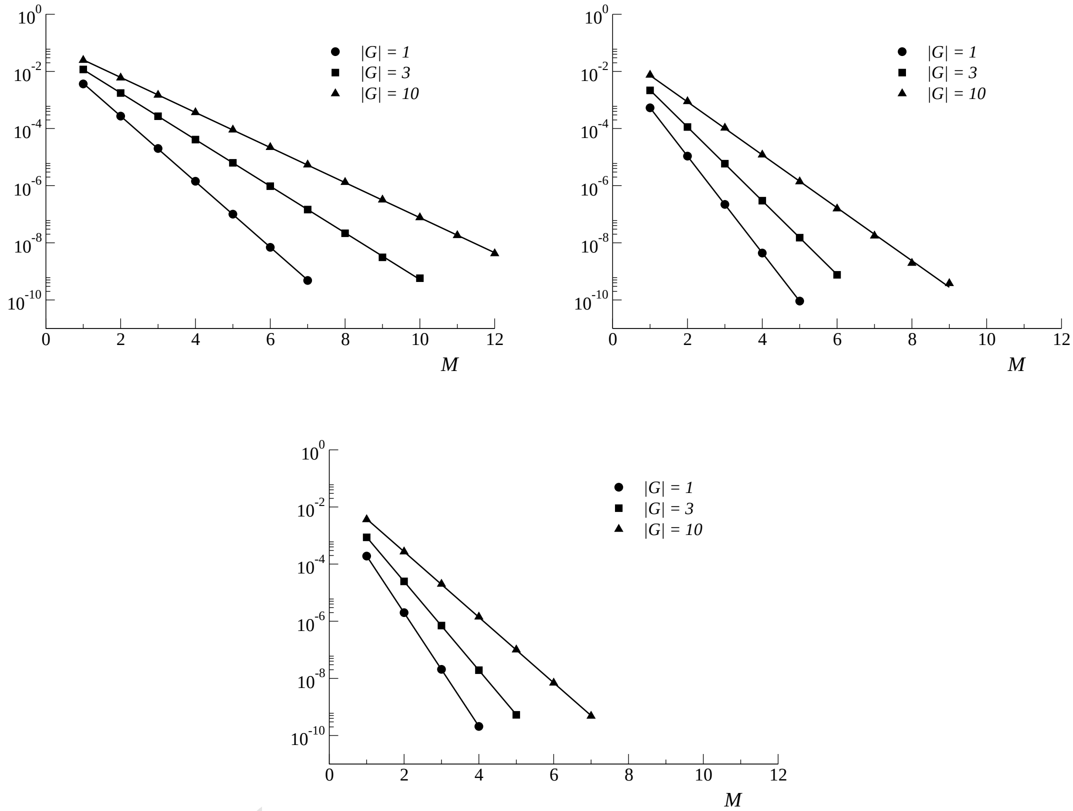

Figure 3: Variation of the POD-errors. Each diagram corresponds to a different location of $\gamma_m = 1, 5$ or 10. In each plot three cases are considered, the conductivities range equals $1, 3$ or 10.

$\lvert G\rvert$	ρ_*	ρ_c	Ratio	ρ_*	ρ_c	Ratio	ρ_*	ρ_c	Ratio
1	5.82	12.81	2.20	9.40	21.95	2.25	41.97	96.54	2.29
3	3.00	6.36	2.12	8.55	19.49	2.28	15.26	35.51	2.32
10	1.86	4.06	2.18	3.73	8.41	2.25	5.83	14.01	2.40

Table 1: Convergence rates, with $\gamma_m = 1, 5$ and 10 (for Data 3).

Test 3: Approximation in stronger norms.

The target is the numerical assessment of the convergence rate of the POD approximation with respect to the natural energy norm of $L^2(G; L^2(0, b; H^1(\Omega)))$. We intend to find out the variations of the following error correspondence

$$M \mapsto \left[\int_G \int_{\mathcal{Q}} |\nabla_x (T - T_M)|^2(\gamma, z)\, d\gamma\, dz \right]^{1/2}.$$

The case selected is related to Data 3. Figure 4 plots the convergence history of the above function together with the $(T - T_M)$ measured in the Lebesgue space $L^2(G, L^2(\mathcal{Q}))$ already provided in Figure 1. Calculations have been done for two sets of discretizations. Mesh 1 corresponds to $\delta t = 10^{-2}$, $N = 64$ and 100 values of the conductivity coefficient while mesh 2 is given by $\delta t = 10^{-3}$, $N = 72$ and 200 values of the conductivity coefficient. In any case, we still recover the optimal exponential convergence rate although the proof is still missing for the stronger (energy) norm.

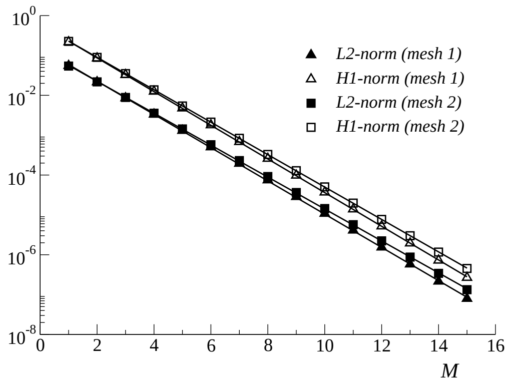

Figure 4: POD-error in norms of $L^2(G, L^2(\mathcal{Q}))$ and $L^2(G; L^2(0, b; H^1(\Omega)))$ (for Data 3).

5 Conclusion

We have studied the approximation of the solutions of the heat equation, understood as a parametrized fields with respect to the conductivity parameter. We have proved that the POD expansion converges with exponential accuracy in the natural L^2 norms associated with the POD expansion. Our analysis can readily be extended to parabolic equations with symmetric elliptic operators. Extension to higher order decompositions and multi-parameters is under study.

References

[1] Adams, Robert A. and Fournier, John J. F., Sobolev Spaces, Academic Press. 2003

[2] Azaïez, M. and Ben Belgacem, F., Karhunen-Loève's truncation error for bivariate functions, Computer Methods in Applied Mechanics and Engineering, Vol 290, pp 57-72, 2015

[3] Berkoz, G. and Holmes, P. and Lumley, J. L., The proper orthogonal decomposition in the analysis of turbulent flows, Annu. Rev. Fluids Mech., Vol 25, pp 539-575, 1993

[4] Bernardi, C. and Maday, Y., Approximations spectrales de problèmes aux limites elliptiques, Mathématiques et applications, Springer, Paris, Berlin, Heidelberg, 1992

[5] Chinesta, F. and Keunings, R. and Leygue, A., The Proper Generalized Decomposition for Advanced Numerical Simulations: A Primer, Springer Publishing Company, Incorporated, 2013

[6] Chinesta F., Ladevese P. and Cueto E., A Short Review on Model Order Reduction Based on Proper Generalized Decomposition, Archives of Computational Methods in Engineering, Vol 18, pp 395-404, 2011

[7] Cohen, A. and DeVore, R. A. and Schwab Ch., Analytic regularity and polynomial approximation of parametric and stochastic elliptic PDEs, Analysis and Applications, Vol 09, pp 11-47, 2011

[8] Diestel, J. and Uhl, J. J. , Vector measures, AMS, 1977

[9] Epureanu, B. I. and Tang, L. S. and Paidoussis, M. P., Coherent structures and their influence on the dynamics of aeroelastic panels , International Journal of Non-Linear Mechanics , Vol 39, pp 977-991, 2004

[10] Ghanem, R. and Spanos, P. , Stochastic finite elements: a spectral approach. Springer-Verlag. 1991.

[11] Golub, G. H. and Loan, C. F. Van, Matrix Computations 3rd, The Johns Hopkins University Press, 1996.

[12] Haasdonk, B., Convergence Rates of the POD-Greedy Method, Modlisation Mathmatique et Analyse Numrique, M2AN, Vol 47, pp 859-873, 2013

[13] Holmes, P. and Lumley, J. L. and Berkooz, G. , Coherent Structures, Synamical Systems and Symmetry , Cambridge Monographs on Mechanis, Cambridge University Press, Cambridge, 1996

[14] Hotelling, H., Analysis of a complex of statistical variables into principal componentse, Journal of Educational Psychology, Vol 24,pp 417-441, 498-520 , 1933

[15] Jolliffe, I. T., Principal Component Analysis, Springer, 1986

[16] Knopp, K. and Bagemihl, F. Theory of Functions, Vol. 1, Dover books on mathematics, Dover Publications 1996

[17] Kunoth, A. and Schwab, Ch., Analytic Regularity and GPC Approximation for Control Problems Constrained by Linear Parametric Elliptic and Parabolic PDEs, SIAM Journal on Control and Optimization, Vol 51, pp 2442–2471, 2013

[18] Lions, J. L. and Magenes, E., Problèmes aux Limites Non Homogènes et Applications, Dunod Vol 2, pp 253-263, 1968

[19] Little, G. and Reade, J. B., Eigenvalues of analytic kernels., SIAM J. Math. Anal, Vol 15, pp 133-136, 1984

[20] M. M. Loève, Probability Theory, Van Nostrand, Princeton, NJ, 1988

[21] Muller, M. , On the POD Method. An Abstract Investigation with Applications to Reduced-Order Modeling and Suboptimal Control, Ph D Thesis, Georg-August Universität, Göttingen, 2008

[22] Pearson, K., On lines and planes of closest fit system of points in space, Philo. Mag. J. Sci., Vol 2, pp 559-572, 1901

[23] Rozza, G and Huynh, D.B.P. and Patera, A.T., Reduced Basis Approximation and a Posteriori Error Estimation for Affinely Parametrized Elliptic Coercive Partial Differential Equations., Arch Comput Methods Eng, Vol 15, pp 229-275, 2008

[24] Stewart, G. W., On the Early History of the Singular Value Decomposition., SIAM Review, vol 35, pp 551-566, 1993

[25] Willcox, K. and Peraire, J., Balanced Model Reduction via the Proper Orthogonal Decomposition, AIAA, Vol 40, pp 2323-2330, 2002

[26] Yano, M., A Space-Time Petrov–Galerkin Certified Reduced Basis Method: Application to the Boussinesq Equations, SIAM J. Sci. Comput., Vol 36, pp 232-266, 2013