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Abstract

In this work we discuss the Dynamically Orthogonal (DO) approximation of time dependent partial differential equations with random data. The approximate solution is expanded at each time instant on a time dependent orthonormal basis in the physical domain with fixed and small number of terms. Dynamic equations are written for the evolution of the basis as well as the evolution of the stochastic coefficients of the expansion.

We analyze the case of a linear parabolic equation with random data and derive a theoretical bound for the approximation error of the S -terms DO solution by the corresponding S -terms best approximation, i.e. the truncated S -terms Karhunen-Loève expansion at each time instant, under the assumption that the latter is continuously differentiable in time. Properties of the DO approximations are analyzed on simple cases of deterministic equations with random initial data. Numerical tests are presented that confirm the theoretical bound and show potentials and limitations of the proposed approach.

Keywords: Dynamically Orthogonal approximation, parabolic PDEs with random parameters, Dynamical Low Rank approximation.

1 Introduction

Many physical and engineering problems can be properly described by mathematical models, typically of differential type. However, in many situations, the input parameters may be affected by uncertainty due e.g. to measurement errors, limited data availability or intrinsic variability of the phenomenon itself. A convenient way to characterize uncertainty consists in describing the uncertain parameters as random variables or space and/or time varying random fields. Starting from a suitable Partial Differential Equation (PDE) model, the aim of the Uncertainty Quantification is to assess the effects of the uncertainty by computing the statistics of the solutions or of some quantities of interest. Several approaches have been proposed and analyzed

in the last decades. We name the Monte Carlo method [5, 7], Quasi Monte Carlo [6, 37] and the corresponding Multilevel versions [36], or the approaches based on deterministic approximations of the parameters-to-solution map (response function) such as the generalized Polynomial Chaos [8, 9, 27, 44] in its Galerkin [10, 42, 43] and collocation versions [1–3, 23, 24].

In this work we focus on a reduced basis method to approximate the solution. We consider a general type of time dependent PDE with random data of the form:

$$\begin{cases} \frac{\partial u(x,t,\omega)}{\partial t} = \mathcal{L}(u(x,t,\omega), \omega), & x \in D, t \in \mathcal{T}, \omega \in \Omega, \\ \mathcal{B}(u(\sigma, t, \omega)) = h(\sigma, t), & \sigma \in \partial D, t \in \mathcal{T}, \omega \in \Omega, \\ u(x, t = 0, \omega) = u_0(x, \omega), & x \in D, \omega \in \Omega, \end{cases} \quad (1)$$

where $x \in D \subset \mathbb{R}^d$ is the spatial coordinate, t is the time variable in $\mathcal{T} \equiv [0, T]$ and ω is the random elementary event in the complete probability space $(\Omega, \mathcal{A}, \mathcal{P})$. In addition \mathcal{L} is a general (linear or non linear) differential operator and \mathcal{B} is an operator defining the boundary conditions. Here the randomness can appear in the operator \mathcal{L} as a random parameter or forcing term as well as in the initial datum. A possible approach to approximate the solution consists in expanding u on a deterministic (Proper Orthogonal Decomposition- POD [26, 45, 46]) or stochastic (gPC [4, 9, 21]) set of orthogonal basis functions, performing a Galerkin projection and computing the coefficients at any time step. Specifically the POD method requires a set of pre-computed snapshots for different parameter values and time instants. However, since the dependence of the solution on the random parameters may significantly vary in time, any approximation which makes use of time fixed basis functions (either deterministic or stochastic), necessarily requires during the evolution an increasing number of terms to maintain a proper level of accuracy and, in general, needs a very high computational effort. Several adaptive and greedy type techniques have been proposed in the literature to (partially) overcome this problem, e.g. time-dependent gPC [38, 39] and Generalized POD [40, 41, 47]. On the other hand, in many cases, the collection of all solutions at a given time corresponding to all possible outcomes of the input random processes can still be well approximated in a low dimensional subspace, which however, will change at each time instant.

It is well known that the optimal S -dimensional subspace, in L^2 sense, is the one which is spanned by the first S terms of the Karhunen-Loève decomposition of the solution [10, 22, 27]. The main practical difficulty is that such subspace is, in general, not easy to characterize a priori and might significantly change in time. Therefore the idea of the approach proposed here is to approximate the solution on an evolving subspace, exploiting the structure of the differential equation. In other words, the approximate solution is expanded on a dynamical deterministic orthonormal basis with stochastic coefficients which evolve in time as well, i.e.:

$$u_S(x, t, \omega) = \bar{u}_S(x, t) + \sum_{i=1}^S Y_i(t, \omega) U_i(x, t), \quad (2)$$

Here $\bar{u}_S(x, t) \simeq \mathbf{E}[u(x, t, \cdot)]$ is the approximated expected value, U_1, \dots, U_S are $L^2(D)$ -orthonormal deterministic basis functions and Y_1, \dots, Y_S are zero mean stochastic variables. The approximate solution (2) is obtained by suitably projecting the residual of the differential equation (non linear

Galerkin projection) and aims to be close enough to the Karhunen-Loève decomposition, even if it does not coincide, in general, with it.

This approach is not new; it has been introduced in [18] and named “Dynamically Orthogonal” approximation (DO) and applied in [19,20] to the approximation of fluid equations with random initial data. Analogous formulations are also used in [28,29,35]. On the other hand, similar ideas have been developed in a quite different context, namely in chemistry and quantum dynamics, for the approximation of the deterministic Schrödinger equations by the Multi-Configuration time-dependent Hartree method (MCTDH, [13,14]) and the Dirac-Frenkel Variation principal [30,31]. There, the goal is to look for an approximate solution written in separable form as product of functions depending on one space variable only, whereas in the DO approach presented here, we aim at separating the space variables from the stochastic ones. The discrete analogue of the MCTDH method consists in looking for a Dynamical Low Rank approximation of a deterministic evolution matrix or tensor equation [11,12,17]. A few theoretical results are available on the accuracy and error estimates for either the MCTDH approximation of Schrödinger equations or Dynamical Low Rank approximation of matrix equations [11,14].

Our first goal in this paper is to establish a precise link between the DO approach (as proposed in [18]) and the Dynamical Low Rank approximation analyzed e.g. in [11]. This allows us to “import” some of the theoretical results developed in [11,14] to our situation of a parabolic equation with random parameters. In particular, we reinterpret the DO equations given in [18–20] as a Galerkin projection onto the tangent space to the manifold of the rank S functions of the form (2). Using curvature bounds for such manifold, given in [14], we show that the DO approximation error for a linear parabolic equation with random input data can be bounded in terms of the best rank S approximation of the solution (Karhunen-Loève expansion), at each time instant, under the assumption that the latter is differentiable in time. This assumption is actually unavoidable and corresponds to the requirement that the eigenvalues of the Karhunen-Loève decomposition do not cross in time. By means of simple examples with a deterministic linear operator and random initial datum, we highlight how and when the crossing of the eigenvalues negatively effects the DO approximation. In particular we show in which cases, for a deterministic operator, the DO solution is exact and on the other hand, when the DO error can not be properly bounded by the best approximation error. Finally we describe the numerical method that we have adopted in this work and the technique utilized to deal with singular covariance matrices. We conclude with some numerical examples in which we specifically address: *i*) a deterministic linear parabolic equation with random initial condition, *ii*) a linear parabolic equation with stochastic coefficient and deterministic initial datum, *iii*) a non-linear parabolic equation of reaction-diffusion type.

The outline of the paper is as follows: in Section 2 we introduce the mathematical problem and basic notations; in Section 3 we describe the DO approximation, we show the analogy with the dynamical low rank approach and we give a variational interpretation of it. In Section 4 the DO approximation is applied to a linear stochastic parabolic equation and an analysis of the DO approximation error is provided. In Section 5 we analyze the case of a linear deterministic operator. Finally in Section 6 we describe the numerical discretization of the DO equations and we present several numerical test cases that will show when the DO approximation is effective and when is not.

2 Problem setting

Let $D \subset \mathbb{R}^d$, $1 \leq d \leq 3$, be an open bounded domain and $(\Omega, \mathcal{A}, \mathcal{P})$ a complete probability space, where Ω is the set of outcomes, \mathcal{A} a σ -algebra and $P : \mathcal{A} \rightarrow [0, 1]$ a probability measure. The problem considered in this paper is the following time dependent stochastic PDE:

$$\frac{\partial u(x, t, \omega)}{\partial t} = \mathcal{L}(u(x, t, \omega), \omega), \quad x \in D, t \in \mathcal{T}, \omega \in \Omega, \quad (3)$$

where \mathcal{L} is a general (linear or non-linear) differential operator, $x \in D$ is the spatial coordinate and t is the time variable in $\mathcal{T} \equiv [0, T]$. Additionally, the initial state of the problem is described by

$$u(x, t = 0, \omega) = u_0(x, \omega), \quad x \in D, \omega \in \Omega, \quad (4)$$

and the (deterministic) boundary condition is given by

$$\mathcal{B}(u(\sigma, t, \omega)) = h(\sigma, t), \quad \sigma \in \partial D,$$

where \mathcal{B} is a linear differential or algebraic operator. We specifically address the parabolic case in which \mathcal{L} is an elliptic second order differential operator in the space variable x . For a random function $v(x, t, \omega)$, we define its mean value as

$$\bar{v}(x, t) = \mathbb{E}[v(x, t, \cdot)] = \int_{\Omega} v(x, t, \omega) d\mathcal{P}(\omega),$$

as well as the L^2 inner product in the physical space

$$\langle u(\cdot, t, \omega), v(\cdot, t, \omega) \rangle = \int_D u(x, t, \omega) v(x, t, \omega) dx.$$

In what follows we use the notation

$$u^*(x, t, \omega) = u(x, t, \omega) - \mathbb{E}[u(x, t, \cdot)]$$

We assume that all the random fields considered in this paper are square integrable for any $t \in \mathcal{T}$, that is,

$$\int_D \mathbb{E}[u^2(x, t, \cdot)] dx < +\infty \quad \forall t \in \mathcal{T}.$$

As the approaches considered in this work have a strong relationship with the Karhunen-Loève expansion, we review some basic properties of the latter. To begin with, let us define the covariance function of a space-dependent random field $u(x, \omega)$ as

$$\text{Cov}_u(x, y) = \mathbb{E}[u^*(x, \cdot) u^*(y, \cdot)], \quad x, y \in D.$$

It is well known that any second order random field $u(x, \omega)$, with continuous and positive definite covariance function $\text{Cov}_u : \overline{D} \times \overline{D} \rightarrow \mathbb{R}$, can be represented as an infinite sum of random variables, by means of the Karhunen-Loève expansion [10]. To this end, we introduce the compact and self-adjoint operator $T_u : L^2(D) \rightarrow L^2(D)$, which is defined by

$$T_u v(\cdot) = \int_D \text{Cov}_u(x, \cdot) v(x) dx, \quad \forall v \in L^2(D). \quad (5)$$

Then, consider the sequence of non-negative decreasing eigenvalues of T_u , $\{\mu_i\}_{i=1}^\infty$, and the corresponding sequence of orthonormal eigenfunctions, $\{Z_i\}_{i=1}^\infty$, satisfying

$$T_u Z_i = \mu_i Z_i, \quad \langle Z_i, Z_j \rangle = \delta_{ij} \quad \forall i, j \in \mathbb{N}^+, \quad (6)$$

where δ_{ij} is the Kronecker symbol. In addition, define the mutually uncorrelated real random variables

$$\gamma_i(\omega) := \frac{1}{\sqrt{\mu_i}} \int_D u^*(x, \omega) Z_i(x) dx \quad \forall i \in \mathbb{N}^+, \quad (7)$$

with zero mean and unit variance, i.e. $\mathbb{E}[\gamma_i] = 0$ and $\mathbb{E}[\gamma_i \gamma_j] = \delta_{ij}$ for $i, j \in \mathbb{N}^+$. Then, the truncated Karhunen-Loève expansion of the stochastic function u , which we denote by z_S , is defined by

$$z_S(x, \omega) = \bar{u}(x) + \sum_{i=1}^S \sqrt{\mu_i} \gamma_i(\omega) Z_i(x), \quad \forall S \in \mathbb{N}^+. \quad (8)$$

By Mercer's theorem [22], it follows that

$$\lim_{S \rightarrow \infty} \sup_{x \in D} \mathbb{E}[(u(x, \cdot)) - z_S(x, \cdot)]^2 = \lim_{S \rightarrow \infty} \sup_{x \in D} \sum_{i=S+1}^{\infty} \mu_i Z_i^2(x) = 0.$$

Observe that the S random variables in (7), describing the approximate random function z_S (8), are weighted differently due to the decay of the eigenvalues of the Karhunen-Loève expansion. The decay properties of eigenvalues and eigenvectors has been investigated e.g. in the works [10, 32].

In the case of a time-varying random field $u(x, t, \omega)$, the truncated Karhunen-Loève expansion at each fixed $t \in \mathcal{T}$ would read

$$z_S(x, \omega, t) = \bar{u}(x, t) + \sum_{i=1}^S \sqrt{\mu_i(t)} \gamma_i(t, \omega) Z_i(x, t), \quad \forall S \in \mathbb{N}^+ \quad (9)$$

with $\langle Z_i(\cdot, t), Z_j(\cdot, t) \rangle = \delta_{ij}$, $\forall t \in \mathcal{T}$.

3 Dynamically Orthogonal approximation

Several approaches have been proposed in the literature to numerically compute the random solution $u(x, t, \omega)$ of PDEs with stochastic input data. For instance, in a generalized Polynomial Chaos (gPC) approach (see e.g. [8, 9, 27]), after parameterizing the probabilistic space by a sequence of random variables $\{\eta_i\}_{i \geq 1}$, the solution is expanded on a fixed basis of orthogonal polynomials in η_i with space and time varying coefficients:

$$v_S(x, t, \omega) = \bar{v}_S(x, t) + \sum_{i=1}^S V_i(x, t) \Phi_i(\eta_1(\omega), \eta_2(\omega), \dots) = \bar{v}_S(x, t) + \sum_{i=1}^S V_i(x, t) \tilde{\Phi}_i(\omega),$$

and $\mathbb{E}[\tilde{\Phi}_i \tilde{\Phi}_j] = \delta_{ij}$.

Unlike the gPC approach, the Dynamically Orthogonal (DO) approximation, first introduced in [18], utilizes a more general expansion

$$u_S(x, t, \omega) = \bar{u}_S(x, t) + \sum_{i=1}^S U_i(x, t) Y_i(t, \omega). \quad (10)$$

Namely, both the spatial basis $\{U_i(x, t)\}_{i=1}^S$ and the random basis $\{Y_i(t, \omega)\}_{i=1}^S$ are time dependent and either U_i or Y_i are kept orthogonal at all times, thus aiming to mimic the Karhunen-Loève expansion (9). Note that the above approximations are finite sums where the index S represents the approximation level.

In what follows we focus on the case where the spatial basis $\{U_i\}_{i=1}^S$ is kept orthogonal at all times. The uniqueness of the DO approximation (10) is guaranteed by the following *dynamically orthogonal* conditions [18], [19], [20]:

$$\mathbb{E}[Y_i(t, \cdot)] = 0, \quad \langle U_i(\cdot, t), U_j(\cdot, t) \rangle = \delta_{ij}, \quad \left\langle \frac{\partial U_i(\cdot, t)}{\partial t}, U_j(\cdot, t) \right\rangle = 0, \quad 1 \leq i, j \leq S, \quad \forall t \in \mathcal{T}. \quad (11)$$

Given problem (3), by using together the Galerkin projection onto the subspaces spanned by the basis functions in (10) and the DO conditions (11), one gets the following DO system [18], [19], [20]:

$$\frac{\partial \bar{u}_S(x, t)}{\partial t} = \mathbb{E}[\mathcal{L}(u_S(x, t, \cdot))] \quad (12)$$

$$\sum_{i=1}^S \mathbf{C}_{ij}(t) \frac{\partial U_i(x, t)}{\partial t} = \Pi_{\mathcal{U}}^{\perp} \mathbb{E}[\mathcal{L}(u_S(x, t, \cdot)) Y_j(t, \cdot)] \quad j = 1, \dots, S \quad (13)$$

$$\frac{\partial Y_i(t, \omega)}{\partial t} = \langle \mathcal{L}^*(u_S(\cdot, t, \omega), \omega), U_i(\cdot, t) \rangle \quad i = 1, \dots, S \quad (14)$$

where

$$\begin{aligned} \mathbf{C}_{ij}(t) &= \mathbb{E}[Y_i(t, \cdot) Y_j(t, \cdot)], \quad \forall i, j = 1, \dots, S, \\ \mathcal{L}^*(u(x, t, \omega), \omega) &= \mathcal{L}(u(x, t, \omega), \omega) - \mathbb{E}[\mathcal{L}(u(x, t, \cdot))] \end{aligned}$$

and $\Pi_{\mathcal{U}}^{\perp}$ is the projection operator from the space $L^2(D)$ to the orthogonal complement of the S dimensional subspace $\mathcal{U} = \text{span}\{U_1, \dots, U_S\}$, namely,

$$\Pi_{\mathcal{U}}^{\perp}[v] = v - \Pi_{\mathcal{U}}[v] = v - \sum_{i=1}^S \langle v, U_i \rangle U_i, \quad \forall v \in L^2(D).$$

The associated boundary conditions have the form

$$\mathcal{B}(\bar{u}_S(\sigma, t)) = h(\sigma, t), \quad \sigma \in \partial D \quad (15)$$

$$\sum_{i=1}^S \mathbf{C}_{ij}(t) \mathcal{B}(U_i(\sigma, t)) = 0, \quad \sigma \in \partial D, \quad j = 1, \dots, S \quad (16)$$

and the corresponding initial conditions are given by

$$\bar{u}_S(x, 0) = \bar{u}_0(x) = \mathbb{E}[u_0(x, \cdot)], \quad U_i(x, 0) = Z_{i0}(x), \quad Y_i(0, \omega) = \langle u_0(\cdot, \omega) - \bar{u}_0, Z_{i0} \rangle, \quad (17)$$

where $\{Z_{i0}(x)\}_{i=1}^S$ are the spatial basis functions appearing in the Karhunen-Loève expansion of $u_0(x, \omega)$.

Note that the DO equations (12)-(14) are coupled together, in general. By solving this system, one easily gets the approximation of the mean and of the total variance of the solution:

$$\mathbb{E}[u(x, t, \cdot)] \approx \mathbb{E}[u_S(x, t, \cdot)] = \bar{u}_S(x, t), \quad \text{Var}_T[u](t) \approx \text{Var}_T[u_S](t) = \sum_{i=1}^S \mathbb{E}[Y_i^2(t)].$$

where the total variance is defined as $\text{Var}_T[u](t) = \int_D \mathbb{E}[(u(x, t, \cdot) - \bar{u}(x, t, \cdot))^2] dx$. Concerning the numerical approximation of the DO system (12)-(14), many approaches can be followed, among which the Finite Elements or the Finite Difference methods for spacial discretization and the Stochastic Collocation [1, 3, 24], gPC [9, 25] or (Quasi) Monte Carlo [5, 7] methods for the stochastic discretization. Any time splitting scheme can be adopted for the time derivative discretization, but care should be taken in respecting exactly or with good accuracy, the DO conditions (11) at each time step.

3.1 Dynamically Double Orthogonal approximation

The DO conditions (11) in the derivation of the DO approach are somehow unsymmetric as only the deterministic fields $\{U_i\}_{i=1}^S$ are required to be orthogonal. An alternative approach consists in considering a double orthogonal basis $\{\tilde{U}_i\}_{i=1}^S$ and $\{\tilde{Y}_i\}_{i=1}^S$ and the general formulation:

$$u(x, t, \omega) \approx \tilde{u}_S(x, t, \omega) = \tilde{u}_S(x, t) + \sum_{i,j=1}^S A_{ij}(t) \tilde{U}_i(x, t) \tilde{Y}_j(t, \omega) = \tilde{u}_S + \tilde{\mathbf{U}}^T \mathbf{A} \tilde{\mathbf{Y}}, \quad (18)$$

with notations

$$\tilde{\mathbf{U}} = (\tilde{U}_1, \dots, \tilde{U}_S)^T, \quad \mathbf{A} = (A_{ij})_{i,j=1}^S, \quad \tilde{\mathbf{Y}} = (\tilde{Y}_1, \dots, \tilde{Y}_S)^T.$$

Here we require that both $\{\tilde{U}_i\}_{i=1}^S$ and $\{\tilde{Y}_i\}_{i=1}^S$ are dynamically orthonormal, or rather:

$$\mathbb{E}[\tilde{Y}_i(t, \cdot)] = 0, \quad \forall 1 \leq i \leq S, \quad (19)$$

$$\langle \tilde{U}_i(\cdot, t), \tilde{U}_j(\cdot, t) \rangle = \delta_{ij}, \quad \mathbb{E}[\tilde{Y}_i(\cdot, t), \tilde{Y}_j(\cdot, t)] = \delta_{ij}, \quad \forall 1 \leq i, j \leq S, \quad (20)$$

$$\left\langle \frac{\partial \tilde{U}_i(\cdot, t)}{\partial t}, \tilde{U}_j(\cdot, t) \right\rangle = 0, \quad \mathbb{E} \left[\frac{\partial \tilde{Y}_i(\cdot, t)}{\partial t}, \tilde{Y}_j(\cdot, t) \right] = 0, \quad \forall 1 \leq i, j \leq S. \quad (21)$$

Analogously to what has been done in the DO approximation, one can easily derive the following dynamically double orthogonal (DDO) system:

$$\frac{\partial \tilde{u}_S(x, t)}{\partial t} = \mathbb{E} [\mathcal{L}(\tilde{u}_S(x, t, \cdot))], \quad (22)$$

$$\frac{d}{dt} \mathbf{A}(t) = \mathbb{E} \left[\left\langle \mathcal{L}^*(\tilde{u}_S(\cdot, t, \cdot)), \tilde{\mathbf{U}}^T(\cdot, t) \right\rangle \mathbf{Y}(\cdot, t)^T \right], \quad (23)$$

$$\mathbf{A}^T(t) \frac{\partial \tilde{\mathbf{U}}(x, t)}{\partial t} = \Pi_{\tilde{\mathcal{U}}}^\perp \mathbb{E} \left[\tilde{\mathbf{Y}}(\cdot, t) \mathcal{L}^*(\tilde{u}_S(\cdot, t, \cdot)) \right] \quad (24)$$

$$\mathbf{A}(t) \frac{\partial \tilde{\mathbf{Y}}(t, \omega)}{\partial t} = \Pi_{\tilde{\mathcal{Y}}}^\perp \left\langle \mathcal{L}^*(\tilde{u}_S(\cdot, t, \omega), \omega), \tilde{\mathbf{U}}(\cdot, t)^T \right\rangle, \quad (25)$$

where $\mathcal{L}^*(u) = \mathcal{L}(u) - \mathbb{E}[\mathcal{L}(u)]$ and $\Pi_{\tilde{\mathcal{Y}}}^\perp$ is the projection operator from the space $L^2(\Omega)$ to the orthogonal complement of the S dimension subspace $\tilde{\mathcal{Y}} = \text{span}(\tilde{Y}_1, \dots, \tilde{Y}_S)$. The related initial and boundary conditions can be obtained by the same way as in (16) and (17). The decomposition (18) and the corresponding system (22)-(25) have been proposed in [11, 12] for a dynamically low rank approximation of a time dependent differential matrix/tensor equation. An analogous formulation in infinite dimensional setting is derived in [13, 14], related to the multi-configuration time-dependent Hartree approach (MCTDH), in the quantum dynamics framework. We remark that for time dependent SPDEs, a Dynamically bi-orthogonal method (DyBO), which has a close relation with the DDO approximation, has been introduced in [28, 29]. As our error analysis relies on the symmetric property of the DDO approach, we will show in the following the equivalence between the DDO and the DO approximations. Note that in the DDO system (22)-(25), the equation for the mean function coincides with equation (12) in the DO system. Furthermore, letting $\mathbf{Y} = \mathbf{A}\tilde{\mathbf{Y}}$, it is easy to show that the approximation $\tilde{u}_S = \bar{u}_S + \tilde{\mathbf{U}}^T \mathbf{Y}$ satisfies the DO system. Indeed, by using together equations (23) and (25), we have

$$\begin{aligned} \frac{\partial \mathbf{Y}}{\partial t} &= \frac{d\mathbf{A}}{dt} \tilde{\mathbf{Y}} + \mathbf{A} \frac{\partial \tilde{\mathbf{Y}}}{\partial t} \\ &= \mathbb{E} \left[\left\langle \mathcal{L}^*(\tilde{u}_S), \tilde{\mathbf{U}}^T \right\rangle \tilde{\mathbf{Y}}^T \right] \tilde{\mathbf{Y}} + \Pi_{\tilde{\mathcal{Y}}}^\perp \left\langle \mathcal{L}^*(\tilde{u}_S), \tilde{\mathbf{U}}^T \right\rangle \\ &= \mathbb{E} \left[\left\langle \mathcal{L}^*(\tilde{u}_S), \tilde{\mathbf{U}}^T \right\rangle \tilde{\mathbf{Y}}^T \right] \tilde{\mathbf{Y}} + \left\langle \mathcal{L}^*(\tilde{u}_S), \tilde{\mathbf{U}}^T \right\rangle - \mathbb{E} \left[\left\langle \mathcal{L}^*(\tilde{u}_S), \tilde{\mathbf{U}}^T \right\rangle \tilde{\mathbf{Y}}^T \right] \tilde{\mathbf{Y}} \\ &= \left\langle \mathcal{L}^*(\tilde{u}_S), \tilde{\mathbf{U}}^T \right\rangle, \end{aligned} \quad (26)$$

which coincides with equation (14) in the DO system. Moreover, by multiplying both sides of (24) by \mathbf{A} we obtain

$$\mathbf{A} \mathbf{A}^T \frac{\partial \tilde{\mathbf{U}}}{\partial t} = \Pi_{\tilde{\mathcal{U}}}^\perp \mathbb{E} [\mathbf{Y} \mathcal{L}^*(\tilde{u}_S)]. \quad (27)$$

Note that the covariance matrix of \mathbf{Y} is

$$\mathbf{C} = \mathbb{E}[\mathbf{Y}\mathbf{Y}^T] = \mathbb{E}[\mathbf{A}\tilde{\mathbf{Y}}(\mathbf{A}\tilde{\mathbf{Y}})^T] = \mathbf{A}\mathbf{A}^T. \quad (28)$$

Thus, the equation (27) coincides with (13) in the DO system. Using similar techniques, one can show that the corresponding initial and boundary conditions for the DO system and the DDO

system also coincide. On the other hand, if $u_S = \bar{u}_S + \mathbf{U}^T \mathbf{Y}$ is a solution of the DO system (12)-(14), then defining \mathbf{A} as the square root of \mathbf{C} one can show by the same arguments as above that $u_S = \bar{u}_S + \mathbf{U}^T \mathbf{A} \tilde{\mathbf{Y}}$ with $\tilde{\mathbf{Y}} = \mathbf{A}^{-1} \mathbf{Y}$ is a solution of the DDO system (22)-(25). In particular, $\tilde{\mathbf{Y}}$ is a vector of orthonormal random variables in $L^2(\Omega)$. We thus conclude that the DO and the DDO formulations produce the same approximate solution.

3.2 An equivalent Variational Formulation

Let $\mathcal{H} \subset L^2(D)$ be a suitable Hilbert space and \mathcal{H}' its dual. We assume that equation (3) can be set in $\mathcal{H}' \otimes L^2(\Omega)$ and it admits a unique solution $u(t) \in \mathcal{H} \otimes L^2(\Omega)$ for any $t \in \mathcal{T}$.

Definition 3.1. We define a S -rank random field as a function $u_S \in \mathcal{H} \otimes L^2(\Omega)$ taking the following form:

$$u_S = \bar{u}_S + u_S^* = \bar{u}_S(x) + \mathbf{U}^T(x) \mathbf{Y}(\omega),$$

where

- $\bar{u}_S(x) \in \mathcal{H}$,
- $\mathbf{U} = (U_1, \dots, U_S)^T \in [\mathcal{H}]^S$ is a vector with orthonormal components in $L^2(D)$,
- $\mathbf{Y} = (Y_1, \dots, Y_S)^T \in [L^2(\Omega)]^S$ is a vector of random components in $L^2(\Omega)$ with zero mean and non singular covariance matrix $\mathbf{C} = \mathbb{E}[\mathbf{Y}\mathbf{Y}^T]$. (Referring to the DDO formulation, this implies that the matrix \mathbf{A} is non singular).

We denote by $\mathcal{M}_S(\mathcal{H} \otimes L^2(\Omega))$, or simply \mathcal{M}_S if no ambiguity arises on the functional spaces, the manifold of all S -rank zero mean random fields $u_S^* \in \mathcal{H} \otimes L^2(\Omega)$ and by $\mathcal{T}_{u_S^*} \mathcal{M}_S$ its tangent space at $u_S^* = \mathbf{U}^T \mathbf{Y} \in \mathcal{M}_S$.

The following propositions hold, suitably adapted to our framework from [11, 14].

Proposition 3.1. The tangent space $\mathcal{T}_{u_S^*} \mathcal{M}_S$ consists of the elements $\delta u_S^* \in \mathcal{H} \otimes L^2(\Omega)$ of the form:

$$\delta u_S^* = \mathbf{U}^T \delta \mathbf{Y} + \delta \mathbf{U}^T \mathbf{Y} \quad (29)$$

where $\delta \mathbf{Y}$ and $\delta \mathbf{U}$ are uniquely determined in the representation (29) if we impose the orthogonality conditions analogous to (11):

$$\langle \delta \mathbf{U}, \mathbf{U}^T \rangle = 0, \quad \mathbb{E}[\delta \mathbf{Y}] = \mathbf{0} \quad (30)$$

where $\mathbf{0}$ is the zero vector in \mathbb{R}^S .

Proposition 3.2. For all $v \in \mathcal{H} \otimes L^2(\Omega)$ and $u_S^* \in \mathcal{M}_S$, the orthogonal projection $P_{u_S^*}$ onto the tangent space $\mathcal{T}_{u_S^*} \mathcal{M}_S$ of v is given by

$$P_{u_S^*}(v) = P_{u_S^*}(v^*) = \mathbf{U}^T \langle v^*, \mathbf{U}^T \rangle + (\Pi_{\mathcal{U}}^\perp \{ \mathbb{E}[v^* \mathbf{Y}^T] \} \mathbf{C}^{-1})^T \mathbf{Y},$$

where \mathbf{C}^{-1} is the inverse of the covariance matrix $\mathbf{C} = \mathbb{E}[\mathbf{Y}\mathbf{Y}^T]$, that has full rank, by definition of S -rank function.

Then directly from Proposition 3.1 and 3.2 one can easily derive the following formulas for $P_{u_S^*}$ and $P_{u_S^*}^\perp$:

Proposition 3.3. *The orthogonal projection onto the tangent space $\mathcal{T}_{u_S^*}\mathcal{M}_S$ at $u_S^* = \mathbf{U}^T\mathbf{Y} = \mathbf{U}^T\mathbf{A}\tilde{\mathbf{Y}}$ is given by*

$$P_{u_S^*}^\perp v = \Pi_{\mathcal{U}}^\perp \otimes \Pi_{\tilde{\mathcal{Y}}}^\perp v, \quad (31)$$

where $\mathcal{U} = \text{span}\{U_1, \dots, U_S\}$, $\tilde{\mathcal{Y}} = \text{span}\{\tilde{Y}_1, \dots, \tilde{Y}_S\}$.

Furthermore observe that the governing equation (3) can be formulated as:

$$\frac{\partial \bar{u}(x, t)}{\partial t} = \mathbb{E}[\mathcal{L}(u(x, t, \cdot))], \quad \text{in } \mathcal{H}' \quad (32)$$

$$\frac{\partial u^*(x, t, \omega)}{\partial t} = \mathcal{L}^*(u(x, t, \omega), \omega) \quad \text{in } \mathcal{H}' \otimes L^2(\Omega) \quad (33)$$

with $u^* = u - \bar{u}$. Then the DO approach corresponds to a Galerkin formulation according to which the residual of the governing equation (33) is projected onto the tangent space $\mathcal{T}_{u_S^*(t)}\mathcal{M}_S$ in $u_S^*(t)$ at each time instant (see Dirac-Frenkel variational principle [30, 31]). We can define the following variational formulation for the DO approach:

Proposition 3.4. *At each $t \in \mathcal{T}$, find $u_S(\cdot, t, \cdot) = \bar{u}_S(\cdot, t) + u_S^*(\cdot, t, \cdot)$ with $(\bar{u}_S, u_S^*) \in \mathcal{H} \times \mathcal{M}_S$ such that:*

$$\mathbb{E} \left[\left\langle \frac{\partial u_S(\cdot, t, \cdot)}{\partial t} - \mathcal{L}(u_S(\cdot, t, \cdot)), v \right\rangle \right] = 0, \quad \forall v = \bar{v} + v^*, (\bar{v}, v^*) \in \mathcal{H} \times \mathcal{T}_{u_S^*(t)}\mathcal{M}_S \quad (34)$$

which can be equivalently written as

$$\frac{\partial u_S(x, t, \omega)}{\partial t} = \mathbb{E}[\mathcal{L}(u_S(x, t, \cdot))] + P_{u_S^*(t)}(\mathcal{L}^*(u_S(x, t, \omega)))$$

with $\mathcal{L}^*(u_S) = \mathcal{L}(u_S) - \mathbb{E}[\mathcal{L}(u_S)]$.

The approximate solution $u_S^* = u_S - \bar{u}_S$ is therefore forced to belong to the S dimensional manifold \mathcal{M}_S at all times. The same conclusion holds for the DDO approximate solution \tilde{u}_S as, by the above discussion, the two approaches lead to the same solution. We point out that the DO solution (34) does not coincide, in general, with the best S-rank approximation (denoted by z_S in (9)) which instead minimizes the approximation error in L^2 sense at each time instant, i.e.

$$z_S(t) = \bar{u}(\cdot, t) + \operatorname{argmin}_{w \in \mathcal{M}_S} \mathbb{E} \left[\|u^*(\cdot, t, \cdot) - w(\cdot, \omega)\|_{L^2(D)}^2 \right], \quad \forall t \in \mathcal{T}. \quad (35)$$

It is well known that the best S-rank approximation corresponds indeed to the truncated Karhunen-Loève expansion, with S terms. Observe that in the best S-rank approximation (35) the solution u^* of the equation (33) is projected onto the manifold \mathcal{M}_S , whereas in (34) the residual of the equation (33) is projected onto the tangent space $\mathcal{T}_{u_S^*(t)}\mathcal{M}_S$. However, the DO formulation takes inspiration from the Karhunen-Loève decomposition. It aims at developing an analogous type

of approximation without directly computing the Karhunen-Loève decomposition. In fact the DO method evolves a dynamically low rank approximation and adapts at each time instant the spatial basis as well the stochastic variables to what best describes the structure of the solution. This makes the method numerically accessible and effective in terms of approximation error at any time instant for long time integration.

3.3 Properties of the manifold

In this subsection, we shall discuss some properties of the manifold \mathcal{M}_S , which will play an important role in the next section when analyzing the convergence properties of the DO approach. Given the equivalence between the DO and DDO formulations, shown in Section 3.1 here we will use either formalism depending on what is more convenient for the presentation.

Definition 3.2. Denoted with \mathbf{A} the square root of the covariance matrix $\mathbf{C} = \mathbb{E}[\mathbf{Y}\mathbf{Y}^T]$, the singular values of a S -rank function $u_S = \bar{u}_S + \mathbf{U}^T \mathbf{Y}$ are defined as the singular values of \mathbf{A} :

$$\sigma(u_S) := \sigma(\mathbf{A}) = \sqrt{\text{eig}(\mathbf{C})}.$$

Equivalently for the DDO formulation, $u_S = \bar{u}_S + \mathbf{U}^T \mathbf{A} \tilde{\mathbf{Y}}$, the singular values of u_S are by definition the singular values of \mathbf{A} .

In the following, we denote with $\|\cdot\|_0 := \|\cdot\|_{L^2(D) \otimes L^2(\Omega)}$ the norm in $L^2(D) \otimes L^2(\Omega)$. The norm for a function vector \mathbf{U} is defined as usual, namely, $\|\mathbf{U}\|_0 = (\sum_i \|U_i\|_{L^2(D)}^2)^{1/2}$. We also denote with $\|\cdot\|_{\mathcal{F}}$ and $\|\cdot\|_2$ the Frobenius and the spectral norm of a matrix, respectively. Note that, with such definition we have $\|u_S^*\|_0 = \|\mathbf{A}\|_{\mathcal{F}}$, for $u_S^* = \tilde{\mathbf{U}}^T \mathbf{A} \tilde{\mathbf{Y}} \in \mathcal{M}_S$.

We introduce now a useful lemma concerning the properties of the operator $P_{u_S^*}$ and the curvature estimates for the manifold \mathcal{M}_S . This lemma is taken from [14] with just small adjustments to the notations and settings used here. We skip the proof as it would follow very closely the one in [14]. Analogous results are achieved in [11], where the authors considered a very similar approach for matrix equations in finite dimensional spaces.

Lemma 3.1. Consider the manifold $\mathcal{M}_S(L^2(D) \otimes L^2(\Omega))$. Let $u_S^* = \mathbf{U}^T \mathbf{Y} \in \mathcal{M}_S$ such that the smallest nonzero singular value satisfies $\sigma_s(u_S^*) \geq \rho > 0$, and let $v_S^* = \mathbf{V}^T \mathbf{Z} \in \mathcal{M}_S$ with $\|u_S^* - v_S^*\|_0 \leq \frac{1}{8}\rho$. Then, $\forall w \in L^2(D) \otimes L^2(\Omega)$, the following bounds hold

$$\|(P_{u_S^*} - P_{v_S^*})w\|_0 \leq 8\rho^{-1} \|u_S^* - v_S^*\|_0 \cdot \|w\|_0, \quad (36)$$

$$\|P_{u_S^*}^\perp(u_S^* - v_S^*)\|_0 \leq 4\rho^{-1} \|u_S^* - v_S^*\|_0^2. \quad (37)$$

Further we observe that any linear deterministic bounded operator applied to a S -rank function, does not increase its rank.

Proposition 3.5. Let \mathcal{V}_1 and \mathcal{V}_2 be two Hilbert spaces such that $\mathcal{V}_2 \subseteq \mathcal{V}_1 \subseteq L^2(D)$ and $\mathcal{B} : \mathcal{V}_1 \rightarrow \mathcal{V}_2$ a linear bounded operator. For any $u_S = \bar{u}_S + u_S^*$ with $(\bar{u}_S, u_S^*) \in \mathcal{V}_1 \times \mathcal{M}_S(\mathcal{V}_1 \otimes L^2(\Omega))$, we have that $\mathcal{B} \otimes \mathbb{I}u_S = \mathcal{B}\bar{u}_S + \mathcal{B} \otimes \mathbb{I}u_S^*$ with $(\mathcal{B}\bar{u}_S, \mathcal{B} \otimes \mathbb{I}u_S^*) \in \mathcal{V}_2 \times \mathcal{T}_{u_S^*} \mathcal{M}_S(\mathcal{V}_2 \otimes L^2(\Omega))$.

Proof. It is enough to observe that $(\mathcal{B} \otimes \mathbb{I})u_S^* = \sum_{i=1}^S (\mathcal{B}U_i)Y_i$ and it can be expanded as:

$$\begin{aligned} (\mathcal{B} \otimes \mathbb{I})u_S^* &= \sum_{i=1}^S \Pi_{\mathbf{U}}(\mathcal{B}U_i)Y_i + \sum_{i=1}^S \Pi_{\mathcal{U}}^\perp(\mathcal{B}U_i)Y_i \\ &= \sum_{i=1}^S \left(\sum_{j=1}^S \langle \mathcal{B}U_i, U_j \rangle U_j \right) Y_i + \sum_{i=1}^S \Pi_{\mathcal{U}}^\perp(\mathcal{B}U_i)Y_i \\ &= \sum_{j=1}^S \left(\sum_{i=1}^S \langle \mathcal{B}U_i, U_j \rangle Y_i \right) U_j + \sum_{i=1}^S \Pi_{\mathcal{U}}^\perp(\mathcal{B}U_i)Y_i = \mathbf{U}^T \delta \mathbf{Y} + \delta \mathbf{U}^T \mathbf{Y} \end{aligned} \quad (38)$$

where $\delta \mathbf{Y} = \langle \mathcal{B}(\mathbf{U}^T) \mathbf{Y}, \mathbf{U} \rangle$ and $\delta \mathbf{U} = \Pi_{\mathcal{U}}^\perp(\mathcal{B}\mathbf{U})$ is orthogonal to \mathbf{U} by construction. \square

4 Application to stochastic parabolic equations

In this section, we consider the DO approach for the following linear stochastic parabolic equation:

$$\frac{\partial u(x, t, \omega)}{\partial t} - \nabla \cdot (a(x, \omega) \nabla u(x, t, \omega)) = f(x, t, \omega), \quad x \in D, t \in \mathcal{T}, \omega \in \Omega, \quad (39)$$

$$u(\sigma, t, \omega) = 0 \quad \sigma \in \partial D, t \in \mathcal{T}, \omega \in \Omega, \quad (40)$$

$$u(x, 0, \omega) = u_0(x, \omega), \quad x \in D, \omega \in \Omega, \quad (41)$$

where $a(x, \omega) : D \times \Omega \rightarrow \mathbb{R}$ is a random field with continuous and bounded covariance function and D is an open, bounded and Lipschitz domain. We say that u is a weak solution of problem (39)-(41) if it satisfies the initial condition $u = u_0$ at $t = 0$ and if, at any $t \in \mathcal{T}$, $u(\cdot, t, \cdot) \in H_0^1(D) \otimes L^2(\Omega)$ and

$$\mathbb{E} \left[\left\langle \frac{\partial u(\cdot, t, \cdot)}{\partial t}, v \right\rangle \right] + \mathbb{E} \left[\langle a \nabla u(\cdot, t, \cdot), \nabla v \rangle \right] = \mathbb{E} \left[\langle f(\cdot, t, \cdot), v \rangle \right] \quad \forall v \in H_0^1(D) \otimes L^2(\Omega). \quad (42)$$

A sufficient condition to guarantee the existence and uniqueness of the solution u consists in assuming that $f \in L^2(\mathcal{T}, L^2(D) \otimes L^2(\Omega))$, $u_0 \in L^2(D) \otimes L^2(\Omega)$ and the diffusion coefficient $a(x, \omega)$ is bounded and uniformly coercive almost surely, i.e.

$$\exists a_{min}, a_{max} \in (0, +\infty) : P(\omega \in \Omega : a(x, \omega) \in [a_{min}, a_{max}], \forall x \in \bar{D}) = 1. \quad (43)$$

Then by standard arguments applied for almost every $\omega \in \Omega$ (see also [4]), it is straightforward to show that there exists a unique solution $u \in L^2(\mathcal{T}, H_0^1(D) \otimes L^2(\Omega))$ with $\frac{\partial u}{\partial t} \in L^2(\mathcal{T}, H^{-1}(D) \otimes L^2(\Omega))$ and by standard energy estimates the following a priori bound holds $\forall T \in \mathcal{T}$:

$$\|u(T)\|_{L^2(D) \otimes L^2(\Omega)}^2 + a_{min} \|u\|_{L^2(\mathcal{T}, H_0^1(D) \otimes L^2(\Omega))}^2 \leq \|u_0\|_{L^2(D) \otimes L^2(\Omega)}^2 + \frac{c_p^2}{a_{min}} \|f\|_{L^2(\mathcal{T}, L^2(D) \otimes L^2(\Omega))}^2, \quad (44)$$

where c_p denotes the constant appearing in the Poincaré inequality.

For the error analysis of the DO method that will be presented in the next section, we need some extra regularity on the exact solution u as well as its DO approximation u_S . We make the following assumption: (For simplicity of notation we denote with \dot{u} the time derivative of u)

Assumption 1.

- $u, u_S \in L^2(\mathcal{T}, H^2(D) \cap H_0^1(D) \otimes L^2(\Omega))$
- $\dot{u}, \dot{u}_S \in L^2(\mathcal{T}, L^2(D) \otimes L^2(\Omega))$

We give here an informal discussion on why this assumption is reasonable under mild extra requirements on the data of the problem (39)-(41). In particular, while regularity results on the exact solution u can be proved by standard techniques, it is not obvious whether analogous results should hold for the DO solution u_S , because of the projection on the tangent manifold. Consider the pure Neumann problem $\partial u_n = 0$ on $\partial\Omega$ and look first at the exact problem (39)-(41) (with Neumann boundary conditions instead of Dirichlet ones). Under the assumption that $\nabla a \in L^\infty(D \times \Omega)$ and $\nabla \dot{u}(0) \in L^2(D) \otimes L^2(\Omega)$, by taking $v = -\Delta u$ in (42) and integrating in time we get:

$$\begin{aligned} \|\nabla u(T)\|_{L^2(D) \otimes L^2(\Omega)}^2 + a_{min} \|\Delta u\|_{L^2(\mathcal{T}, L^2(D) \otimes L^2(\Omega))}^2 &\leq \frac{2}{a_{min}} \|\nabla a\|_{L^\infty(D \times \Omega)} \|\nabla u\|_{L^2(\mathcal{T}, L^2(D) \otimes L^2(\Omega))}^2 \\ &\quad + \frac{2}{a_{min}} \|f\|_{L^2(\mathcal{T}, L^2(D) \otimes L^2(\Omega))}^2 \\ &\quad + \|\nabla \dot{u}(0)\|_{L^2(D) \otimes L^2(\Omega)}^2, \end{aligned} \quad (45)$$

which implies, in light of (44), that u is bounded in $L^2(\mathcal{T}, H^2(D) \otimes L^2(\Omega))$. In order to derive a bound on the time derivative of u , let us now take $v = \dot{u}$ in (42) and integrate in time. We get the following a priori estimate:

$$\|\dot{u}\|_{L^2(\mathcal{T}, L^2(D) \otimes L^2(\Omega))}^2 + a_{min} \|\nabla u(T)\|_{L^2(D) \otimes L^2(\Omega)}^2 \leq a_{max} \|\nabla u_0\|_{L^2(D) \otimes L^2(\Omega)}^2 + \|f\|_{L^2(\mathcal{T}, L^2(D) \otimes L^2(\Omega))}^2 \quad (46)$$

which shows that $\dot{u} \in L^2(\mathcal{T}, L^2(D) \otimes L^2(\Omega))$. Therefore the regularity properties in Assumption 1 on u are sound provided that $\nabla a \in L^\infty(D \times \Omega)$ and $u(0), \dot{u}(0) \in H^1(D) \otimes L^2(\Omega)$. Observe that, since the truncated Karhunen-Loève expansion inherits the spatial regularity of u [32], estimates (45) and (46) are valid for z_S as well, for any $S \in \mathbb{N}$. By following the same approach as before, we investigate now the regularity of the DO solution u_S . The weak formulation of the DO method reads: *At each time $t \in \mathcal{T}$, find $u_S = \bar{u}_S + u_S^*$ with $(\bar{u}_S, u_S^*) \in H^1(D) \times \mathcal{M}_S(H^1(D) \otimes L^2(\Omega))$ such that*

$$\mathbb{E}[\langle \dot{u}_S(\cdot, t, \cdot), v \rangle] + \mathbb{E}[\langle a \nabla u_S(\cdot, t, \cdot), \nabla v \rangle] = \mathbb{E}[\langle f(\cdot, t, \cdot), v \rangle], \mathcal{M}_S \quad (47)$$

$$\forall v = \bar{v} + v^*, (\bar{v}, v^*) \in H^1(D) \times \mathcal{T}_{u_S^*(t)}.$$

We now take as before $v = -\Delta u_S$ in (47). The key now is to observe that thanks to the Proposition 3.5, $v^* = -\Delta u_S^* \in \mathcal{T}_{u_S^*} \mathcal{M}_S$ so that it is a suitable test function. By the same argument we can take $v = \dot{u}_S$ as a test function. Then, proceeding as before, one can derive the same bounds (45) and (46) for the DO solution as well. This shows that the regularity assumption (Assumption 1) are also sound for the DO solution u_S under the same conditions on the data: $\nabla a \in L^\infty(D \times \Omega)$ and $u(0), \dot{u}(0) \in H^1(D) \otimes L^2(\Omega)$.

Remark 4.1. *The informal arguments that we have used to derive the bounds (45) and (46) for the exact solution as well as its DO approximation u_S can be made rigorous e.g. by using the so called Faedo-Galerkin method that consists on working with a sequence of Galerkin approximations of the solution u , which satisfy the governing equation projected in finite dimensional subspaces, and weakly converge to u (see e.g. [33, 34]).*

4.1 Analysis of DO approximation error

We are now ready to prove the convergence result for the DO approximation of the stochastic parabolic equation (39)-(41). The proof will follow closely the one by Lubich et al. in [11] for the error analysis of the Dynamical Low Rank approximation of time dependent data matrices. For notation simplicity, we denote

$$\mathcal{L}(u) := \nabla \cdot (a \nabla u) + f, \quad \mathcal{L}^*(\cdot) = \mathcal{L}(\cdot) - \mathbb{E}[\mathcal{L}(\cdot)]. \quad (48)$$

We suppose that the problem (39)-(41) admits a unique solution u in $L^2(\mathcal{T}, H^2(D) \cap H_0^1(D) \otimes L^2(\Omega))$ and that there exists a continuously differentiable best S -rank approximation $z_S = \bar{z} + z_S^*$ of the solution u at any $t \in \mathcal{T}$. In light of what discussed in the previous section we can argue that also the truncated Karhunen-Loève expansion z_S and the DO approximate solution u_S will in general belong to $L^2(\mathcal{T}, H^2(D) \cap H_0^1(D) \otimes L^2(\Omega))$ and, in particular, the quantities $\|\mathcal{L}(u)\|_0$, $\|\mathcal{L}(z_S)\|_0$ and $\|\mathcal{L}(u_S)\|_0$ will be bounded, which is a necessary condition for our proof of the quasi-optimality of the DO approximate solution. We will estimate the error of the DO approximate solution in terms of the best approximation error $\|u - z_S\|_{H^1(D) \otimes L^2(D)}$ as long as this remains small enough compared with the smallest singular value of z_S .

Theorem 4.1. *Suppose that a continuously differentiable best S -rank approximation $z_S(t)$ of the exact solution $u(t)$ of (39)-(41) exists in $(H^2(D) \cap H_0^1(D)) \otimes L^2(\Omega)$ for $0 \leq t \leq \bar{t}$ and the smallest singular value of $z_S(t)$ is uniformly bounded from below, with lower bound $\sigma(z_S(t)) \geq \rho > 0, \forall t \in [0, \bar{t}]$. Then there exists $0 < \hat{t} \leq \bar{t}$ such that the approximation error of the DO solution $u_S = \bar{u}_S + u_S^*$ with initial value $u_S(0) = z_S(0)$ is bounded by*

$$\|u_S(t) - z_S(t)\|_0^2 + a_{\min} \int_0^t |u_S(\tau) - z_S(\tau)|_1^2 d\tau \leq 2\alpha e^{2\beta(t)} \int_0^t \|z_S(\tau) - u(\tau)\|_1^2 d\tau, \quad (49)$$

for all $0 < t \leq \hat{t}$, with

$$\begin{aligned} \beta(t) &= 4\rho^{-1} \int_0^t (4\|\mathcal{L}^*(z_S(\tau))\|_0 + \|\mathcal{L}^*(u(\tau))\|_0 + \|\mathcal{L}^*(u_S(\tau))\|_0 + \|z_S^*(\tau)\|_0^2) d\tau, \\ \alpha &= \max \left\{ \frac{a_{\max}^2}{2a_{\min}}, 4\rho^{-1} \right\}, \end{aligned} \quad (50)$$

where $\|\cdot\|_1, |\cdot|_1$ denote respectively the norm and semi-norm in $H^1(D) \otimes L^2(\Omega)$, provided that all the terms in (49) are well defined.

Proof. Thanks to the assumptions of boundedness of \dot{u} and \dot{z}_S and being $u_S(0) = z_S(0)$, we have that for any $t \in [0, \bar{t}]$

$$\begin{aligned} \|u_S(t) - z_S(t)\|_0^2 &= \left\| \int_0^t (\dot{u}_S(\tau) - \dot{z}_S(\tau)) d\tau \right\|_0^2 \\ &\leq t \int_0^t \|\dot{u}_S(\tau) - \dot{z}_S(\tau)\|_0^2 d\tau \leq 2t \underbrace{(\|\dot{u}_S\|_{L^2([0,t],L^2(D)) \otimes L^2(\Omega)}^2 + \|\dot{z}_S\|_{L^2([0,t],L^2(D)) \otimes L^2(\Omega)}^2)}_{A(t)} \end{aligned} \quad (51)$$

therefore, for $\hat{t} = \min(\bar{t}, \frac{\rho^2}{2.8^2 A(\bar{t})})$ the distance between u_S and z_S remains bounded by $\frac{1}{8}\rho$, as required in Lemma 3.1.

For the best approximation z_S it must hold that $\mathbb{E}[z_S] = \mathbb{E}[u]$ and $\mathbb{E}[\dot{z}_S] = \mathbb{E}[\mathcal{L}(u)]$. Moreover $(z_S - \mathbb{E}[z_S]) - (u - \mathbb{E}[u])$ must be orthogonal to the tangent space $\mathcal{T}_{z_S^*} \mathcal{M}_S$, that is:

$$P_{z_S^*}((z_S - \mathbb{E}[z_S]) - (u - \mathbb{E}[u])) = P_{z_S^*}(z_S - u) = 0 \quad (52)$$

For $z_S^* \in \mathcal{M}_S$, we denote with $\mathbf{D}_{z_S^*} P[\delta z_S^*]$ the Gateaux derivative of the projection operator in z_S^* , i.e.

$$\mathbf{D}_{z_S^*} P[\delta z_S^*] = \lim_{\varepsilon \rightarrow 0} \frac{P_{z_S^* + \varepsilon \delta z_S^*} - P_{z_S^*}}{\varepsilon}. \quad (53)$$

Observe that $\frac{d}{dt} P_{z_S^*}(t) = \mathbf{D}_{z_S^*} P[\dot{z}_S^*]$. We differentiate the relation (52) with respect to t and we then obtain:

$$P_{z_S^*}(\dot{z}_S - \dot{u}) + \mathbf{D}_{z_S^*} P[\dot{z}_S^*](z_S - u) = 0, \quad (54)$$

Since we have $P_{z_S^*}(\dot{z}_S) = P_{z_S^*}(\dot{z}_S^*) = \dot{z}_S^* = \dot{z}_S - \mathbb{E}[\dot{z}_S]$ the above equation becomes

$$\begin{aligned} \dot{z}_S &= \mathbb{E}[\dot{z}_S] + P_{z_S^*}(\dot{u}) - \mathbf{D}_{z_S^*} P[\dot{z}_S^*](z_S - u) \\ &= \mathbb{E}[\mathcal{L}(u)] + P_{z_S^*}(\mathcal{L}^*(u)) - \mathbf{D}_{z_S^*} P[\dot{z}_S^*](z_S - u) \end{aligned} \quad (55)$$

Since the DO solution satisfies

$$\dot{u}_S = \mathbb{E}[\mathcal{L}(u_S)] + P_{u_S^*}(\mathcal{L}^*(u_S)), \quad (56)$$

by subtracting equations (55) and (56) we get

$$\dot{u}_S - \dot{z}_S = \mathbb{E}[\mathcal{L}(u_S)] - \mathbb{E}[\mathcal{L}(u)] + P_{u_S^*}(\mathcal{L}^*(u_S)) - P_{z_S^*}(\mathcal{L}^*(u)) + \mathbf{D}_{z_S^*} P[\dot{z}_S^*](z_S - u).$$

By adding and subtracting $(P_{u_S^*} - P_{z_S^*})(\mathcal{L}^*(z_S))$ we obtain

$$\begin{aligned} \dot{u}_S - \dot{z}_S &= \mathbb{E}[\mathcal{L}(u_S)] - \mathbb{E}[\mathcal{L}(u)] + (P_{u_S^*} - P_{z_S^*})(\mathcal{L}^*(z_S)) + P_{z_S^*}(\mathcal{L}^*(z_S) - \mathcal{L}^*(u)) \\ &\quad + [I - P_{u_S^*}^\perp](\mathcal{L}^*(u_S) - \mathcal{L}^*(z_S)) + \mathbf{D}_{z_S^*} P[\dot{z}_S^*](z_S - u). \end{aligned}$$

and then

$$\begin{aligned} \dot{u}_S - \dot{z}_S &= (P_{u_S^*} - P_{z_S^*})(\mathcal{L}^*(z_S)) + P_{z_S^*}(\mathcal{L}^*(z_S) - \mathcal{L}^*(u)) + \mathbf{D}_{z_S^*} P[\dot{z}_S^*](z_S - u) \\ &\quad + (\mathcal{L}(u_S) - \mathcal{L}(z_S)) - P_{u_S^*}^\perp(\mathcal{L}^*(u_S) - \mathcal{L}^*(z_S)) + \mathbb{E}[\mathcal{L}(z_S)] - \mathbb{E}[\mathcal{L}(u)]. \end{aligned}$$

By taking the inner product with $u_S - z_S$, on both sides, we obtain

$$\begin{aligned}
\mathbb{E}[\langle \dot{u}_S - \dot{z}_S, u_S - z_S \rangle] &= \overbrace{\mathbb{E}[\langle (P_{u_S^*} - P_{z_S^*})(\mathcal{L}^*(z_S)), u_S - z_S \rangle]}^{T_1} + \overbrace{\mathbb{E}[\langle \mathcal{L}(u_S) - \mathcal{L}(z_S), u_S - z_S \rangle]}^{T_2} \\
&\quad + \overbrace{\mathbb{E}[\langle P_{z_S^*}(\mathcal{L}^*(z_S) - \mathcal{L}^*(u)), u_S - z_S \rangle]}^{T_3} + \mathbb{E}[\langle \mathbb{E}[\mathcal{L}(z_S)] - \mathbb{E}[\mathcal{L}(u)], u_S - z_S \rangle] \\
&\quad + \overbrace{\mathbb{E}[\langle \mathbf{D}_{z_S^*} P[\dot{z}_S^*](z_S - u), u_S - z_S \rangle]}^{T_4} + \overbrace{\mathbb{E}[\langle -P_{u_S^*}^\perp(\mathcal{L}^*(u_S) - \mathcal{L}^*(z_S)), u_S - z_S \rangle]}^{T_5}
\end{aligned} \tag{57}$$

We now estimate separately each term on the right hand side of (57). Lemma 3.1 implies that:

$$\begin{aligned}
T_1 : \mathbb{E}[\langle (P_{u_S^*} - P_{z_S^*})(\mathcal{L}^*(z_S)), u_S - z_S \rangle] &= \mathbb{E}[\langle \mathcal{L}^*(z_S), (P_{u_S^*} - P_{z_S^*})(u_S - z_S) \rangle] \\
&\leq 8\rho^{-1} \|\mathcal{L}^*(z_S)\|_0 \|u_S - z_S\|_0^2
\end{aligned} \tag{58}$$

$$T_2 : \mathbb{E}[\langle \mathcal{L}(u_S) - \mathcal{L}(z_S), u_S - z_S \rangle] \leq -a_{min} \|\nabla u_S - \nabla z_S\|_0^2 \leq -a_{min} |u_S - z_S|_1^2 \tag{59}$$

For the term T_3 , since

$$\begin{aligned}
\mathbb{E}[\langle P_{z_S^*}(\mathcal{L}^*(z_S) - \mathcal{L}^*(u)), u_S - z_S \rangle] &= \mathbb{E}[\langle \mathcal{L}^*(z_S) - \mathcal{L}^*(u), u_S - z_S \rangle] \\
&\quad - \mathbb{E}[\langle \mathcal{L}^*(z_S) - \mathcal{L}^*(u), P_{z_S^*}^\perp(u_S - z_S) \rangle]
\end{aligned}$$

we have

$$\begin{aligned}
T_3 : \mathbb{E}[\langle P_{z_S^*}(\mathcal{L}^*(z_S) - \mathcal{L}^*(u)), u_S - z_S \rangle] &+ \mathbb{E}[\langle \mathbb{E}[\mathcal{L}(z_S)] - \mathbb{E}[\mathcal{L}(u)], u_S - z_S \rangle] \\
T_3 &= \mathbb{E}[\langle \mathcal{L}(z_S) - \mathcal{L}(u), u_S - z_S \rangle] - \mathbb{E}[\langle \mathcal{L}^*(z_S) - \mathcal{L}^*(u), P_{z_S^*}^\perp(u_S - z_S) \rangle]
\end{aligned}$$

and then

$$T_3 \leq a_{max} |z_S - u|_1 |u_S - z_S|_1 + 4\rho^{-1} (\|\mathcal{L}^*(z_S)\|_0 + \|\mathcal{L}^*(u)\|_0) \|u_S - z_S\|_0^2 \tag{60}$$

Analogously

$$\begin{aligned}
T_5 : \mathbb{E}[\langle P_{u_S^*}^\perp(\mathcal{L}^*(u_S) - \mathcal{L}^*(z_S)), u_S - z_S \rangle] &\leq \|\mathcal{L}^*(u_S) - \mathcal{L}^*(z_S)\|_0 \|P_{u_S^*}^\perp(u_S - z_S)\|_0 \\
&\leq 4\rho^{-1} (\|\mathcal{L}^*(z_S)\|_0 + \|\mathcal{L}^*(u_S)\|_0) \|u_S - z_S\|_0^2.
\end{aligned} \tag{61}$$

Also we have:

$$\|\mathbf{D}_{z_S^*} P[\dot{z}_S^*](z_S - u)\|_0 = \lim_{dt \rightarrow 0} \frac{P_{z_S^* + dt \dot{z}_S^*} - P_{z_S^*}}{dt}(z_S - u) \leq 8\rho^{-1} \|\dot{z}_S^*\|_0 \|z_S - u\|_0,$$

and hence:

$$T_4 : \mathbb{E}[\langle \mathbf{D}_{z_S^*} P[\dot{z}_S^*](z_S - u), u_S - z_S \rangle] \leq 8\rho^{-1} \|\dot{z}_S^*\|_0 \|z_S - u\|_0 \|u_S - z_S\|_0. \tag{62}$$

Finally by combining (59)-(62) and denoting $\epsilon = u_S - z_S$, we obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\epsilon\|_0^2 + \frac{1}{2} a_{min} |\epsilon|_1^2 &\leq \{16\rho^{-1} \|\mathcal{L}^*(z_S)\|_0 + 4\rho^{-1} \|\mathcal{L}^*(u)\|_0 + 4\rho^{-1} \|\mathcal{L}^*(u_S)\|_0 \\ &\quad + 4\rho^{-1} \|\dot{z}_S^*\|^2\} \|\epsilon\|_0^2 + \frac{a_{max}^2}{2a_{min}} |z_S - u|_1^2 \\ &\quad + 4\rho^{-1} \|z_S - u\|_0^2 \end{aligned} \quad (63)$$

The result now follows using the Gronwall inequality. \square

Remark 4.2. *Improved upper bounds can be investigate under stronger assumptions as in [11]. Smaller errors over longer time intervals can be obtained if, not only the error $u - z_S$, but also its derivative is small.*

5 Deterministic equation with stochastic initial datum

To have a better understanding of the DO approximation, let us have now a closer look at the following simple problem

$$\dot{u}(x, t, \omega) - \Delta u(x, t, \omega) = 0 \quad x \in D, t \in \mathcal{T}, \omega \in \Omega, \quad (64)$$

$$u(\sigma, t, \omega) = 0 \quad \sigma \in \partial D, t \in \mathcal{T}, \omega \in \Omega, \quad (65)$$

$$u(x, 0, \omega) = u_0(x, \omega) \quad x \in D, \omega \in \Omega \quad (66)$$

For sake of simplicity we assume $\mathbb{E}[u_0] = 0$. However observe that in case of a deterministic linear operator the equation for the mean in the DO system (12)-(14) is completely decoupled from the others, which implies that nothing changes in the following analysis for any $\bar{u}_0 \neq 0$.

5.1 Case I: exactness of the DO approximation

We assume that the initial datum u_0 is in the manifold \mathcal{M}_S . According to the Karhunen-Loève decomposition, u_0 can be expanded as:

$$u_0(x, \omega) = \sum_{i=1}^S \sqrt{\mu_i} \gamma_i(\omega) Z_i(x) \quad (67)$$

Let $\{\lambda_i\}_{i=1}^{\infty}$ and $\{\Phi_i\}_{i=1}^{\infty}$ be respectively the eigenvalues and the eigenfunctions of the Laplace operator, then the exact solution of problem (64) with initial datum (67) is simply given by:

$$u(x, t, \omega) = \sum_{i=1}^S \sqrt{\mu_i} \gamma_i(\omega) \left[\sum_{k=1}^{\infty} \langle Z_i, \Phi_k \rangle e^{-\lambda_k t} \Phi_k(x) \right]. \quad (68)$$

Observe that u is in the manifold \mathcal{M}_S and the truncated Karhunen-Loève expansion of rank S is actually exact for all times. The exact solution belongs indeed to \mathcal{M}_S at any time instant, hence

it coincides with its best S -rank approximation z_S . We show here that the DO approximate solution is exact as well. First of all we have that the time derivative \dot{u} is in manifold \mathcal{M}_S :

$$\dot{u}(x, t, \omega) = - \sum_{i=1}^S \sqrt{\mu_i(0)} \gamma_i(\omega) \left[\sum_{k=1}^{\infty} \langle Z_i, \Phi_k \rangle \lambda_k e^{-\lambda_k t} \Phi_k(x) \right].$$

Moreover we observe that, in light of Proposition 3.4, Δu belongs to $\mathcal{T}_u \mathcal{M}_S$ at each time instant, indeed:

$$\Delta u = \sum_{i=1}^S \langle \Delta u, U_i \rangle U_i + \sum_{i=1}^S \mathbb{E}[\Pi_U^\perp(\Delta u) Y_i] Y_i$$

which implies that the projection of Δu onto the tangent space $\mathcal{T}_u \mathcal{M}_S$ is actually equal to Δu itself. In particular, since the projection of the governing equation (64) onto the tangent space $\mathcal{T}_u \mathcal{M}_S$ coincides with the governing equation, we have that the DO solution u_S satisfies the exact equation (64). Finally the fact that $u_0 = z_S(0) = u_S(0)$ ensures that the three solutions coincide at each time. Formally the same conclusion can be achieved by looking at the evolution equations of z_S and u_S . As shown in (55) and (56) we have that:

$$\dot{z}_S = P_{z_S}(\mathcal{L}(u)) - \mathbf{D}_{z_S} P[\dot{z}_S](z_S - u) \quad (69)$$

$$\dot{u}_S = P_{u_S}(\mathcal{L}(u_S)) \quad (70)$$

with initial condition $u_0 = z_S(0) = u_S(0)$. Since $u(t) = z_S(t)$ at each time, the second term on the right side of the equation (69) is equal to zero, i.e.:

$$\dot{z}_S = P_{z_S}(\mathcal{L}(z_S)) = \mathcal{L}(z_S) \quad (71)$$

$$\dot{u}_S = P_{u_S}(\mathcal{L}(u_S)) = \mathcal{L}(u_S). \quad (72)$$

The two functions satisfy the same evolution equation with equal initial condition which implies that they are equal at each times.

Remark 5.1. *More generally, if the differential operator $\mathcal{L}(\cdot)$ in (3) is a linear deterministic operator and the initial condition u_0 is in \mathcal{M}_S , then u belongs to \mathcal{M}_S and the DO approximate solution (with rank equal to S) coincides with the exact solution at each time instant.*

Proposition 5.1. *If the initial condition $u_0 \in \mathcal{M}_S$ is a linear combination of S eigenfunctions $\Phi = (\Phi_1, \dots, \Phi_S)^T$ of the Laplace operator, then the DO method coincides to the Proper Orthogonal Decomposition method (see e.g. [27] chapter 2) in which the governing equation is projected in the fixed (time independent) subspace spanned by Φ . Indeed the deterministic basis functions do not evolve in time and the DO solution u_S is given by $u_S(x, t, \omega) = \mathbf{U}^T(x, t) \mathbf{Y}(t, \omega)$ with:*

$$\mathbf{U}(x, t) = \mathbf{U}(x, 0), \quad \mathbf{Y}(t, \omega) = \mathbf{\Upsilon}(0) e^{-\mathbf{\Lambda} t} \mathbf{\Upsilon}(0)^\top \mathbf{Y}(0, \omega), \quad (73)$$

where $\mathbf{\Lambda}$ is the diagonal matrix of the eigenvalues of the Laplace operator associated to Φ , i.e. $-\Delta \Phi = \mathbf{\Lambda} \Phi$, and $\mathbf{\Upsilon}(t)$ is the transformation matrix $\Upsilon(t)_{i,j} = \langle U_i(\cdot, t), \Phi_j \rangle$ between the basis of modes \mathbf{U} and the basis of eigenfunctions Φ .

Proof. First of all we recall that, since $u_0 \in \mathcal{M}_S$, the exact solution is in \mathcal{M}_S . Moreover it is in the span of the S eigenfunctions $\Phi = (\Phi_1, \dots, \Phi_S)^T$ at any time instant. Indeed, being $u_0(x, \omega) = \Phi(x)^T \Upsilon(0) \mathbf{Y}(0, \omega)$, the exact solution is given by:

$$u(x, t, \omega) = \Phi(x)^T e^{-\Lambda t} \Upsilon(0)^T \mathbf{Y}(0, \omega)$$

As previously discussed, we have that the DO solution coincides to the exact solution. Then it is easy to verify that $u = \mathbf{U}^T \mathbf{Y}$ and the couple (\mathbf{U}, \mathbf{Y}) in (73) satisfies the DO system. To this end, observe that the covariance matrix of the solution can be explicitly calculated as follows:

$$\begin{aligned} \mathbf{C}(t) &= \Upsilon(0) e^{-\Lambda t} \Upsilon(0)^T \mathbb{E}[\mathbf{Y}(0) \mathbf{Y}(0)^T] \Upsilon(0) e^{-\Lambda t} \Upsilon(0)^T \\ &= \Upsilon(0) e^{-\Lambda t} \Upsilon(0)^T \mathbf{C}(0) \Upsilon(0) e^{-\Lambda t} \Upsilon(0)^T \end{aligned} \quad (74)$$

The initial covariance matrix $\mathbf{C}(0)$ is assumed to have full rank and since $\Upsilon(0) e^{-\Lambda t} \Upsilon(0)^T$ is strictly positive definite, $\mathbf{C}(t)$ remains invertible at any $t \in \mathcal{T}$. This implies that $\mathbf{C}(t)$ can be simplified in (13) and then DO system is reduced to:

$$\begin{cases} \frac{d\Upsilon(t)}{dt} = [\Upsilon(t) \Lambda \Upsilon(t)^T \Upsilon(t) - \Upsilon(t) \Lambda] = 0 \\ \frac{\partial \mathbf{Y}(t, \omega)}{\partial t} = -\Upsilon(t) \Lambda \Upsilon(t)^T \mathbf{Y}(t, \omega). \end{cases} \quad (75)$$

where we use that $\Upsilon(t)$ is a square orthogonal matrix. By integrating in time we get the result. \square

5.2 Case II: effect of truncation - z_S is continuously time differentiable

We now consider an initial datum $u_0 \notin \mathcal{M}_S$. Assuming $u_0 \in L^2(D) \otimes L^2(\Omega)$ it can be expanded according to the Karhunen-Loève decomposition as:

$$u_0(x, \omega) = \sum_{i=1}^{\infty} \sqrt{\mu_i} \gamma_i(\omega) Z_i(x) \quad (76)$$

Analogously the exact solution u of problem (64) with initial condition (76) can be in general decomposed at each time t as:

$$u(x, t, \omega) = \sum_{i=1}^{\infty} \sqrt{\mu'_i(t)} \gamma'_i(\omega, t) Z'_i(x, t). \quad (77)$$

In order to apply the DO method, the initial datum is approximated by the first S terms of the series (76), whose sum $z_S(0)$ corresponds to the best rank- S approximation of u_0 in norm $L^2(D) \otimes L^2(\Omega)$ (S -rank truncated Karhunen-Loève expansion). In the same way, we denote with $z_S(t)$ the best rank- S approximation of the exact solution at time $t > 0$, i.e.:

$$z_S(x, t, \omega) = \sum_{i=1}^S \sqrt{\mu'_i(t)} \gamma'_i(\omega, t) Z'_i(x, t) \quad (78)$$

where we assumed that the coefficient μ'_i are ordered in decreasing order at each time t :

$$\mathbb{E}[\mu'_1(\cdot, t)] \geq \mathbb{E}[\mu'_2(\cdot, t)] \geq \dots \geq \mathbb{E}[\mu'_S(\cdot, t)].$$

In other words the triplet $(\gamma'_i(\omega, t), \mu'_i(t), Z'_i(x, t))$ is the one with the i^{th} biggest coefficient $\mu'_i(t)$ at time t . In addition, we denote with $\mu_i(t)$ the trajectory of the i^{th} term of the Karhunen-Loève decomposition of u_0 or, rather, the evolution of the term that at $t = 0$ has the i^{th} biggest variance. Observe that the function

$$u_S(x, t, \omega) = \sum_{i=1}^S \sqrt{\mu_i(t)} \gamma_i(\omega, t) Z_i(x, t) \quad (79)$$

is the exact solution of the problem (64) with initial condition $z_S(0)$ (the best S -rank approximation of u_0):

$$u_{0S}(x, \omega) = z_S(x, 0, \omega) = \sum_{i=1}^S \sqrt{\mu_i(0)} \gamma_i(\omega, 0) Z_i(x, 0) \in \mathcal{M}_S. \quad (80)$$

and differs, in general, from $z_S(t)$. Moreover, from what previously discussed, since u_{0S} is in a S dimensional manifold the DO solution coincides to (79). This shows that the DO method, differently to the best S -rank approximation, may be affected by the truncation of the initial datum. Indeed the DO solution of problem (64) with initial condition u_0 will be always equal to the exact solution of the same problem with initial datum u_{0S} , that is generally different to u and z_S as well.

We consider first the case in which the best S -rank approximation z_S is continuously differentiable in time, as in the hypothesis of Theorem 4.1. For the problem we are analyzing this regularity assumption implies that the S^{th} eigenvalue of the correlation operator is differentiable in time, which can be translated in practice by requiring that the maximum neglected eigenvalue μ'_{S+1} of the correlation operator, would never cross the trajectories μ_1, \dots, μ_S at any time. Under this assumption the best rank- S approximation z_S coincides to (79) and the approximation error is given by

$$\epsilon_S(t) = \sum_{i=S+1}^{\infty} \mu'_i(t) = \sum_{i=S+1}^{\infty} \mu_i(t). \quad (81)$$

We see that, for a deterministic linear operator $\mathcal{L}(\cdot)$, the continuous time differentiability of z_S is a sufficient condition for the DO solution to coincide to the best rank S approximation.

5.3 Case III: effect of truncation - z_S is not continuously time differentiable

We remove any hypothesis of regularity on the evolution of the eigenvalues of the correlation operator. This implies that the trajectories of μ_i, μ_j may cross each other at any time instant, for any $i, j \in \mathbb{N}$. In particular, if the S^{th} eigenvalue of the correlation operator is not continuously time differentiable, which means that $\mu'_k(t)$ would cross $\mu_i(t)$ at some $t \in \mathcal{T}$, for some $i = S+1, \dots, \infty$ and $k = 1, \dots, S$, then the best approximation z_S will not be continuously differentiable

in time. In this case the DO approximate solution and the best rank- S approximation do not coincide:

$$\begin{aligned} z_S(x, t, \omega) &= \sum_{i=1}^S \gamma'_i(\omega, t) \sqrt{\mu'_i(t)} Z'_i(x, t) \\ u_S(x, t, \omega) &= \sum_{i=1}^S \gamma_i(\omega, t) \sqrt{\mu_i(t)} Z_i(x, t) \end{aligned} \quad (82)$$

The DO approximation error is then strictly larger than the best approximation error:

$$\epsilon_S^{DO}(t) = \sum_{i=1}^S \mu_i(t) > \sum_{i=1}^S \mu'_i(t) = \epsilon_S(t). \quad (83)$$

and we do not have any control on it in terms of best approximation error. However observe that the DO approximation error is always bounded by the initial truncation error:

$$\epsilon_S^{DO}(t) \leq \epsilon_S(0), \quad \forall t \in \mathcal{T}. \quad (84)$$

5.4 An Illustrative Example

Consider the following problem:

$$\begin{cases} \frac{\partial u(x, t, \omega)}{\partial t} - \frac{\partial^2 u(x, t, \omega)}{\partial x^2} = 0 & x \in (0, 2\pi), t \in [0, T], \omega \in \Omega \\ u(0, t; \omega) = u(2\pi, t; \omega) = 0 & t \in [0, T], \omega \in \Omega \\ u(x, 0; \omega) = \alpha_1(\omega) \frac{1}{\sqrt{\pi}} \sin(x) + \alpha_2(\omega) \frac{1}{\sqrt{\pi}} \sin(2x) & x \in (0, 2\pi), \omega \in \Omega \end{cases} \quad (85)$$

where α_1, α_2 are independent uniform random variables with zero mean and variance $\mathbb{E}[\alpha_1^2] = 1$, $\mathbb{E}[\alpha_2^2] = 2$. As one can easily verify, the exact solution as well the total variance can be calculate analytically, i.e.:

$$u(x, t, \omega) = \alpha_1(\omega) e^{-t} \frac{1}{\sqrt{\pi}} \sin(x) + \alpha_2(\omega) e^{-4t} \frac{1}{\sqrt{\pi}} \sin(2x), \quad \text{Var}_T[u](t) = \mathbb{E}[\alpha_1^2] e^{-2t} + \mathbb{E}[\alpha_2^2] e^{-8t}. \quad (86)$$

Observe that $u(x, 0, \omega)$ is a 2-rank function in the span of the first two eigenfunctions of the Laplace operator. Consequently the exact solution evolves in the manifold \mathcal{M}_2 at any time instant, the DO method degenerates to the POD method and, with $S = 2$, both the DO and the Karhunen-Loève solutions coincide with the exact solution.

Think now that we want to approximate the solution in a manifold of dimension 1. The initial datum is approximated according to the Karhunen-Loève decomposition by the principal component with largest variance, i.e. $z_1(x, 0, \omega) = u_1(x, 0, \omega) = \alpha_2(\omega) \frac{1}{\sqrt{\pi}} \sin(2x)$, and the DO method develops the following approximate solution:

$$u_1(x, t, \omega) = \alpha_2(\omega) e^{-4t} \frac{1}{\sqrt{\pi}} \sin(2x) \quad x \in [0, 2\pi], t \in [0, T], \omega \in \Omega \quad (87)$$

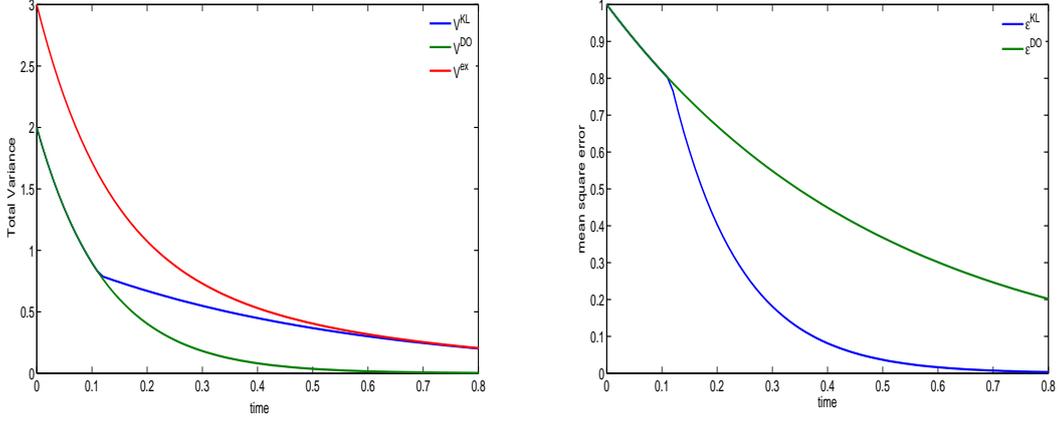


Figure 1: On the left: Evolution of the total variance $\text{Var}_T(t)$ of the exact solution as well as the KL and DO approximate solution with $S = 1$. On the right: Time evolution of the mean square error $\epsilon(t)$ of the DO method with $S = 1$, compared to the best approximation error.

On the contrary the Karhunen-Loève approximate solution is given by:

$$z_1(x, t, \omega) = \begin{cases} \alpha_2(\omega) e^{-4t} \frac{1}{\sqrt{\pi}} \sin(2x) & \text{for } t \in [0, T] : \mathbb{E}[\alpha_1^2] e^{-2t} \leq \mathbb{E}[\alpha_2^2] e^{-8t} \\ \alpha_1(\omega) e^{-t} \frac{1}{\sqrt{\pi}} \sin(x) & \text{for } t \in [0, T] : \mathbb{E}[\alpha_1^2] e^{-2t} > \mathbb{E}[\alpha_2^2] e^{-8t} \end{cases} \quad (88)$$

That is not continuously time differentiable at $t^* = \frac{1}{6} \log\left(\frac{\mathbb{E}[\alpha_1^2]}{\mathbb{E}[\alpha_2^2]}\right)$. Figure 1 shows the evolution of the exact and approximate total variance (left) and the mean square error of the DO method compared to the best 1-rank approximation.

One can see that the error of the DO method is bounded by the initial truncation error and goes asymptotically to zero as t goes to infinity, but it is strictly larger than the best approximation error as soon as the eigenvalues cross each other. Indeed, while the best approximation error asymptotically goes to zero with exponential rate given by the second eigenvalue of the Laplace operator, i.e.:

$$\epsilon(t)_{KL} = \min(\mathbb{E}[\alpha_1^2] e^{-2t}, \mathbb{E}[\alpha_2^2] e^{-8t}) \quad \text{and} \quad \epsilon(t)_{KL} = \mathbb{E}[\alpha_2^2] e^{-8t} \quad \text{for } t > t^*,$$

the exponential rate of DO approximation error is given by the smallest eigenvalue of the Laplace operator:

$$\epsilon(t)_{DO} = \mathbb{E}[\alpha_1^2] e^{-2t} = \begin{cases} \epsilon_{KL}(t) & \text{for } t \in [0, T] : t \leq t^* \\ \frac{\mathbb{E}[\alpha_1^2]}{\mathbb{E}[\alpha_2^2]} e^{6t} \epsilon_{KL}(t) & \text{for } t \in [0, T] : t > t^* \end{cases} \quad (89)$$

which shows that the DO error can not be bounded uniformly by the Karhunen-Loève error. This result does not contradict Theorem 4.1. Indeed at time t^* the truncated Karhunen-Loève expansion with rank $S = 1$ is not differentiable in time, so one important assumption in the Theorem 4.1 is not fulfilled.

6 Numerical examples

In this section, we will give some numerical examples to verify the performance of the DO approximation. Thus, we need to numerically solve the following DO system:

$$\frac{\partial \bar{u}_S(x, t)}{\partial t} = \mathbb{E} [\mathcal{L}(u_S(x, t, \cdot))] \quad (90)$$

$$\sum_{i=1}^S \mathbf{C}_{ij}(t) \frac{\partial U_i(x, t)}{\partial t} = \Pi_{\mathcal{U}}^\perp \mathbb{E} [\mathcal{L}(u_S(x, t, \cdot)) Y_j(t, \cdot)], \quad j = 1, \dots, S, \quad (91)$$

$$\frac{\partial Y_i(t, \omega)}{\partial t} = \langle \mathcal{L}^*(u_S(\cdot, t, \omega), \omega), U_i(\cdot, t) \rangle, \quad i = 1, \dots, S \quad (92)$$

6.1 Numerical discretization

For what concerns the numerical discretization of the system (90)-(92) we use the Finite Element method in the physical space, for equations (90)-(91), and Stochastic Collocation method (see e.g. [1, 2]) for equation (92). We assume that the input data are functions of a uniformly distributed random vector $\boldsymbol{\eta} = (\eta_1, \dots, \eta_N)$ so that the stochastic space $(\Omega, \mathcal{A}, \mathcal{P})$ is parametrized by $\boldsymbol{\eta}$ and replaced by $(\mathbf{\Lambda}, \mathcal{B}(\mathbf{\Lambda}), f(\boldsymbol{\eta})d\boldsymbol{\eta})$ where $\mathbf{\Lambda}$, $\mathcal{B}(\mathbf{\Lambda})$ and f denote respectively the domain, the Borel σ -algebra and the density function of $\boldsymbol{\eta}$. For the discretization in time we use a backward Euler scheme in which however eventual non linear terms are computed explicitly. Both the covariance matrix and the projection operator in (90) are treated explicitly, this allow us to linearize and completely decouple equations (90)-(91) from equations (92). In particular, the projection onto the orthogonal space in (91) is done on a basis freezed at the previous time step whereas the update of the random variables $\{Y_i\}$ in (91) is done on the newly computed basis. The splitting scheme is therefore of ‘‘Gauss-Seidel’’ type. Let \mathcal{U}_h denote the finite element space of continuous piecewise linear functions on a regular triangulation of the spatial domain D with mesh size h , $\{\xi_{\mathbf{i}} \in \mathbf{\Lambda}\}$ the set of N_y tensorized Gauss-Legendre collocation points and Δt the time step. Then the DO approximate solution at time $t^n = n\Delta t$ is discretized as follow:

$$u_{S,h,N_y}^n(x, \boldsymbol{\eta}) = \sum_{j=1}^{N_h} \bar{U}_j^n \rho_j(x) + \sum_{i=1}^S \left(\sum_{j=1}^{N_h} U_{j,i}^n \rho_j(x) \sum_{k=1}^{N_y} Y_{k,i}^n \mathcal{L}_k(\boldsymbol{\eta}) \right)$$

where $\{\rho_i\}_{i=1}^{N_h}$ and $\{\mathcal{L}_k\}_{k=1}^{N_y}$ are respectively the finite elements basis functions in D and the multivariate tensorized Lagrange polynomials on the grid $\{\xi_{\mathbf{k}}\}$ in $\mathbf{\Lambda}$. Observe that the first moment of the DO approximate solution at $t = t^n$ corresponds to the function $\bar{U}_h^n(x) = \sum_{j=1}^{N_h} \bar{U}_j^n \rho_j(x)$ and the total variance can be easily computed as the sum of the variances of the stochastic coefficients $\{Y_i\}$, i.e.:

$$\text{Var}_T[u_{S,h,N_y}^n] = \sum_{i=1}^S \text{Var}[Y_i^n] = \sum_{i=1}^S \sum_{k=1}^{N_y} Y_i^n(\xi_k)^2 w_k$$

where $\{w_k\}_{k=1}^{N_y}$ are the weights of the Gaussian quadrature formula associated to the collocation points of the stochastic grid. (For further details concerning other possible types of stochastic

grids we refer to [2,3]). Moreover the computation of the covariance of the stochastic coefficients is explicitly required in the equations (91). Indeed the equations for the deterministic basis functions $\{U_i\}$ are coupled together by the covariance matrix. A “natural” option to decouple the equations consists in multiplying both sides in (91) by the inverse of the covariance matrix. Unfortunately this is often not possible, since the covariance matrix $\mathbf{C}(t^n) = \mathbf{C}^n$ may be singular or very ill conditioned at some time instant t^n . A straightforward example is provided by any system of PDEs with stochastic coefficients and deterministic initial data: the DO approximate solution will require $S \geq 1$ number of modes, in general, even if the initial covariance matrix is identically equal to zero and then singular at least for the very first iteration. Furthermore the rank of the covariance matrix typically evolves in time whatever the initial condition is. For instance in the very simple case of linear diffusion equations with no forcing terms, the rank tends asymptotically to zero as t goes to infinity whereas for non linear problem it may drastically increases or decreases during the time evolution. This makes unsuitable also the direct use of the pseudo-inverse of \mathbf{C}^n , since such approach automatically sets to zero the “non active” deterministic basis functions and then prevents the rank from increasing. Instead of multiplying both sides of (91) by the pseudo-inverse of \mathbf{C} , denoted by \mathbf{C}^\dagger , we reformulate directly the problem in this form:

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{C}^\dagger \Pi_{\mathcal{U}}^\perp \mathbb{E}[\mathbf{Y} \mathcal{L}(u_s)],$$

that is equivalent to solve (91) when the covariance matrix has full rank. From a numerical point of view the strategy that we have adopted in this work, is based on diagonalizing the covariance matrix at each time step in order to completely decouple the system of equation (91). Indeed, even if the covariance matrix at $t = 0$ is diagonal, the DO method does not preserve in general the un-correlation of the stochastic coefficients for $t > 0$. For a better understanding let us write equation (91) in algebraic form with notations:

$$\begin{aligned} \mathbf{U}^n \in \mathbb{R}^{N_x \times S} : U_{i,j}^n &= U_j(x_i, t^n), & \mathbf{Y}^n \in \mathbb{R}^{N_y \times S} : Y_{i,j}^n &= Y_j(\xi_i, t^n) \\ \mathbf{F}^n \in \mathbb{R}^{N_x \times N_y} : \mathbf{F}_{jk}^n &= \langle \mathcal{L}(u_S(\cdot, \xi_k, t^n)), \rho_j \rangle \end{aligned}$$

Furthermore we denote with \mathbb{M} the Finite Element mass matrix and with $\mathbb{E}_{N_y}[\cdot]$ the discretized expected value, computed by the quadrature formula on the collocation points $\{\xi_k\}_{k=1}^{N_y}$. Then the algebraic formulation of system (91) is the following:

$$\mathbb{M} \mathbf{U}^{n+1} \mathbf{C}^n = \mathbb{M} \mathbf{U}^n \mathbf{C}^n + (\mathbb{I} - \mathbb{M} \mathbf{U}^n \mathbf{U}^{nT}) \mathbb{E}_{N_y}[\mathbf{F}^* \mathbf{Y}^n] \quad (93)$$

where \mathbf{F}^* denotes that the diffusion term is always treated implicitly, while eventual non linear terms are computed at $t = t^n$. Let $\mathbf{V}^n = (v_1^n, \dots, v_S^n) \in \mathbb{R}^{S \times S}$ be the matrix of eigenvectors of \mathbf{C}^n and $\mathbf{\Sigma}^n \in \mathbb{R}^{S \times S} : \Sigma_{ij}^n = \delta_{ij} \mu_i^n$ the matrix of eigenvalues, such that $\mathbf{C}^n \mathbf{V}^n = \mathbf{V}^n \mathbf{\Sigma}^n$. Then multiplying both sides in (93) by \mathbf{V}^n we get:

$$\mathbb{M} \mathbf{U}^{n+1} \mathbf{V}^n \mathbf{\Sigma}^n = \mathbb{M} \mathbf{U}^n \mathbf{V}^n \mathbf{\Sigma}^n + (\mathbb{I} - \mathbb{M} \mathbf{U}^n \mathbf{U}^{nT}) \mathbb{E}_{N_y}[\mathbf{F}^* \mathbf{Y}^n \mathbf{V}^n]$$

Observe that $\mathbf{Z}^n = \mathbf{Y}^n \mathbf{V}^n$ is a vector of uncorrelated random variables with variance $\mathbb{E}_{N_y}[(Z_i^n)^2] = \mu_i^n$. Finally we solve:

$$\mathbb{M} \mathbf{U}^{n+1} \mathbf{V}^n = \mathbb{M} \mathbf{U}^n \mathbf{V}^n + (\mathbb{I} - \mathbb{M} \mathbf{U}^n \mathbf{U}^{nT}) \mathbb{E}_{N_y}[\mathbf{F}^* \mathbf{Y}^n \mathbf{V}^n] \mathbf{\Sigma}^{\dagger n} \quad (94)$$

where $\Sigma^{\dagger n}$ is the pseudoinverse of Σ^n with tolerance ϵ , that is:

$$\Sigma_{ij}^{\dagger n} = \begin{cases} \delta_{ij} \mu_i^n & \mu_i^n > \epsilon \mu_{max}^n \\ 0 & \text{otherwise} \end{cases}$$

Roughly speaking we impose that only the “directions” associated to the eigenvalues $\mu_i^n > \epsilon \mu_{max}^n$ evolve, while the others remain constant. An alternative integrator for the low rank approximation of time dependent matrix is proposed in [16]. This is based on a suitable splitting of the orthogonal projector onto the tangent space.

As already mentioned, the DO method explicitly requires the deterministic basis functions to be orthonormal in $L^2(D)$. At the continuous level the orthonormality is preserved at any time instant thanks to condition (11). On the other hand, many numerical schemes, including the one discussed here, will not preserve the orthonormality of the discrete basis (see e.g. [15] for a discussion on orthogonality preserving numerical schemes). We therefore re-orthogonalize at each time step the spatial basis $\{U_i\}$ by means of a QR factorization (where the matrix Q is orthogonal with respect to the continuous $L^2(D)$ inner product, i.e. $Q^T M Q = \mathbb{I}$).

6.2 Linear parabolic problem with random initial conditions

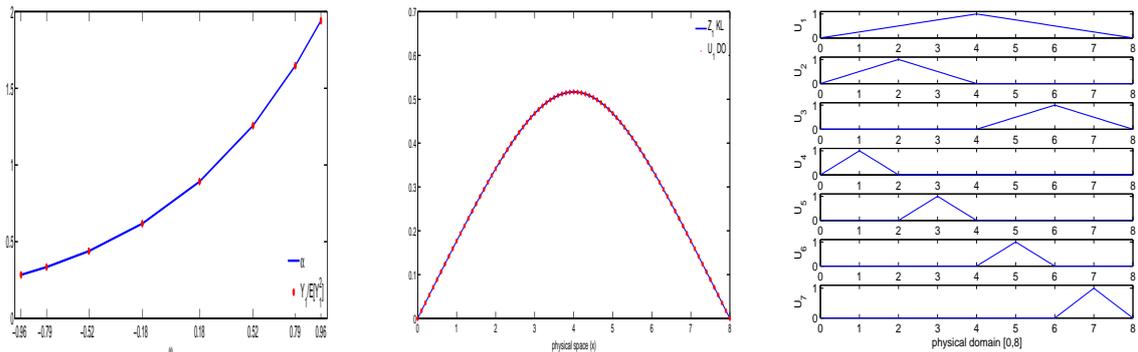


Figure 2: Left: The random variable $\alpha(\eta)$, blue, and $Y_1(t)$ (scaled by the variance $\mathbb{E}[Y_1(t)^2]$), red markers, at the collocation points. Middle: The first mode with $S = 1$ (red markers) and the principal component Z_1 (blue) at $T=1$. Right: Hierarchical basis function.

We start by considering the following simple problem already discussed in Section 5:

$$\begin{aligned} \frac{\partial u(x, t, \omega)}{\partial t} - \frac{\partial^2 u(x, t, \omega)}{\partial^2 x} &= 0, & x \in [0, 8], t \in \mathcal{T}, \omega \in \Omega \\ u(0, t; \omega) = u(8, t, \omega) &= 0, & t \in \mathcal{T}, \omega \in \Omega \end{aligned} \quad (95)$$

where the initial condition is a random field. Here we take

$$u_0(x, \omega) = \alpha(\omega) u_{01}(x) = \alpha(\omega) \frac{1}{4} | -x + 4 | + 1$$

where $\alpha(\omega) = e^{\eta(\omega)} - \mathbb{E}[e^\eta]$ and $\eta(\omega)$ is a uniformly distributed random variable in $[-1, 1]$. It is easy to see that the exact solution is a stochastic field with the same distribution of $\alpha(\omega)$. Analytically it can be calculated as $u_{ex}(x, \omega, t) = \alpha(\omega)\psi(x, t)$, being ψ the solution of the deterministic diffusion PDE with initial condition $\psi(x, 0) = u_{01}(x)$. By normalizing the field $\psi(x, t)$ the solution can be rewritten in accordance with the Karhunen-Loève decomposition, having only one principal component $Z_1(x, t) = \psi(x, t)/\|\psi(\cdot, t)\|_0$ and one stochastic coefficient $\gamma_1(\omega, t) = \alpha(\omega)\|\psi(\cdot, t)\|_0$. We can easily verify that the couple (Z_1, γ_1) satisfy the DO system (12)-(13) with $S = 1$:

$$\begin{cases} \dot{Z}_1 = \frac{\dot{\psi}}{\|\psi\|_0} - \left\langle \frac{\dot{\psi}}{\|\psi\|_0}, \frac{\psi}{\|\psi\|_0} \right\rangle \frac{\psi}{\|\psi\|_0} = \Delta Z_1 - \langle \Delta Z_1, Z_1 \rangle Z_1 = \Pi_{\mathcal{Z}}^\perp \{\Delta Z_1\} \\ \dot{\gamma}_1 = \left\langle \frac{\dot{\psi}}{\|\psi\|_0}, \frac{\psi}{\|\psi\|_0} \right\rangle \gamma_1 = \langle \Delta Z_1, Z_1 \rangle \gamma_1 \end{cases} \quad (96)$$

and initial condition $Z_1(x, 0) = u_{01}(x)/\|u_{01}\|_0$, $\gamma_1(\omega, 0) = \alpha(\omega)$. This confirms again the exactness of the DO method in case of deterministic operator and initial condition that belongs to a finite dimensional manifold. Now we want to show that the exactness of the DO method is preserved at the discrete level as well: let $u_{h, N_y, \Delta t}$ denote the discrete solution of (95), obtained by using piecewise linear continuous Finite Elements in space with mesh size h , Stochastic Collocation method on N_y Gauss-Legendre points in $\eta(\omega)$ and backward Euler discretization in time with step Δt . We show that the corresponding DO approximate solution coincides with $u_{h, N_y, \Delta t}$. Let \mathbb{M} and \mathbb{K} be respectively the mass and stiffness matrix of the Finite Element discretization and let μ_1^n denotes the variance of the random variable Y_1^n . The algebraic system for the DO solution $u_{1, h, N_y, \Delta t} = U_{1, h, \Delta t} Y_{1, N_y, \Delta t}^T$ with rank one is given by:

$$\mathbb{M}U^{n+1}\mu^n + \Delta t\mathbb{K}U^{n+1}\mu^n = \mathbb{M}U^n\mu^n + \Delta t\mathbb{M}U^nU^{nT}\mathbb{K}U^n\mu^n \quad (97)$$

$$Y^{n+1T} + \Delta tU^n\mathbb{K}U^nY^{n+1T} = Y^{nT} \quad (98)$$

where for simplicity of notation, we have omitted the subscripts. By multiplying the first equation by Y^{n+1} and using (98) we get:

$$\mathbb{M}U^{n+1}Y^{n+1T} + \Delta t\mathbb{K}U^{n+1}Y^{n+1T} = \mathbb{M}U^nY^{n+1T} - \mathbb{M}U^nY^{n+1T} + \mathbb{M}U^nY^{nT} \quad (99)$$

or equivalently:

$$\mathbb{M}u_1^{n+1} + \Delta t\mathbb{K}u_1^{n+1} = \mathbb{M}u_1^n \quad (100)$$

which exactly corresponds to the algebraic system of the discretized problem for $u_{h, N_y, \Delta t}$. Figure 2 (middle) shows that the deterministic basis function U_1 evolves in time and coincides to the principal component Z_1 of the discrete solution $u_{h, N_y, \Delta t}$ at each time step. The stochastic coefficient Y_1 is as well proportional to the initial random parameter, with variance that decreases in time and coincides with the total variance of the solution. Figure 2 (left) shows that Y_1^n , normalized with respect to the variance at time t^n ($\mathbf{E}[(Y_1^n)^2]$), is equal to $\alpha(\omega)$ at each time step.

Finally we aim at analyzing the efficacy of the DO method in case of over-approximation, that occurs when the DO approximate solution is defined in a manifold of dimension larger than the rank of the exact solution. To this purpose we again apply the DO method to problem (95) with

$S > 1$ whereas we have seen that only one mode is really needed. We initialize the deterministic basis functions $\{U_i\}_{i=1}^S$ to a sequence of hierarchical functions as in Figure 2 (right). To preserve the consistency with the initial datum, the first stochastic coefficient is initialized to $\alpha(\omega)$ and all the other coefficients are initialized to zero. Since the DO method requires the deterministic basis functions to be orthonormal in $L^2(D)$, the first step consists in the re-orthonormalizing the initial hierarchical basis functions. From a computational point of view, this is achieved by using the QR decomposition, with respect to the continuous $L^2(D)$ inner product. Let $(\hat{U}_1, \dots, \hat{U}_S)$ denotes the set of orthonormalized basis functions. Then the initial datum is expanded as

$$u_0(x, \omega) = \sum_{i=1}^S \hat{U}_i(x, 0) \hat{Y}_i(\omega, 0) \quad (101)$$

with $\hat{Y}_i(\omega, 0) = 0$ for $i = 2, \dots, S$. As the system evolves in time, all the spatial basis functions evolve and all the random variables become in general different from zero (Figure 3). However the stochastic coefficients $\{\hat{Y}_i\}$ are all linearly dependent and the rank of the covariance matrix $\mathbf{C}_{ij}^n = \mathbb{E}[\hat{Y}_i^{nT} \hat{Y}_j^n]$ remains constantly equal to one at each time step, as long as the total variance of the solution is larger than zero. This confirms that the DO method in the version proposed here, effectively deals with singular covariance matrices in case of over-approximation and is able to identify the effective dimension of the manifold of the solution. Moreover we remark that at each time step only one deterministic PDE is actually solved, thanks to the diagonalization technique discussed in Section 6.1. Also in case of over-approximation we have verified numerically that the DO solution corresponds to the discrete solution $u_{h, N_y, \Delta t}$ at each time step.

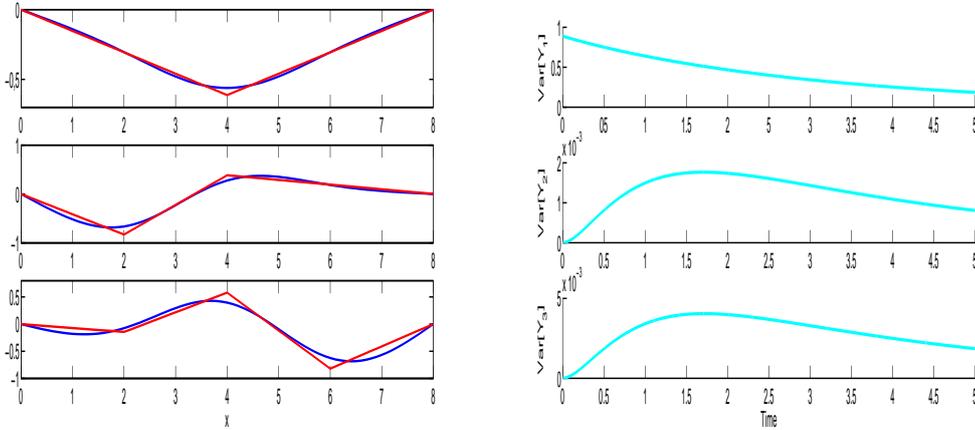


Figure 3: Left: The re-orthogonalized modes at time $T = 0$ (red) and $T = 5$ (blue), with $S = 3$. Collocation points $N_y = 11$, time step $\Delta t = 0.001$, spatial discretization $h = 0.1$ and threshold $\epsilon = 1.e - 16$. Right: Evolution in time of the variance of the stochastic coefficients.

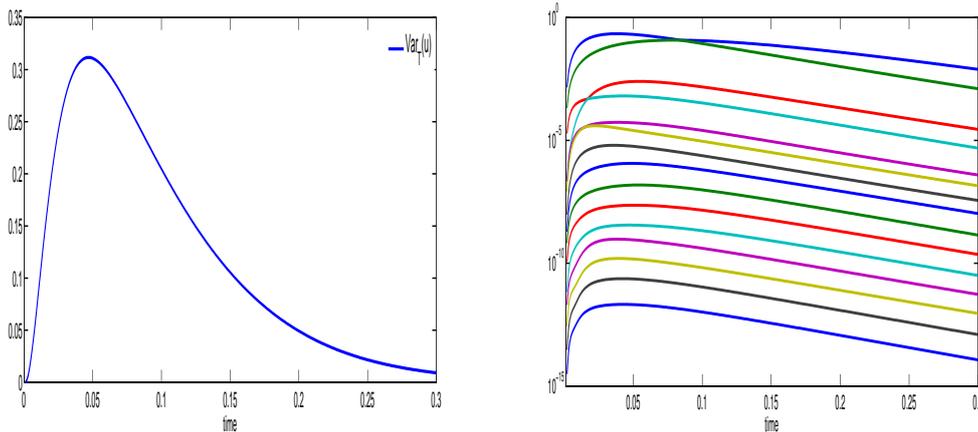


Figure 4: Left: The evolution of the total variance of the solution. Right: Evolution of the first 15 eigenvalues of the correlation operator in log scale

6.3 Linear parabolic problem with random diffusion coefficient

We consider now the following linear parabolic equation:

$$\begin{aligned} \frac{\partial u(x, t, \omega)}{\partial t} - \operatorname{div}\left(a(x, \omega) \frac{\partial u(x, t, \omega)}{\partial x}\right) &= 0, & x \in [0, 1], t \in \mathcal{T}, \omega \in \Omega \\ u(0, t, \omega) = u(1, t, \omega) &= 0, & t \in \mathcal{T}, \omega \in \Omega \end{aligned} \quad (102)$$

where now $\mathcal{L}(\cdot)$ is actually a stochastic differential operator, being the diffusion coefficient a a random field on $(\Omega, \mathcal{A}, \mathcal{P})$ taking values in $L^\infty(D)$. This means that the eigenvalues and the eigenfunctions of $\mathcal{L}(\cdot)$ are random fields in $(\Omega, \mathcal{A}, \mathcal{P})$ as well. For reasons of existence and uniqueness of the solution we assume $a(\cdot, \omega)$ to be a strictly positive and bounded function over D for each random event $\omega \in \Omega$. Here we consider a coefficient having the following form:

$$a(x, \omega) = \bar{a}(x) + \sum_{i=1}^2 (\eta_{2i-1}(\omega) \cos(i\pi x) + \eta_{2i}(\omega) \sin(i\pi x))$$

where $\bar{a} = 1.45$ and η_1, \dots, η_4 are zero mean uniform independent random variables with variance $\mathbb{E}[\eta_i^2] = (1/3) \cdot 10^{-i+1}$. On the other hand, the initial condition is taken to be a deterministic function and is given by:

$$u_0(x) = 10 \sin(\pi x)$$

By this choice we can also verify the stability of the DO method in case of an initial zero rank covariance matrix and emphasize the differences with respect to the type of problems discussed in Section 5.1 and 6.2. Here the solution $u(x, t, \omega)$ is actually a function of the random variables $\boldsymbol{\eta} = (\eta_1, \dots, \eta_4)$. Figure 4 (left) shows the evolution of the total variance of the solution.

At each time step, we can introduce the parameter-to-solution map $u(\cdot, t, \boldsymbol{\eta}) : [-1, 1]^4 \rightarrow H_0^1(D)$. Defining now the set $\mathcal{V}(t) = \{u(\cdot, t, \boldsymbol{\eta}), \boldsymbol{\eta} \in [-1, 1]^4\} \subset H_0^1(D)$, at each time step the solution $u(\cdot, t, \boldsymbol{\eta}(\omega))$ is in $\mathcal{V}(t)$ for all $\omega \in \Omega$. The manifold $\mathcal{V}(t)$ is a multidimensional manifold which,

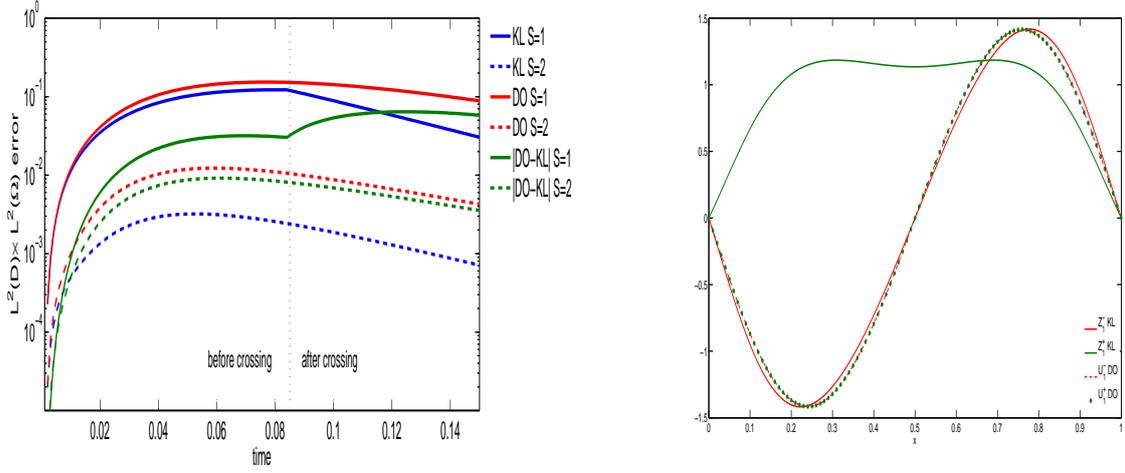


Figure 5: Left: The best approximation error (blue) and the error of the DO approximate solution (red) in the $L^2(D) \times L^2(\Omega)$ norm with $S = 1$ (solid line) and $S = 2$ (dotted line), in log scale. In green the $L^2(D) \times L^2(\Omega)$ norm of the difference between the DO and the Karhunen-Loève solutions with $S = 1$ (solid line) and $S = 2$ (dotted line). Right: The first mode of the Karhunen-Loève expansion and DO solution at the time step just before (red) and after the crossing of eigenvalues (green solid line-Karhunen-Loève, green markers-DO).

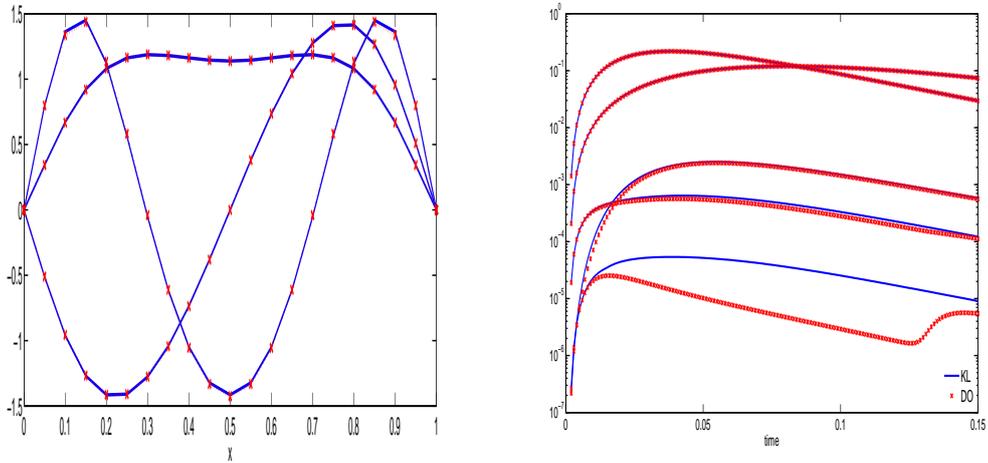


Figure 6: Left: The first three modes of the DO approximate solution (red markers) with $S = 5$ and of the Karhunen-Loève expansion (blue, solid line) just after the crossing t^* . Right: The eigenvalues of the covariance matrix of the stochastic coefficient of the DO solution (red markers) with $S = 5$ and the first 5 eigenvalues of the covariance operator of the reference solution (blue, solid line), in log scale. Note that the first DO and KL modes and eigenvalues are almost indistinguishable.

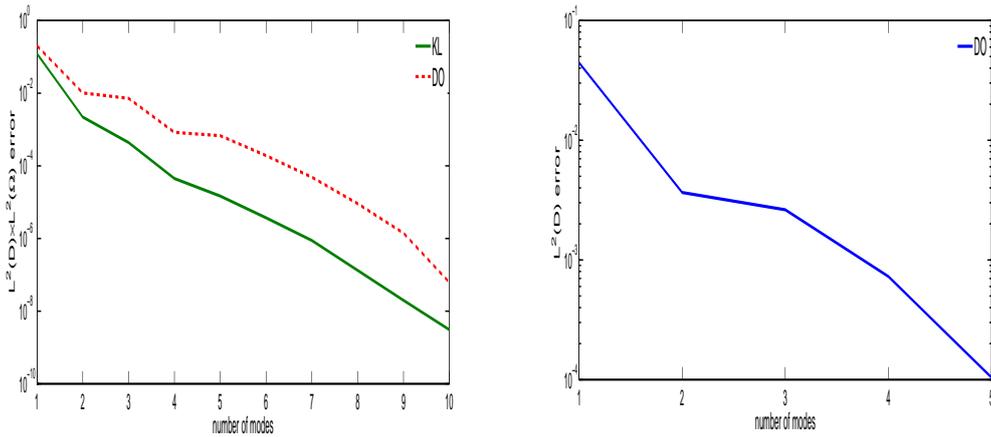


Figure 7: Left: The best approximation error (green) and the error of the DO approximate solution (red, dotted line) in $L^2(D) \times L^2(\Omega)$ norm w.r.t. the number of modes at time $T = 0.1$. Right: The $L^2(D)$ -error on the mean of the DO approximate solution w.r.t. the number of modes, at time $T = 0.1$

in this example, evolves in time. First of all we compute and analyze the Karhunen-Loève decomposition of the numerical reference solution computed with a very accurate (and costly) Stochastic Collocation method. The analysis of the Karhunen-Loève decomposition is very useful to understand what we can expect from the DO method. Moreover, it allows us to directly compare the DO solution with the best approximation. In Figure 4 (right) we see the evolution of the eigenvalues of the covariance operator. Observe that only few of them reach remarkable values. This immediately shows that the solution u can be well approximated in a low rank format. On the other hand, notice that the first two eigenvalues cross each other at time $t^* \approx 0.08$. This implies that the 1-truncated Karhunen-Loève expansion is not continuously differentiable in time at the crossing. Hence Theorem 4.1 only applies for $t < t^*$, for $S = 1$. On the other hand, the case $S = 2$ seems to be smooth (at least up to the final computational time $T = 0.3$). Similar considerations apply to successive modes, for $S = 3, 4, S = 5, 6$, etc.

The numerical results confirm the theoretical ones given in Section 4 and are consistent with the observations above. Figure 5 (left) shows the approximation error in the $L^2(D) \times L^2(\Omega)$ norm of the truncated Karhunen-Loève expansion as well as the DO solution, with rank $S = 1$ (solid line) and $S = 2$ (dotted line). We see that the approximation error of the DO solution with rank equal to 1 is proportional to the best approximation error only until the first two eigenvalues of the Karhunen-Loève expansion cross each other. Before the crossing, the difference in the $L^2(D) \times L^2(\Omega)$ norm between the DO solution and the truncated Karhunen-Loève expansion with rank 1 is bounded by the best approximation error so the error of the DO method is well controlled by the error of the Karhunen-Loève expansion. After the crossing, the bound clearly degenerates. The problem is due to the evolution of the first mode of the Karhunen-Loève expansion which is no longer continuous in time. In Figure 5 (right) we see the first mode of the Karhunen-Loève expansion in two consecutive time step, just before and after the crossing. By using only

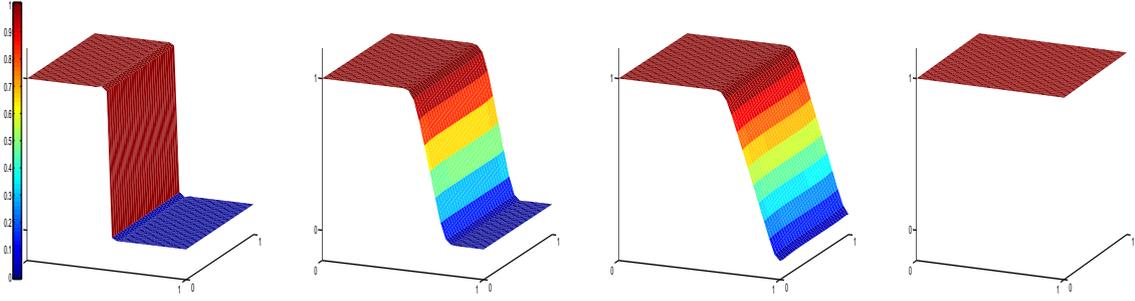


Figure 8: Mean solution at time $t = 0$ (left), $t = 0.35$ (middle-left), $t = 1$ (middle-right) and $t = 2$ (right). Discretization parameters: Gauss-Legendre collocation points $N_y = 41$, spatial discretization $h = 0.03$, time step $\Delta t = 0.001$

one mode, the DO method is not able to follow accurately the evolution of the first mode of the Karhunen-Loève expansion after the crossing. Indeed the hypothesis of continuous differentiability of the rank-1 Karhunen-Loève approximation is not fulfilled and Theorem 4.1 can not be applied after the crossing. However this problem can be overcome by using an approximation with rank larger than 1, as we can see in Figure 6 (left). The plot shows the first three modes of the DO approximate solution which are very close to those of the Karhunen-Loève expansion even after the crossing t^* . Moreover the evolution of the eigenvalues of the covariance matrix related to the DO solution, is comparable to the evolution of the eigenvalues of the covariance operator of the exact solution (Figure 6, right). For what concerns the $L^2(D) \times L^2(\Omega)$ error (Figure 7, left) and the $L^2(D)$ error on the mean (Figure 7, right), good levels of accuracy can be achieved by using only few modes. Moreover, the plot clearly shows an exponential convergence rate with respect to the number of modes.

6.4 Parabolic equation with non linear reaction term

To conclude we consider a reaction-driven non linear parabolic operator with stochastic coefficient. The problem is defined as follows:

$$\begin{aligned} \frac{\partial u(\mathbf{x}, t, \omega)}{\partial t} - \mu \Delta u(\mathbf{x}, t, \omega) &= f(u(\mathbf{x}, t, \omega)), & \mathbf{x} \in D = [0, 1]^2, t \in \mathcal{T}, \omega \in \Omega, \\ \frac{\partial u}{\partial \mathbf{n}}(\boldsymbol{\sigma}, t, \omega) &= 0, & \boldsymbol{\sigma} \in \partial D, t \in \mathcal{T}, \omega \in \Omega \\ u(\mathbf{x}, 0, \omega) &= \begin{cases} 1 & \text{if } x_1 \leq 0.5, \\ 0 & \text{if } x_1 > 0.5. \end{cases} & \mathbf{x} \in D, \omega \in \Omega, \end{aligned}$$

The reaction term is a cubic polynomial in u , i.e. $f(u) = \beta u(u - 1)(\alpha(\omega) - u)$, with constant excitation rate β and stochastic threshold potential $\alpha(\omega)$. We assume $\alpha(\omega)$ to be a uniformly distributed random variable. The initial condition is instead deterministic and it is represented by a step function equal to one for values of coordinate x_1 smaller than 0.5 and zero otherwise. The solution is a traveling wave, whose direction and speed, proportional to β , is determined

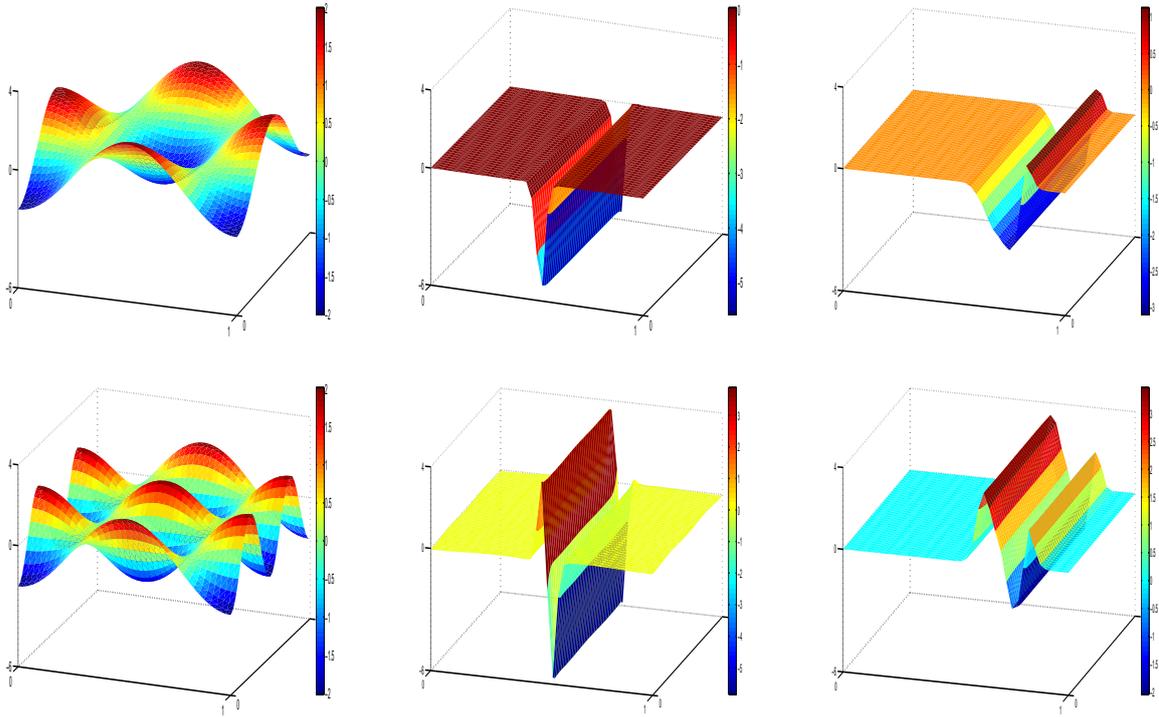


Figure 9: First (top) and second (bottom) mode of the DO approximate solution at time $t = 0$ (left), $t = 0.05$ (middle) and $t = 0.5$ (right) with a number of modes $S = 6$, excitation rate $\beta = 100$ and threshold potential $\alpha(\omega)$ uniform r.v. in $[0, 0.4]$. Discretization parameters: Gauss-Legendre collocation points $N_y = 41$, spatial discretization $h = 0.05$, time step $\Delta t = 0.001$

by the value of the random variable α . After a while, the wave exits the computational domain and the solution tends to the constant function $u = 1$ if $\alpha(\omega) < 0.5$, and $u = 0$ if $\alpha(\omega) > 0.5$, irrespectively of the initial datum. Therefore for $t \gg 0$ the solution is at most a rank-1 function and is deterministic if either $\alpha(\omega) < 0.5$ or $\alpha(\omega) > 0.5 \forall \omega \in \Omega$. Figure 8 shows the evolution of the expected value of the solution, by assuming $\alpha(\omega) < 0.5$. Observe that the solution is a function of the random variable α . By defining as before the parameter-to-solution map $u(\cdot, t, \alpha) : [-1, 1] \rightarrow H^1(D)$ and the set $\mathcal{V}(t) = \{u(\cdot, t, \alpha), \alpha \in [-1, 1]\} \subset H^1(D)$, at each $t \in \mathcal{T}$ the solution $u(\cdot, t, \alpha(\omega))$ is in the one dimensional manifold $\mathcal{V}(t)$ for all $\omega \in \Omega$. However the manifold $\mathcal{V}(t)$ evolves in time, driven by the non linear reaction term, and may feature a complex structure for large times. In the DO approach, we try to approximate such manifold by a linear combination of S modes. The number of basis functions that the DO approximate solution needs to well describe the solution depends obviously on the complexity of the manifold $\mathcal{V}(t)$.

We analyze here the performance of the DO approach. First of all, since the initial condition is deterministic, we have arbitrarily initialized the modes to a set of orthonormal functions. Due to the zero Neumann boundary conditions, we have chosen S orthonormal cosine functions of increasing frequency, i.e. $u_{\mathbf{i}}(x_1, x_2) = k_{\mathbf{i}} \cos(i_1 \pi x_1) \cos(i_2 \pi x_2)$ (where $k_{\mathbf{i}}$ is the normalization

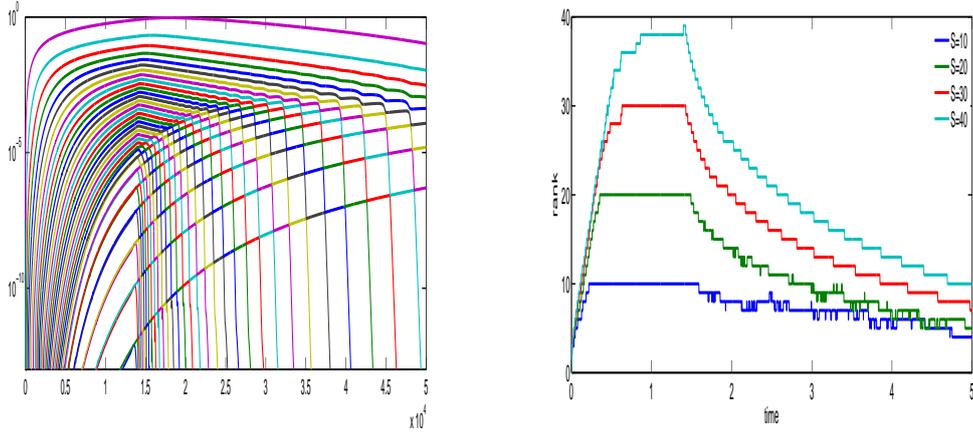


Figure 10: On the left: Evolution of the eigenvalues of the covariance matrix of the DO approximate solution (in logarithmic scale) with $S = 40$. Right: Evolution of the rank of the covariance matrix with number of modes $S = 10/20/30/40$ and excitation rate $\beta = 100$. Discretization parameters: Gauss-Legendre collocation points $N_y = S$, spatial discretization step $h = 0.05$, time step $dt = 0.001$.

constant). Figure 9 shows the first two deterministic basis functions at different time iterations. Observe that the modes adapt very fast to the structure of the problem and assume values different than zero only around the front of the traveling wave. On the other, by analyzing the evolution of the eigenvalues of the covariance matrix, we see that good levels of accuracy can be achieved only if a relative large number of modes is used. Figure 10 (left) shows that several eigenvalues reach remarkable values and many of them cross each other. This poses a serious limitation in the use of low rank formats for this type of problems, which is intrinsically due to the nature of the problem and the structure of the solution. This is confirmed also by the analysis of the effective

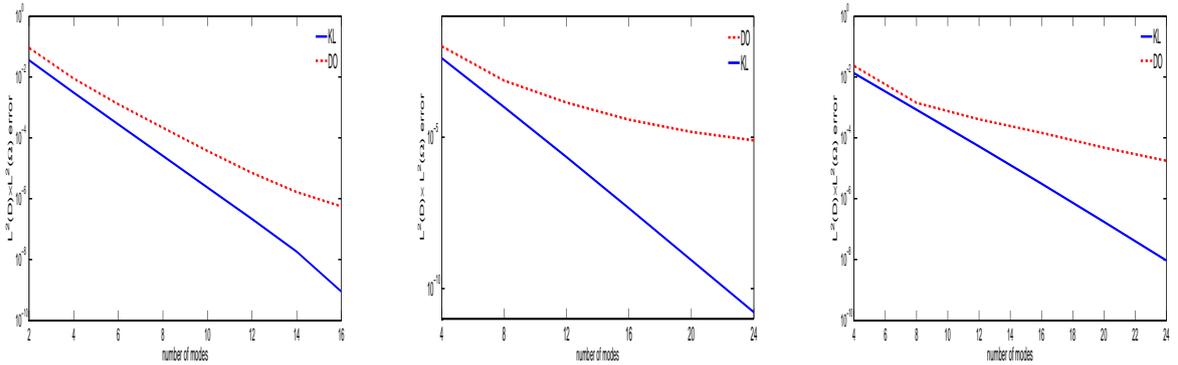


Figure 11: Error in norm $L^2(D) \times L^2(\Omega)$ of the DO (red, dotted line) and the truncated Karhunen-Loève (blue, solid line) approximate solution w.r.t. the number of modes. (log scale). Left: $\beta = 10$, $dt = 1.e - 3$, $T=3$. Middle: $\beta = 100$, $dt = 1.e - 3$, $T = 0.5$. Right: $\beta = 100$, $dt = 1.e - 3$, $T = 0.7$.

rank of the DO approximate solution. Figure 10 (right) shows the evolution of the rank of the DO approximate solution, for different values of S . Being the rank of the covariance matrix bounded by the number of collocation points that are used in the stochastic discretization, in the plot we consider a number of collocation points at least equal to S . We see that for $S < 40$ the rank tends to reach the saturation level S , whereas it does not exceed 39 by using $S > 40$. However that bound is influenced by the space discretization and tends to slightly increase by refining the deterministic discretization parameter. Furthermore the bound is related to the value of the excitation rate β , which affects the “sharpness” of the front. When the excitation rate is small, e.g $\beta \approx 10$, the maximum rank achieved is relatively smaller (≈ 22). In the latter case indeed the reaction has weaker predominance on the diffusion term and the solution has less step gradients. Looking at the solution for larger times, when the front is about to exit the computational domain, the total variation of the solution decreases, and the rank decreases as well. If, on the one hand, these results show the ability of the DO method to capture the effective dimension of the solution at each time step, on the other hand they also show the need of using a large number of modes. Figure 11 shows the $L^2(D) \times L^2(\Omega)$ error of the DO approximate solution (red, dotted line) and of the truncated Karhunen-Loève expansion (blue, solid line) with respect to the number of modes. We observe that in both cases, high levels of accuracy may be achieved only for large values of S . Furthermore the rate of convergence of the DO method is slower than the one of the truncated Karhunen-Loève expansion. This is due to the fast increasing/decreasing of the eigenvalues of the covariance matrix, that makes them frequently cross each other. As discussed in Section 4, this fact may negatively affect the performance of the DO method. On the other hand numerical evidence reveals that better performances for these types of problems can be achieved when the stochastic input concerns the initial condition instead of the coefficients of the reaction-operator.

Conclusion

In this work we established and formalized a link between the DO approximation of PDEs with random initial datum and the MCTDH method proposed for the approximation of deterministic Schrödinger equations, or the discrete analogue Dynamical Low Rank approximation of evolution matrix or tensor equations. We have reinterpreted the DO approximation as a Galerkin projection onto the tangent space to the manifold \mathcal{M}_S of all rank S functions, at any time instant and in light of the theoretical results developed in [11, 14] for the MCTDH method and the Dynamical Low Rank approximation, we investigated the properties of the manifold \mathcal{M}_S for a linear parabolic equation with random parameters. Specifically we exploited the curvature bounds of \mathcal{M}_S to show that the DO approximation error can be bounded in terms of the best rank S approximation of the solution, at each time instant, under the assumption that the latter is differentiable in time. On the other hand, we have seen that the regularity assumption on the Karhunen-Loève decomposition is actually a necessary condition to maintain an effective control on the DO approximation error. As confirmed by the numerical results, the DO approximation error is properly bounded in terms of best approximation error as long as the eigenvalues of Karhunen-Loève expansion included in the S rank approximation, do not cross the ones which

have been initially omitted. In conclusion our work sets the bases for a theoretical analysis of the DO approximation for random PDEs and provides indication of the effectiveness of the DO method for different types of problems.

Acknowledgements

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