POLITECNICO DI MILANO

Scuola di Ingegneria dei Sistemi

Corso di Studi in Ingegneria Matematica

Dynamical low rank approximation of time dependent PDEs with random parameters

Relatore: Prof. Fabio Nobile
Correlatore: Dott. Tao Zhou

Laureanda: Eleonora Musharbash
766995

Anno Accademico 2011-2012

Contents

List of Figures

Sommario

Questo lavoro si pone, nell'ambito dell' "Uncertainty Quantification", lo studio di EDP tempo dipendenti caratterizzate da parametrico condizioni iniziali stochastiche, con il particolare fine di sviluppare soluzioni approssimanti con dimensionalità ridotta. L' approaccio adottato, che prende il nome di "Dynamically Orthogonal Field" (DO), consiste nell'assumere la soluzione approssimante espansa in termini di serie, con basi deterministiche e coefficienti stocastici, entrambi tempo dipendenti in modo tale da evolvere in accordo con la soluzione. L'obiettivo è quello di riuscire ad utilizzare una espansione con pochi termini che descrivano globalmente la struttura della soluzione ad ogni istante temporale. Questo concetto si traduce nel nostro caso in un sistema accoppiato di equazioni di evoluzione, stocastiche quelle per i coefficienti e deterministiche per le basi e la media della funzione approssimante. Tale sistema può essere ricavato direttamente dalla EDP stocastica che governa il problema, tramite un opportuno approccio alla Galerkin. Mostreremo inoltre che tale approccio corrisponde dal punto di vista numerico con la 'Dynamically Double Orthogonal" (DDO), in quanto entrabi forniscono la stessa soluzione se si adotta una formulazione alla Galerkin. Tale fatto risulta rilevante in quanto sono presenti in letterature stime di quasi ottimalità per l'approssimazione DDO in dimensione finita, ovvero errore limitato da quello di migliore approssimazione sotto opportune ipotesi e con le opportune norme. Alla luce di questo abbiamo indagato la relazione tra soluzione approssimate (DO) a rango N e la migliore approssimazione a rango N tramite test numerici e considerazioni teoriche per il caso semplice di EDP paraboliche con diffusione lineare. Tale modello di equazioni sarà inoltre utilizzato per testare il reale funzionamento del metodo e l'influenza dai vari parametri di discretizzazione. Concludiamo il lavoro applicando l'approccio DO a PDE tempo dipendenti con termine di reazione non lineare, specificatamente ispirate ai modelli di attività bioletrica per le cellule cardiache, distinguendo nei test numerici il caso di condizione iniziale o parametri stocastici.

Abstract

In this thesis we focus on parabolic PDEs in which some of the parameters or the initial data are not exactly quantified "a priori". In this framework the problem is described in terms of random variables in the probability space; in particular, the solutions are assumed to be spatial and time dependent random fields.

When the number of stochastic variables is large, an important issue consists in reducing the dimensionality of the problem for the approximation of the solution. This represents a challenging task when the probability structure of the solution evolves in time. In view of that we consider the Dynamically Orthogonal Field (DO) approach according to which the approximate solution is described in terms of deterministic basis functions and stochastic coefficients, both of them evolving in time. In particular they adapt to the solution in a way that reduces the dimension of the approximation. The key point consists in not building an approximation through fixed bases either in the deterministic or physical space but in looking directly for an approximate rank N solution that is achieved by a Galerkin projecting of the governing equation. The method results in a system of evolution equations that defines the solution at any time instant in order to maintain the effectiveness of the approximation also for long time integration. One can find in literature equivalent formulation in a finite element setting for which convergence analysis and error estimates are provided. In particular, we show that the DO approach is strongly related to the Dynamically Double Orthogonal decomposition (DDO) since both methods provide the same numerical solution when the Galerkin approach is adopted.

The rest of the thesis is divided in two parts. In the first one we focus on parabolic linear diffusion equations for which we give theoretical results on the convergence rate and numerical examples to test the accuracy of the method. In the second one we consider parabolic equations with non linear reaction term, particularly inspired by electrical models of biological tissues.

Introduction

In the last decades many engineering and physical problems have been described by mathematical models and reproduced in numerical simulation. This approach basically consists in investigating the phenomena to find all the relevant variables, formulating mathematical equations to describe the principles that link these variables each other and then discretizing and solving the problem via numerical methods. However each of these steps is pron to many sources of error and uncertainty. In particular in several situations the analysis of the problem is compromised by incomplete knowledge or it is characterized by intrinsic variability. Exact experimental measurement are indeed not always available or they might not characterize completely the system. One can think for instance to geological problems, where the study of the mechanical proprieties of the soil can not be supported by complete data. The measurement of the physical quantities like viscosity, permeability or density are often not precise or not available point-wise. In other cases the uncertainty is instead intrinsic in the phenomena as some quantities can not be predicted. This occurs for example in the weather forecasting framework where the initial conditions are never exactly known "a priori". In addition there are other situations in which the model is required to preserve the variability of the phenomena. This is the case of models for the electrical signals in biological tissues, in which the parameters depend on each individual and can change in time, based on the age and the occurrence of many situation among which diseases, stress and changes of the life-style. The limitations of the deterministic approach can be overcame by characterizing and quantifying the impact of the uncertainties on the mathematical modeling and consequently on the numerical predictions. By following this approach the problem is reformulated under probability structures in order to predict and quantify both the expected outcome and its variability. The resulting mathematical model is often described by partial differential equations where the data and the parameters are modeled as random variables or random fields that may have spatial or temporal structures. Specifically in this thesis we focus on dynamical systems governed by stochastic partial differential equations where the randomness is generated by the initial condition or it arises from the parameters in the differential operator. Since in this framework the dimension of the stochastic space is often large or infinite, a challenging task consists in developing numerical methods that efficiently describe the evolution of the stochastic system at an affordable computational cost.

In this thesis we focus on numerical methods that aim at finding an approximate solution

in a low dimensional manifold that evolve in time. Specifically we analyze the Dynamically Orthogonal Filed approach (DO), proposed in [16] [17] and also in [12], [10] with a slightly different formulation in finite dimensional setting. The Dynamically Orthogonal field approach consists basically in a low rank approximation method according to which the numerical solution is built as a linear combination of few basis functions that try to catch the principal features of the stochastic field. Contrary to most of the methods proposed in literature this approach provides an approximate representation of the solution where both the stochastic and deterministic components changes in time in order to adapt to the process evolution. This feature makes the model effective also for long time integration.

In the light of the strong relation between the Dynamically Orthogonal Filed approach and the dynamical Singular Value Decomposition (SVD), we propose an analysis and implementation of the method specifically for stochastic parabolic equations with diffusion-reaction term. In particular the thesis is organized as follows:

- **Chapter 1** we review the spectral approach in the uncertainty quantification framework with a brief description of the main methods proposed in the literature for the forward uncertainty quantification,

- **Chapter 2** we illustrate the DO approach and show the equivalence with the Double Dynamically Orthogonal decomposition. In the light of that we report some results on the convergence analysis of the approximation in the finite dimensional setting, obtained in [12],

- **Chapter 3** We apply the DO method to a linear parabolic PDE with either stochastic initial datum or stochastic diffusion coefficient. In particular we analyze the relation between the DO expansion and the expansion of the solution on the eigenfunction of the differential operator. We detail then the discretization of the DO system by Finite Element in space and Finite Difference in time and present same numerical tests that confirm the theoretical findings. We discus the computational aspects of the method, that has been implemented in Matlab.

- **Chapter 4** we apply the DO method to stochastic parabolic equations with non linear reaction term describing the electric signal in biological tissues. By distinguishing the case in which the initial datum or the parameters of the operator are stochastic, we compare the DO approximate solution with the best rank N approximation.

- **Conclusion** we discuss the results achieved in this work, the key points of the DO approach and the suitable further developments.

Chapter 1

Problem Background

In this chapter we introduce the necessary background concerning the problem discussed in the thesis. We give a brief overview of some of the stochastic modeling methods recently developed in the literature for the uncertainty quantification and, in particular, the Stochastic Collocation method that will be used hereafter.

1.1 Notation

Let $(\Omega, \mathcal{F}, \mathcal{P})$ be a complete probability space where Ω is the set of outcomes, $\mathcal{F} \subset 2^{\Omega}$ the σ-algebra of events and $\mathcal{P} : \mathcal{F} \to [0,\, 1]$ the associated probability measure. A real-valued random variable on $(\Omega, \mathcal{F}, \mathcal{P})$ is a function $\xi = \xi(\omega) : \Omega \to \mathbb{R}$ that associates one numerical value to each realization $\omega \in \Omega$. We indicate with $\mathbb{E}[\xi]$ the mean, or expected value, of ξ and generally with $\mathbb{E}[\xi^k]$ the k-th moment:

$$\mathbb{E}[\xi^k] = \int_{\Omega} \xi^k(\omega)\, d\mathcal{P}(\omega) \tag{1.1}$$

The space of all the stochastic variables with finite second moment, denoted by $\mathrm{L}^2_{\mathrm{P}}(\Omega)$:

$$\mathrm{L}^2_{\mathrm{P}}(\Omega) = \left\{ \xi : \Omega \to \mathbb{R} : \mathbb{E}[\xi^2] < \infty \right\} \tag{1.2}$$

is an Hilbert space with associated inner product given by:

$$< \xi_1,\, \xi_2 >_{\mathrm{L}^2_{\mathrm{P}}(\Omega)} = \mathbb{E}[\xi_1 \xi_2] = \int_{\Omega} \xi_1(\omega), \xi_2(\omega)\, d\mathcal{P}(\omega) \tag{1.3}$$

Given two jointly distributed random variable $\xi_1,\, \xi_2 \in \mathrm{L}^2_{\mathrm{P}}(\Omega)$ we define the covariance and the variance respectively as:

$$\begin{aligned} \mathbb{C}(\xi_1, \xi_2) &= \mathbb{E}[(\xi_1 - \mathbb{E}[\xi_1])(\xi_2 - \mathbb{E}[\xi_2])], \\ \mathbb{V}ar(\xi_1) &= \mathbb{E}[(\xi_1 - \mathbb{E}[\xi_1])^2], \end{aligned} \tag{1.4}$$

and we remind that $\mathbb{E}[(\xi_1 - \mathbb{E}[\xi_1])^2] = \mathbb{E}[\xi_1^2] - \mathbb{E}[\xi_1]^2$.

Furthermore, given a spatial domain $D \subset \mathbb{R}^n$ (with $n = 1, 2, 3$) we call deterministic function any function defined in D with value in R. The infinite set of all the square integrable functions in D, $L^2(D)$, form a Hilbert space with inner product denoted by $< \cdot, \cdot >$. Specifically:

$$L^2(D) = \left\{ u : D \to \mathbb{R} : \int_D u^2(\mathbf{x}) \, d\mathbf{x} < \infty \right\} \tag{1.5}$$

Moreover we define $H^1(D)$ the Hilbert space of all square integrable functions in D with square integrable distributional derivatives.

$$H^1(D) = \left\{ u : D \to \mathbb{R} : \int_D \big(u(\mathbf{x})\big)^2 + |\nabla u|^2(\mathbf{x}) \, d\mathbf{x} < \infty \right\} \tag{1.6}$$

and $H_0^1(D) \subset H^1(D)$ the subspace of the functions with zero trace on the boundary.

Given the deterministic and the stochastic space, a random filed is defined as a real valued function on the product space:

$$u(\mathbf{x}, \omega) : D \times \Omega \to \mathbb{R} \tag{1.7}$$

where $\mathbf{x}$ denotes the space coordinate. For any fixed $\mathbf{x} \in D$, $u(\mathbf{x}, \cdot)$ is a random variable and conversely, fixed the event $\omega \in \Omega$, $u(\cdot, \omega)$ is called realization of the stochastic filed. Similarly to what seen before, we can define the expected value and the covariance operator that in this case become functions of the deterministic variable $\mathbf{x}$:

$$\begin{aligned} \bar{u}(\mathbf{x}) &= \mathbb{E}[u(\mathbf{x}; \cdot)] & \mathbf{x} \in D \\ C_{uv}(\mathbf{x}, \mathbf{y}) &= \mathbb{E}\big[\big(u(\mathbf{x}; \cdot) - \bar{u}(\mathbf{x})\big)\big(v(\mathbf{y}; \cdot) - \bar{v}(\mathbf{y})\big)\big] & \mathbf{x}, \mathbf{y} \in D \end{aligned} \tag{1.8}$$

The set of all square integrable random fields form a Hilbert space, denoted by $\mathcal{H}$ i.e.:

$$\mathcal{H} = \left\{ u : D \times \Omega \to \mathbb{R} : \int_\Omega \int_D \big(u(\mathbf{x}; \xi)\big)^2 \, d\mathbf{x} \, d\mathcal{P}(\omega) < \infty \right\} \tag{1.9}$$

with associated inner product $< u, v >_{\mathcal{H}} = \mathbb{E}[< u, v >]$.

All the previous definitions can be generalized to time dependent stochastic fields:

$$u(\mathbf{x}, t, \omega) : D \times [0, T] \times \Omega \to \mathbb{R} \tag{1.10}$$

where t is the temporal variable and $[0, T] \subset \mathbb{R}$ is the time interval. We introduce also the Banach spaces $L^\infty([0, T], \mathcal{H})$ and $L^2([0, T], \mathcal{H})$ defined as:

$$\begin{aligned} L^\infty([0, T], \mathcal{H}) &= \left\{ u : D \times [0, T] \times \Omega \to \mathbb{R} : \mathbb{E}\big[\int_D u^2(\mathbf{x}, t; \cdot) \, d\mathbf{x}\big] < \infty \; \forall t \in [0, T] \right\} \\ L^2([0, T], \mathcal{H}) &= \left\{ u : D \times [0, T] \times \Omega \to \mathbb{R} : \int_{[0, T]} \mathbb{E}\big[\int_D u^2(\mathbf{x}, \cdot; \cdot) \, d\mathbf{x}\big] \, dt < \infty \right\} \end{aligned}$$
$$\tag{1.11}$$

Under the "finite dimensional noise assumption" the stochastic space is parametrized by a random vector $\vec{\xi} = [\xi_1, ..., \xi_s]$ and it assumed to have finite dimension s. Let Γ_i be the support of ξ_i and $\mathbf{\Gamma} = \Gamma_1 \times ... \times \Gamma_s \subset \mathbb{R}^s$ the support of $\vec{\xi}$, then the abstract probability space $(\Omega, \mathcal{F}, \mathcal{P})$ can be replaced by $(\mathbf{\Gamma}, \mathcal{B}(\mathbf{\Gamma}), f(\vec{\xi})d\vec{\xi})$ where $\mathcal{B}(\mathbf{\Gamma})$ denoted the Borel $\sigma-$algebra and $f(\vec{\xi})$ is the joint probability density function of $\vec{\xi}$. The Hilbert space $\mathrm{L}_P^2(\Omega)$ becomes $\mathrm{L}_f^2(\mathbf{\Gamma})$ defined as:

$$\mathrm{L}_f^2(\mathbf{\Gamma}) = \left\{ y : \Gamma \to \mathbb{R} : \int_{\mathbf{\Gamma}} y^2(\vec{\xi}) f(\vec{\xi}) \, d\vec{\xi} < \infty \right\} \qquad (1.12)$$

Any stochastic field in $u \in \mathcal{H}$ can be also re-defined and expressed in terms of $\vec{\xi}$, $u(\mathbf{x}, \vec{\xi}(\omega))$, with $u(\mathbf{x}, \cdot) \in \mathrm{L}_f^2(\mathbf{\Gamma})$.

1.2   Spectral Representation

The spectral approach aims to describe the uncertainty from a functional point of view. Contrarily to the Monte Carlo Methods that obtains locally informations by sampling, the spectral approach aims to determine the functional dependence that generates the uncertainty. The unknown random variables are generally represented in form of series, and the basis functions are defined in the stochastic space.
We introduce two classical spectral representation approaches for square integrable random fields $u(\mathbf{x}, \omega)$: the Karhunen Loève expansion based on the spectral decomposition of the autocorrelation function and the generalized Polynomial Chaos Expansion which provides the decomposition in terms of orthogonal polynomials in the stochastic space. Thus the approaches will be then generalized for time dependent stochastic fields $u(\mathbf{x}, t, \omega)$.

1.2.1   The Karhunen Loève Expansion

Any square integrable random field $u(\mathbf{x}, t)$ with continuous covariance function can be represented as an infinite sum of uncorrelated random variables. The Karhunen-Loève expansion, see [2], [23], is one of the most common decompositions of a random field and is the analogous of the Principal Component Decomposition (see e.g. [1]) in infinite dimensional setting. It consists of decomposing the random field in terms of uncorrelated random variables, i.e. random variable orthogonal in $\mathrm{L}_P^2(\Omega)$, and $\mathrm{L}^2(\mathrm{D})$-orthonormal deterministic basis functions, i.e.:

$$u(\mathbf{x}; \omega) = \bar{u}(\mathbf{x}) + \sum_{i=1}^{\infty} y_i(\omega) u_i(\mathbf{x}) \qquad (1.13)$$

with

- $< u_i(\mathbf{x}), u_j(\mathbf{x}) > = \delta_{ij}$,
- $\mathbb{E}[y_i] = 0$

- $\mathbb{E}[y_i y_j] = \lambda_i \delta_{ij}$

for all $i, j \in \mathbb{N}_+$ and where δ_{ij} is the Kronecker's symbol, $\delta_{ij} = 1$ if $i = j$ and zero otherwise. We detail the KL expansion in the case of time dependent random fields.

Proposition 1.2.1.
Let $u \in \mathrm{L}^\infty([0, \mathrm{T}], \mathcal{H})$ be a random field with continuous covariance function $C_{u(t)u(t)}(\mathbf{x}, \mathbf{x}')$ for any $t \in [0, \mathrm{T}]$. Let $\Gamma_{u(t)}$ be the linear, symmetric and compact operator defined for any $t \in [0, \mathrm{T}]$ as:

$$v \in \mathrm{L}^2(\mathrm{D}) \to \Gamma_{u(t)u(t)}(v) = \int_{\mathrm{D}} C_{u(t)u(t)}(\mathbf{x}, \mathbf{x}')v(\mathbf{x}') \, d\mathbf{x}' \qquad (1.14)$$

Hence, it admits a decreasing and non-negative sequence of eigenvalues $\{\lambda_i(t)\}_{i \in \mathbb{N}}$ with corresponding eigenfunctions $\{u_i(\mathbf{x}, t)\}_{i \in \mathbb{N}}$ that form an orthonormal basis in $\mathrm{L}^2(\mathrm{D})$ at any t. Moreover it holds:

$$u(\mathbf{x}, t; \, \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{\infty} y_i(t; \, \omega)u_i(\mathbf{x}, t) \qquad (1.15)$$

where $\bar{u}(\mathbf{x}, t) = \mathbb{E}[u(\mathbf{x}, t; \, \omega)]$ and $y_i(t; \, \omega)$ are uncorrelated stochastic processes with zero mean and variance $\mathbb{V}ar[y_i(t; \, \omega)] = \lambda_i(t)$, defined as:

$$y_i(t; \, \omega) = \int_{\mathrm{D}} [u(\mathbf{x}, t; \, \omega) - \bar{u}(\mathbf{x}, t)]u_i(\mathbf{x}, t) \, d\mathbf{x} \qquad (1.16)$$

Furthermore the total variance of u is given by:

$$\int_{\mathrm{D}} \mathbb{V}ar[u(\mathbf{x}, t; \, \cdot)] \, d\mathbf{x} = \sum_{i=1}^{\infty} \lambda_i(t) \qquad (1.17)$$

The expansion (1.13) is an exact representation of the stochastic field u that is decomposed at any time instant in a infinite number of deterministic fields multiplied by scalar stochastic coefficients. The deterministic fields carry all the spatial information while the stochastic coefficients describe the whole stochastic response.

In order to get a computable decomposition, the series (1.15) is truncated and only a finite set of N terms is taken into account. The number of terms N has to be large enough to deliver a good approximation of u, i.e. it has to be chosen in order to include a sufficient percentage of the total variance (1.17). The set of N terms that maximizes the total variance of the approximation is given by the first N elements of the series assuming that the eigenvalues $\{\lambda_i(t)\}_{i \in \mathbb{N}}$ in the spectral decomposition of the covariance operator have been sorted in decreasing order with respect to the variance. Then the truncated Karhunen Loève expansion reads:

$$u_N(\mathbf{x}, t; \, \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N} y_i(t; \, \omega)u_i(\mathbf{x}, t) \qquad (1.18)$$

Observe that the truncated KL expansion is an optimal approximation in the sense that it is the best approximation that can be achieved by N terms in the mean square sense at any time instant.

The approximation u_N converges in mean square sense to u as provided by the Mercer's Theorem and the rate of convergence depends on the decay of the eigenvalues, [4]. In particular it holds:

$$\mathbb{E}\left[\int_{\mathrm{D}} |u(\mathbf{x}, t, \cdot) - u_N(\mathbf{x}, t, \cdot)|^2 \, d\mathbf{x} \right] = \sum_{i=N+1}^{\infty} \lambda_i(t) \to 0 \; when \; N \to \infty \qquad (1.19)$$

for any $t \in [0, \mathrm{T}]$. Moreover the decay of λ_i is related to the spatial regularity of the covariance function: the smoother the covariance is, the faster the eigenvalues $\lambda_i(t)$ decay. Specifically an analytic covariance function has exponential decay of λ_i, while finite Sobolev regularity leads only to an algebraic decay.

An alternative to the Karhunen Loève expansion is given by the Fourier-based decomposition [23], according to which the stochastic field is expanded in terms of trigonometric polynomials.

Consider a stochastic filed $u \in \mathcal{H}$. We say that u is stationary if the covariance function $C_{uu}(\mathbf{x}, \mathbf{x}')$ depends only on the distance $\|\mathbf{x} - \mathbf{x}'\|$, i.e. $C_{uu}(\mathbf{x}, \mathbf{x}') = C_{uu}(\|\mathbf{x} - \mathbf{x}'\|)$. Assume that $u : [0, L]^2 \times \Omega \to \mathbb{R}$ is stationarity and isotropic. For the hypothesis of stationarity the variance of u is assumed to be point-wise equal to σ^2. Moreover let the covariance function $C_{uu}(\mathbf{x}, \mathbf{x}')$ be Lipschitz continuous, it can be expressed in cosinus terms by the Fourier series:

$$C_{uu}(\|\mathbf{x} - \mathbf{x}'\|) = \sigma^2 \sum_{\mathbf{i} \in \mathbb{N}_+^2} c_{\mathbf{k}} \cos(\omega_{k_1}(x_1 - x_1')) \cos(\omega_{k_2}(x_2 - x_2')) \qquad (1.20)$$

with normalized coefficient $c_{\mathbf{k}}$ so that $\sum_{\mathbf{i} \in \mathbb{N}_+^2} c_{\mathbf{k}} = 1$.

Then u admits the following representation:

$$
\begin{aligned}
u(\mathbf{x}; \omega) = \bar{u}(\mathbf{x}) + \sigma \sum_{\mathbf{i} \in \mathbb{N}_+^2} c_{\mathbf{k}} \quad & [y_{\mathbf{i}}^1(\omega) \cos(\omega_{k_1} x_1) \cos(\omega_{k_2} x_2) + \\
& y_{\mathbf{i}}^2(\omega) \sin(\omega_{k_1} x_1) \sin(\omega_{k_2} x_2) + \\
& y_{\mathbf{i}}^3(\omega) \cos(\omega_{k_1} x_1) \sin(\omega_{k_2} x_2) + \\
& y_{\mathbf{i}}^4(\omega) \sin(\omega_{k_1} x_1) \cos(\omega_{k_2} x_2)]
\end{aligned}
\qquad (1.21)
$$

where $\omega_{k_i} = \frac{k_i \pi}{L}$ and the stochastic variables $, y_{\mathbf{i}}^j$, j=1,...,4, are uncorrelated, with zero mean and unit variance . Thanks to the trigonometric polynomials this approach highlights the contribution of each frequency to the total field.

Once more the series needs to be truncated in order to get a computationally suitable representation. Compared to the KL expansion, similar convergence proprieties holds.

In general if u admits a continuous version and is periodic, it can be expanded in Fourier series, or in other words it can be represented by deterministic cosine and sine

terms with stochastic coefficients. Otherwise if u is not periodic, it can be made periodic in a bigger physical domain, e.g if we assume $u(\cdot, \omega)$ defined in $[0,\ L]$ it have to be made periodic with period at least equal to L (or bigger). This technique provides a periodic function that can be expanded in Fourier series but on the other hand this might introduce discontinuities on the boundary of the original domain leading to a degraded convergence rate. It is then worth making the function periodic on a larger domain $[-\delta,\ L+\delta]$ with δ equal to twice or three times the correlation length to minimize this degradation.

1.2.2 Generalized Polynomial Chaos Expansion

The Generalized Polynomial Chaos (gPC) expansion, [23], [1], [2], [26] consists in decomposing the stochastic variables in terms of uncorrelated polynomial functions. Namely the stochastic variable is linearly expanded into a series of fixed stochastic functions multiplied by deterministic coefficients.
Historically in 1938 Wiener first formulated the polynomial chaos expansion, [25], in term of the Hermite polynomials to modelize near-gaussian stochastic processes.
Under the "finite dimensional noise assumption" the probabilistic space is parametrized by a finite number S of random variables $\vec{\xi} = (\xi_1, ..., \xi_S) : \Omega \to \Gamma^S$, where Γ^S is the support of $\vec{\xi}$. Assume that $\vec{\xi}$ is a vector of S centered, normalized, mutually orthogonal Normal random variables and let $\{\psi_i\}_{i\in\mathbb{N}}$ be a sequence of uncorrelated polynomials, i.e.: $\mathbb{E}[\psi_i\psi_j] = \delta_{ij}$ where δ_{ij} is equal to 1 for $i = j$ and 0 otherwise. The uncorrelated relation is transfered in $L^2(\mathbf{\Gamma}, \mathcal{B}(\Gamma), f(\vec{\xi})d\vec{\xi})$ and leads to:

$$\mathbb{E}[\psi_i\psi_j] \ = \ \int_{\mathbf{\Gamma}} \psi_i(\vec{\xi})\psi_j(\vec{\xi})f(\vec{\xi})\,d\vec{\xi} \ = \ \delta_{ij} \tag{1.22}$$

Here f is the joint density function of $\vec{\xi}$, $\mathcal{B}(\mathbf{\Gamma})$ denoted the Borel $\sigma-$algebra and that $\{\psi_i\}_{i\in\mathbb{N}}$ form a complete basis in $L^2(\mathbf{\Gamma}, \mathcal{B}, f(\vec{\xi})d\vec{\xi})$.
Now let u be a square integrable random field. It can be expressed in terms of the random vector $\vec{\xi}$ as $u(\mathbf{x}, \vec{\xi}(\omega))$ and in particular we have $u(\mathbf{x}, \cdot) \in L^2(\mathbf{\Gamma})$. Then, according to the Polynomial Chaos approach, u can be represented as:

$$u(\mathbf{x}, \vec{\xi}(\omega)) = \sum_{i=0}^{\infty} u_i(\vec{x})\psi_i(\vec{\xi}(\omega)) \tag{1.23}$$

where $\{\psi_i(\vec{\xi})\}_{i\in\mathbb{N}}$ correspond to the Hermite polynomials. One can verify that they are orthogonal with respect to the Gaussian measure and moreover that $\mathbb{E}[\psi_i] = 0$ for all $i > 1$.
In order to get a computationally feasible representation, the series (1.23) is truncated and the stochastic field is approximated by the first $N + 1$ terms:

$$u_N(\mathbf{x}, \vec{\xi}(\omega)) = \sum_{i=0}^{N} u_i(\mathbf{x})\psi_i(\vec{\xi}(\omega)) \tag{1.24}$$

One can choose to approximate the expansion by using all the polynomials up to a fixed total degree p that leads to take into account a number of terms:

$$N + 1 = \frac{(S + p)!}{S!p!} \tag{1.25}$$

An alternative approach consists on the tensor product expansion according to which one considers all the combinations of the one-dimensional polynomials with degree lower or equal to a fixed order p. The number of terms included grows exponentially with the dimension of the stochastic space and because of that the method suffers of the so called *curse of dimensionality*. Alternative approaches to overcame this problems are introduced in [21].

The approximation (1.24) introduces a truncation error that depends on p. However the generalization of Cameron and Martin theorem [30] provides that the truncated expansion converges to u in mean square sense when p, and consequently N, goes to infinity, i.e.:

$$\lim_{N \to \infty} \mathbb{E}\Big[\int_{\mathrm{D}} |u_N(\mathrm{x}, \cdot) - u(\mathrm{x}, \cdot)|^2 d\mathbf{x} \Big] \to 0 \tag{1.26}$$

The polynomials $\{\psi_i(\vec{\xi})\}_{0=1,..\infty}$ form indeed a complete basis in $\mathrm{L}^2(\Omega)$. Moreover, by assuming that u is a nearly Gaussian random field, the Hermite polynomials provides that the truncation error is minimized with respect to N, the number of terms in the expansion. In this sense we refer to "optimal" set of polynomial. Observe indeed that any Gaussian random variable can be exactly represented with $p = 1$.

In 2002, Xiu and Karniadakis [26] generalized this idea and applied the concept of orthogonal polynomials to some of the most common probability distributions. Observe that the probability density function plays the role of a weight function in the orthogonality relation (1.22). In the light of the correspondence between the probability density functions and weighting functions, the stochastic polynomials are constructed by using the measure corresponding to the probability law of the random field that one wants to represent. Specifically, once the probability space has been parametrized by $\vec{\xi}$ according to the probability structure of the problem, any square integrable stochastic field $u(\mathbf{x}, \vec{\xi}(\omega))$ is represented by using orthogonal polynomials with respect the probability law of $\vec{\xi}(\omega)$. The Askey scheme [2] provides the correspondence between the common distributions and the associated orthogonal family of polynomials, e.g. Legendre polynomials correspond to uniform distribution. For many more general distributions the set of orthogonal polynomials can be found by the Gram-Schmidt orthogonalization process [27]. However, observe that this approach implicitly requires a priori knowledges on the probability structure of the sources of uncertainty.

The gPC method can be also used to represent time-dependent fields and the decomposition reads:

$$u(\mathbf{x}, t, \vec{\xi}(\omega)) = \sum_{i=0}^{\infty} u_i(\mathbf{x}, t)\psi_i(\vec{\xi}(\omega)) \tag{1.27}$$

where $\{\psi_i(\vec{\xi})\}_{i \in \mathbb{N}}$ are the orthogonal polynomials with respect to $\vec{\xi}$. Observe that the polynomials are time independent. In other words the stochastic structure remains fixed in time and the deterministic coefficients evolve according to the process evolution.

1.3 Methods for forward uncertanty propagation

In this thesis we deal with time-dependent stochastic problems of the form:

$$
\begin{cases}
\dfrac{\partial u(\mathbf{x}, t, \omega)}{\partial t} = \mathcal{L}(u(\mathbf{x}, t, \omega); \omega) & \mathbf{x} \in \mathrm{D},\, t \in [0, \mathrm{T}],\, \omega \in \Omega \\
u(\mathbf{x}, 0, \omega) = u_0(\mathbf{x}, \omega) & \mathbf{x} \in \mathrm{D},\, \omega \in \Omega \\
u(\sigma, t; \omega) = h(\sigma, t; \omega) & \sigma \in \partial\mathrm{D},\, t \in [0, \mathrm{T}],\, \omega \in \Omega
\end{cases}
\tag{1.28}
$$

where $\mathcal{L}$ is a general differential operator.

There exist several approaches according to witch the solution $u(\mathbf{x}, t, \omega)$ can be discretized in order to get a numerical approximation. One of them, the Proper Orthogonal Decomposition, consists of evolving an approximate solution given a set of fixed deterministic basis functions chosen a "priori". On the contrary the generalized polynomial Chaos Expansion approach provides a decomposition of the stochastic field by using fixed basis functions in the random space.

1.3.1 Proper Orthogonal Decomposition

The Proper Orthogonal Decomposition method [2], [1] adopts the idea of the KL expansion and attempts to approximate the solution along the principal components of the stochastic field u. The method results in an approximation of the form:

$$
u_N(\mathbf{x}, t, \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N} y_i(t; \omega) u_i(\mathbf{x})
\tag{1.29}
$$

where $\{y_i(t; \omega)\}_{i=1,...N}$ are stochastic processes and $\{u_i(\mathbf{x})\}_{i=1,...N}$ time-independent orthonormal fields. Following the statistical approach, the sample covariance matrix is computed from experimental data or from direct numerical simulations and the eigenvectors of the correlation matrix are supposed to correspond to the spatial functional basis functions. In other words the technique consists in pre-computing a number of snapshot at different time instant and for several parameter values. The snapshots are then used to estimate the sample correlation matrix and the bases are computed by the SVD decomposition. Alternatively the initial datum is expanded according to the KL decomposition and the first N principal components are used as the time constant physical basis functions.

The solution is approximated in the low dimensional subspace identified by the basis functions $u_1(\mathbf{x}), ...u_N(\mathbf{x})$. Specifically by the Galerkin projection of the original governing equations onto the subspace spanned by the basis functions, one recovers the evolution equations for the unknown stochastic coefficients:

$$
\frac{\partial y_i(t, \omega)}{\partial t} = <\mathcal{L}(u(\cdot, t, \omega), \omega),\, u_i> \qquad \forall i = 1, ...N
\tag{1.30}
$$

The advantage of the POD consists on reducing the dimension of the problem but on the other hand the lack of time dependence on the deterministic basis functions reduces the representation capabilities of the method that might not be effective for non-linear dynamical problems.

1.3.2   gPC based Stochastic Galerkin

The Stochastic Galerkin, [2], [9], [32], [31] is an intrusive method that consists in formulating the governing equations for the deterministic coefficients in the gPC.
According to the gPC approach, the probabilistic space is parametrized by $\vec{\xi}$ and the stochastic filed u is expanded onto the orthonormal polynomials $\{\psi_i\}_{i\in\mathbb{N}}$. The series is then truncated to N terms:

$$u_N(\mathbf{x}, t, \vec{\xi}(\omega)) = \sum_{i=0}^{N} u_i(\mathbf{x}, t)\psi_i(\vec{\xi}(\omega)) \tag{1.31}$$

and it is introduced into the governing equation (1.28). A Galerkin projection into the subspace $\mathcal{V}_N = span < \psi_0, ..., \psi_N >$ yields to a set of $N+1$ deterministic equations.

$$\frac{\partial u_i(\mathbf{x}, t)}{\partial t} = \frac{1}{\alpha_i}\mathbb{E}\big[\mathcal{L}\big(\sum_{k=0}^{\infty} u_k(\mathbf{x}, t)\psi_k\big)\psi_i\big] \tag{1.32}$$

for all $i = 0, ...N$, where $\alpha_i = \mathbb{E}[\psi_i\psi_i]$. The Galerkin projection above ensures that the residual is orthogonal to $\mathcal{W}_N$ at any time instant. The system (1.32) is deterministic and can be solved by any common discretization techniques, e.g. by the finite element method. In this case the solution is approximated in the finite dimensional space $\mathcal{V}_{h,p} = \mathrm{W}_h \otimes \mathcal{V}_N$ where W_h is a finite element space of continuous piecewise polynomials defined on a triangulation $\mathcal{T}_h$ of D, being h the mesh spacing parameter.
On the other hand the equations are often coupled, with dimension equal to $N+1$ times the dimension of the deterministic system, and they require *ad hoc* strategies for the resolution, besides a big effort for what concerns the memory storage.
Moreover we remark that the method might suffers for long time integration. The gPC approach indeed assumes a fixed parametrization of the probability space according to the random inputs. As shown in [8], [14] in some cases, e.g. quadratic non-linearity in the stochastic space, the solution deviates from the distribution of the inputs for later times. It follows that more and more terms in (1.31) are required to well describe the solution in time. In rough words the problem concerns with the fact that the solution is approximated by polynomials fixed in time which do not adapt to the evolution of the probabilistic structure.
A possible solution has been proposed in [13], [14] and it consists in using time dependent polynomials $\{\psi_i(\vec{\xi}, t)\}_{i=0,...N}$ that adapt to the changes of the probability density function.

1.3.3   Stochastic Collocation

The Stochastic Collocation, SC, is in a interpolation method based on Lagrange polynomials, [22], [21], [24], [33].
Given a stochastic differential problem as (1.28), this is evaluated in a set of $N_\mathbf{y}$ points $\{\xi_\mathbf{i} \in \Gamma\}$. That means that for all $\xi_\mathbf{i} \in \Gamma$ one computes the corresponding deterministic

solution $u(., t, \xi_{\mathbf{i}})$ and builds the global polynomial approximation upon those evaluations, i.e.:

$$u(\mathbf{x}, t; \vec{\xi}(\omega)) = \sum_{i=1}^{N_y} u(\mathbf{x}, t)\mathcal{L}_i(\vec{\xi}(\omega)) \tag{1.33}$$

where $\{\mathcal{L}_i(\vec{\xi}(\omega))\}_{i=1}^{N_y}$ are the multivariate Lagrange polynomials. There are several possibilities to choose the collocation points:

- Clenshaw-Curtis points: i.e. the roots of Chebyshev polynomials, $T_k(x) = \cos(k \arccos(x))$. By doubling the number of points each time, this choice produces a nested sets of points with $N_y^k = 2^{k-1} + 1$ and $N_y^1 = 1$.

- Gauss points: the zeros of the orthogonal polynomials in the probability space, i.e. the orthogonal polynomials with respect to the probability density function $f(\xi)$. The result is a grid of non nested points.

- Kronrod-Patterson: the nested sequence of points that maximizes the exactness of the quadrature formula with respect to the weight $f(\xi)$. It gives a set of nested "nearly Gauss" points.

This technique can be based on either full or sparse tensor product approximation space. In oder to detail the method we focus on the former case.
Let Γ be the S-dimensional interval $[-1, 1]^S \in \mathbb{R}^S$ where S is the dimension of the stochastic space. First of all we consider the case with $S = 1$.
We introduce the set of the collocation points on the mono-dimensional interval $\Gamma^1 = [-1, 1]$ such that $\{\xi_1, ...\xi_{N_y}\} \subset [-1, 1]$. Let $\mathcal{W}$ be the Banach space where $u(\xi, \cdot)$ takes values so that we define the one-dimensional Lagrange interpolation operators as:

$$\mathcal{U}^{N_y}(u)(\xi(\omega)) = \sum_{j=1}^{N_y} u(\xi_j)\mathcal{L}_j(\xi(\omega)) \tag{1.34}$$

for all $u \in C^0(\Gamma^1, \mathcal{W})$, where $\mathcal{L}_j$ are the Lagrange polynomials of degree $N_y - 1$:

$$\mathcal{L}_j(\xi) = \prod_{k=1, \, k\neq j}^{N_y} \frac{(y - y_k)}{(y_j - y_k)} \tag{1.35}$$

Observe that the interpolation (1.35) is exact for all the polynomials of degree less than N_y.
Now in the multidimensional case $S > 1$, we introduce a multi-index $\mathbf{i} = (i_1, ..., i_S) \in \mathbb{N}_+^S$. For each $u \in C^0(\Gamma, \mathcal{W})$ and multi-index $\mathbf{i}$ the function is approximated using the full tensor product interpolation:

$$
\begin{aligned}
u_{N_y}^{\mathbf{i}}(\vec{\xi}) &= \left(\mathcal{U}^{i_1} \otimes ... \otimes \mathcal{U}^{i_S}\right)(u)(\vec{\xi}) \\
&= \sum_{j_1=1}^{i_1} ... \sum_{j_S=1}^{i_S} u\left(y_{j_1}, ..., y_{j_S}\right)\left(\mathcal{L}_{j_1}^{i_1}(\xi_1) \otimes ... \otimes \mathcal{L}_{j_S}^{i_S}(\xi_S)\right)
\end{aligned}
\tag{1.36}
$$

where N_y is the total number of collocation points i.e. $N_y = \prod_{k=1}^{S} i_k$.

The great advantage of the SC with respect to the stochastic Galerkin consists on decoupling the problem. In other words, given a stochastic partial differential equation the SC method consists on an approximation by solving N_y decoupled deterministic partial differential equations.

On the other hand the method is affected by what is known as *curse of dimensionality*. The number of collocation points grows exponentially with the dimension of the stochastic space and for large S the tensor product interpolation becomes impracticable. To overcame, at least in part, to this problem sparse grid can be used. For details concerning the sparse grid approximation see [18], [15], [24].

Note that, once the Stochastic Collocation approximation is computed, the evaluation of the moments of u can be simply obtained by applying the quadrature roles to the equation (1.36). In particular the mean function and the total variance can be computed respectively as:

- $\mathbb{E}[u_{N_y}(\mathbf{x}, t; \cdot)] \cong \sum_{k=1}^{N_y} u_k(\mathbf{x}, t; \xi_k) w_k$

- $\mathbb{V}ar[u_{N_y}(\mathbf{x}, t; \cdot)] \cong \sum_{k=1}^{N_y} u_k^2(\mathbf{x}, t; \xi_k) w_k - \mathbb{E}[u_{N_y}(\mathbf{x}, t; \cdot)]^2$

where $w_1, ... w_{N_y}$ are the weights associated to each point of the stochastic grid, i.e.:

$$w_k = \int_{\mathbf{\Gamma}} \mathcal{L}_k(\vec{\xi}(\omega)) f(\vec{\xi}(\omega)) d\vec{\xi}(\omega) \qquad \forall k = 1, ... N_y \qquad (1.37)$$

1.4 Conclusion

To conclude this brief overview we stress that for time dependent problems the POD method, as well as the gPC and the SC are not always able to well describe the solution while the time evolves. This is due to the use of a fixed approximation bases in the random or in the physical space that could require more and more approximation terms or can lead to unacceptable error levels.

Moreover from the computational point of view the gPC method requires to solve a set of deterministic equations that are often coupled and eventually needs *ad hoc* efficient and robust solvers. On the other hand the SC is a non intrusive method and leads to solve uncoupled deterministic problems with the possibility to use pre-existing codes in a "black box" way. Unfortunately the number of collocation points grows exponentially with the dimension of the stochastic space if full tensor grids are used and the method can result in a large number of equations to solve.

In the next chapters we describe an alternative method based on the Dynamical Orthogonal field approach. We will see how it answers to these problems and limitations and what are its advantages and limitations.

Chapter 2

Dynamically Orthogonal Field method

2.1   Dynamically Orthogonal Field approach

In this chapter we illustrate the Dynamically Orthogonal Filed approach that provides an alternative method to effectively describe the solution $u(\mathbf{x}, t; \omega)$ of time dependent stochastic PDE, at any time instant. The DO field methodology was introduced in [16], [19], [17] to deal with ocean flow with random initial data and it was presented as a generalization of the approaches that we have described in the previous chapter, in particular the POD and the gPC ones. Specifically the DO approach aims to evolve a low rank approximation by providing few terms that globally describe the solution u. Contrary to what assumed for the gPC or POD method, the stochastic filed $u(\mathbf{x}, t; \omega)$ is expanded in time dependent terms on both the physical and the stochastic space. Fixing the expansion to N terms, the approximate solution u_N looks as:

$$u_N(\mathbf{x}, t; \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N} y_i(t; \omega) u_i(\mathbf{x}, t) \tag{2.1}$$

where:

- $\bar{u}(\mathbf{x}, t) \cong \mathbb{E}[u(\mathbf{x}, t; \omega)]$,

- $\{u_i(\mathbf{x}, t)\}_{i \in \mathbb{N}}$ is a deterministic orthonormal basis in $\mathrm{L}^2(\mathrm{D})$,

- $\{y_i(t; \omega)\}_{i \in \mathbb{N}}$ is a set of zero mean stochastic processes in $\mathrm{L}^2_P(\Omega)$.

It easy to verify that such decomposition is not unique. Given any orthonormal matrix $v(t) \in \mathbb{R}^{N \times N}$, we can define new deterministic basis function and stochastic coefficients as

- $w_j(\mathbf{x}, t) = \sum_{i=1}^{N} u_i(\mathbf{x}, t) v_{ij}(t)$

- $z_j(t; \omega) = \sum_{i=1}^{N} y_i(t; \omega) v_{ji}(t)$

by obtaining an equivalent representation of u_N where the new deterministic basis functions are still orthonormal in $L^2(D)$. The redundancy of the representation is overcome by imposing the so called *Dynamically Orthogonal condition*:

$$< \frac{\partial u_i(\cdot, t)}{\partial t}, u_j(\cdot, t) > = 0 \qquad \forall i, j = 1, ...N \ \forall t \in [0, \text{T}] \qquad (2.2)$$

In particular the Dynamically Orthonormal condition preserves the orthonormality of the bases:

$$\frac{\partial}{\partial t} < u_i(\cdot, t), u_j(\cdot, t) > = < \frac{\partial u_i(\cdot, t)}{\partial t}, u_j(\cdot, t) > + < \frac{\partial u_j(\cdot, t)}{\partial t}, u_i(\cdot, t) > = 0 \qquad (2.3)$$

$\forall i, j = 1, ...N \ \forall t \in \text{T}$.
Roughly speaking, if we denote by $\mathcal{W}_N(t)$ the subspace spanned by the deterministic basis $\{u_1(\mathbf{x}, t), ..., u_N(\mathbf{x}, t)\}$, the DO condition is a restriction imposed on the subspace where the solution is approximated:

$$\frac{d\mathcal{W}_N(t)}{dt} \perp \mathcal{W}_N(t) \iff < \frac{\partial u_i(\cdot, t)}{\partial t}, u_j(\cdot, t) > = 0 \qquad \forall i, j = 1, ..., N \ \forall t \in [0, \text{T}]$$
$$(2.4)$$

It forces the evolution of the modes to be normal to $\mathcal{W}_N(t)$ since the dynamics of the stochasticity within $\mathcal{W}_N(t)$ can be already described by the random coefficients $y_1, ..., y_N$. In practice, to build an approximate solution of the form (2.1) we can use a Galerkin method where the residual of the equation is projected onto the subspace $\mathcal{W}_N$.
The approach concerns dynamical systems governed by a stochastic *PDE* as

$$\begin{cases} \dfrac{\partial u(\mathbf{x}, t, \omega)}{\partial t} = \mathcal{L}(u(\mathbf{x}, t, \omega); \omega) & \mathbf{x} \in \text{D}, \ t \in [0, \text{T}], \ \omega \in \Omega \\ u(\mathbf{x}, 0, \omega) = u_0(\mathbf{x}, \omega) & \mathbf{x} \in \text{D}, \ \omega \in \Omega \\ u(\sigma, t; \omega) = h(\sigma, t; \omega) & \sigma \in \partial\text{D}, \ t \in [0, \text{T}], \ \omega \in \Omega \end{cases} \qquad (2.5)$$

where $\mathcal{L}$ is a general differential operator and the randomness can arise from the initial or boundary conditions as well as from the parameters appearing in the differential operator. By assuming that the approximate solution expanded as in (2.1) satisfies the DO condition (2.2), a Galerkin projection provides a system of evolution equations for all the components of the expansion (2.1). In view of that, from the original SPDE one derives a set of $N + 1$ deterministic PDEs coupled to N stochastic ordinary differential equations. The first set of equations describes the evolution of the mean and of the deterministic basis functions while the other set governs the dynamic of the stochastic coefficients. Therefore the DO approach automatically evolves a low rank approximation with a number of terms fixed in time, all of them uniquely determined at any time instant and evolving according to the structure of the solution. This makes the approximate solution in (2.1) affective also for long time intervals, as long as the low rank approach is suitable for the problem analyzed.

2.2   Dynamically Orthogonal Field equations

Given a time dependent problem governed by a stochastic *PDE* as in (2.5), we derive now the evolution equations for all the terms in the expansion (2.1). Recall that the deterministic basis $\{u_i(\mathbf{x},t)\}_{i=1}^N$ has to satisfy the *Dynamically Orthogonal condition* at each time $t \in [0,\ T]$.

DO Equations.
Under the assumption of the DO *representation (2.1), (2.2) by performing a Galerkin projection of the equations (2.5) one obtains:*

$$
\begin{cases}
\dfrac{\partial \bar{u}(\mathbf{x},\ t)}{\partial t} \;=\; \mathbb{E}[\mathcal{L}(u(\cdot,t;\ \omega);\ \omega)] \\[2.5ex]
\sum_{i=1}^N \dfrac{\partial u_i(\mathbf{x},\ t)}{\partial t} C_{y_i,y_j}(t) \;=\; \prod_{\mathcal{W}_N(t)^\perp} \mathbb{E}[\mathcal{L}(u(\cdot,t;\ \omega);\ \omega)y_j(t;\ \omega)] \qquad \forall j=1,...N \quad (2.6) \\[2.5ex]
\dfrac{\partial y_i(t;\ \omega)}{\partial t} \;=\; <\mathcal{L}(u(\cdot,t;\ \omega);\ \omega) - \mathbb{E}[\mathcal{L}(u(\cdot,t;\ \omega);\ \omega)],\ u_i(\cdot,t)> \qquad \forall i=1,...N
\end{cases}
$$

where $\mathcal{W}_N(t) = span < u_1(\mathbf{x},t),...,u_N(\mathbf{x},t) >$ *and* $\prod_{\mathcal{W}_N(t)^\perp}$ *is the projection operator onto* $\mathcal{W}_N(t)^\perp$ *defined as:* $\prod_{\mathcal{W}_N(t)^\perp}\big[\mathcal{F}(\mathbf{x})\big] = \mathcal{F}(x) - \sum_{k=1}^N < \mathcal{F}(\cdot),\ u_k(\cdot,t) > u_k(\mathbf{x},t)$. *The associated boundary conditions have the form:*

$$
\begin{aligned}
&\bar{u}(\sigma,t) \;=\; \mathbb{E}[g(\sigma,t;\ \omega)] \\[2ex]
&\sum_{i=1}^N u_i(\sigma,t)C_{y_i,y_j}(t) \;=\; \mathbb{E}[g(\sigma,t;\ \omega)y_j(t;\ \omega)] \qquad\qquad \forall j=1,...N
\end{aligned}
$$

$$(2.7)$$

and initial conditions are given by:

$$
\begin{aligned}
\bar{u}(\mathbf{x},t_0) &= \bar{u}_0(\mathbf{x}) = \mathbb{E}[u_0(\mathbf{x};\ \omega)] & \\
u_i(\mathbf{x},t_0) &= u_{i0}(\mathbf{x}) & \forall i=1,...N \qquad (2.8)\\
y_i(t_0,\omega) &= < u_0(\cdot;\ \omega) - \bar{u}_0(.),\ u_{i0}(\cdot) > & \forall i=1,...N
\end{aligned}
$$

where $\{u_{i0}(\mathbf{x})\}_{i=1,...N}$ *are the eigenfunctions of the covariance operator* $\Gamma_{u_0 u_0}$.

The DO equations can be derived by repleacing the DO expansion in the governig *SPDE* and performing a Galerkin projection in the tensor space $\mathcal{W}_N(t) \otimes \mathcal{V}_N(t)$ where $\mathcal{V}_N(t) = span < y_1(t,\omega),...,y_N(t,\omega)$. In what follows we describe it in details. First of all we substitute the expansion (2.1) in the *SPDE* (2.5) and we obtain:

$$
\frac{\partial \bar{u}(\mathbf{x},t)}{\partial t} + \sum_{i=1}^N \frac{\partial u_i(\mathbf{x},t)}{\partial t}y_i(t;\ \omega) + \sum_{i=1}^N \frac{\partial y_i(t;\ \omega)}{\partial t}u_i(\mathbf{x},t) \;=\; \mathcal{L}(u(\mathbf{x},t;\ \omega);\ \omega) \qquad (2.9)
$$

Since the random coefficients are zero mean stochastic processes, by integrating in Ω, i.e. applying the mean operator, we get the first equation in (2.6).

Considering again the equation (2.9) we calculate the spatial inner product with $u_j(\mathbf{x}, t)$:

$$
< \frac{\partial \bar{u}(\mathbf{x}, t)}{\partial t}, u_j(\mathbf{x}, t) > \quad + \sum_{i=1}^{N} < \frac{\partial u_i(\mathbf{x}, t)}{\partial t} y_i(t; \omega), u_j(\mathbf{x}, t) >
$$
$$
+ \sum_{i=1}^{N} < \frac{\partial y_i(t; \omega)}{\partial t} u_i(\mathbf{x}, t), u_j(\mathbf{x}, t) > = < \mathcal{L}(u(\mathbf{x}, t; \omega); \omega), u_j(\mathbf{x}, t) >
$$
$$(2.10)$$

Since $\{u_i(\mathbf{x}, t)\}_{i=1,\dots N}$ form an orthonormal bases of $\mathcal{W}_N(t) \subset L^2(\mathrm{D})$, i.e.
$< u_i(\mathbf{x}, t), u_j(\mathbf{x}, t) > = \delta_{ij}$, the third term on the left side vanishes for $i \neq j$.
Thanks to the *DO* condition the second term on the left side is always equal to zero.
Therefore we get:

$$
< \frac{\partial \bar{u}(\mathbf{x}, t)}{\partial t}, u_j(\mathbf{x}, t) > + \frac{\partial y_j(t; \omega)}{\partial t} = < \mathcal{L}(u(\mathbf{x}, t; \omega); \omega), u_j(\mathbf{x}, t) > \qquad (2.11)
$$

Observe that by using the first equation in (2.6) we can replace the first term on the left side with $\mathbb{E}[< \mathcal{L}(u(\cdot, t; \omega), u_j(\cdot, t) >]$ and get the third set of equations in (2.6).
Starting again from equation (2.9) this time we consider the inner product with the stochastic variables $\{y_i\}$. Then it holds:

$$
\mathbb{E}[\frac{\partial \bar{u}(\mathbf{x}, t)}{\partial t} y_j(t, \omega)] \quad + \sum_{i=1}^{N} \frac{\partial u_i(\mathbf{x}, t)}{\partial t} C_{y_i, y_j}(t)
$$
$$
+ \sum_{i=1}^{N} u_i(\mathbf{x}, t) C_{\partial_t y_i, y_j}(t) = \mathbb{E}[\mathcal{L}(u(\mathbf{x}, t; \omega); \omega), y_j(t; \omega)] \qquad (2.12)
$$

where $C_{y_i, y_j}(t) = \mathbb{E}[y_i(t; \omega) y_j(t; \omega)]$ and $C_{\partial_t y_i, y_j}(t) = \mathbb{E}[\frac{\partial y_i(t; \omega)}{\partial t} y_j(t; \omega)]$.
Note that, since the $\{y_i(t; \omega)\}_{i=1,\dots N}$ are zero mean stochastic processes the first term on the left side is equal to zero. Then we calculate the spatial inner product with $u_k(\mathbf{x}, t)$.
The second term in (2.12) vanishes because of the orthogonal condition, hence it remains:

$$
C_{\partial_t y_k, y_j}(t) = < \mathbb{E}[\mathcal{L}(u(\cdot, t; \omega); \omega) y_j(t; \omega)], u_k(\cdot, t) > \qquad (2.13)
$$

By using this result in (2.12) we obtain the second set of equations in (2.6).

2.3   Dynamically Double Orthogonal decomposition

According to the DO approach the approximate solution is expanded as in (2.1) where the deterministic basis functions are supposed be orthonormal in $\mathrm{L}^2(\mathrm{D})$ while the stochastic coefficients are possibly correlated. The Double Dynamically Orthogonal approach, DDO [11], adopts intead a slightly different decomposition according to which the stochastic coefficients are required do be orthonormal in $\mathrm{L}_P^2(\Omega)$. Specifically, given $u \in \mathcal{H}$ solution of (2.5), the DDO decomposition of the approximate solution reads:

$$
\tilde{u}_N(\mathbf{x}, t; \omega) = \tilde{\bar{u}}(\mathbf{x}, t) + \sum_{j, i=1}^{N} a_{ij}(t) \tilde{u}_i(\mathbf{x}, t) \tilde{y}_j(t; \omega) \qquad (2.14)
$$

where:

- $< \tilde{u}_i(\mathbf{x}, t),\ \tilde{u}_j(\mathbf{x}, t) >= \delta_{ij},$

- $< \dfrac{\partial \tilde{u}_i(\mathbf{x}, t)}{\partial t},\ \tilde{u}_j(\mathbf{x}, t) >= 0,$

- $\mathbb{E}[\tilde{y}_i(t, \omega)] = 0$

- $\mathbb{E}[\tilde{y}_i(t, \omega)\tilde{y}_j(t,\ \omega)] = \delta_{ij}$

- $\mathbb{E}[\dfrac{\partial \tilde{y}_i(t, \omega)}{\partial t}\tilde{y}_j(t,\ \omega)] = 0$

- $a(t) \in \mathbb{R}^{N \times N}$ invertible

for all $i,\ j = 1, ...N$, at any $t \in [0, \mathrm{T}]$.

The DDO decomposition has been proposed in finite dimensional setting by *Lubich et al.* in [11], [12] to develop dynamically low rank approximations of time dependent matrix equations. By following the same idea of the dynamical SVD decomposition, under the assumption that u_N is expanded as in (2.14), one can recover evolution equations for all the terms in the DDO decomposition. In particular, by applyng a Galerkin projection, the problem (2.5) is reformulated as:

$$\begin{cases} \dfrac{\partial \bar{u}(\mathbf{x},\ t)}{\partial t} = \mathbb{E}[\mathcal{L}(u(\cdot, t;\ \omega);\ \omega)] & \mathbf{x} \in \mathrm{D},\ t \in [0,\ \mathrm{T}],\ \omega \in \Omega \\[2mm] \dfrac{da_{ij}(t)}{dt} = \mathbb{E}\big[< \mathcal{L}(u(\cdot, t;\ \omega);\ \omega) - \mathbb{E}[\mathcal{L}(u(\cdot, t;\ \omega);\ \omega)], \tilde{u}_i(\mathbf{x},\ t) > \tilde{y}_j(t;\ \omega)\big] \\[1mm] \hspace{9cm} \forall i,\ j = 1, ...N \\[2mm] \sum_{k=1}^{N} \dfrac{\partial \tilde{u}_k(\mathbf{x},\ t)}{\partial t} a_{ki}(t) = \prod_{\mathcal{W}_N^{\perp}} \mathbb{E}\big[\big(\mathcal{L}(u(\cdot, t;\ \omega);\ \omega) - \mathbb{E}[\mathcal{L}(u(\cdot, t;\ \omega);\ \omega)]\big)\tilde{y}_i(t;\ \omega)\big] \\[1mm] \hspace{9cm} \forall i = 1, ...N \\[2mm] \sum_{k=1}^{N} a_{ik}(t)\dfrac{\partial \tilde{y}_k(t;\ \omega)}{\partial t} = \prod_{\mathcal{V}_N^{\perp}} \big[< \mathcal{L}(u(\cdot, t;\ \omega);\ \omega) - \mathbb{E}[\mathcal{L}(u(\cdot, t;\ \omega);\ \omega)], \tilde{u}_i(\cdot, t) > \big] \\[1mm] \hspace{9cm} \forall i = 1, ...N \end{cases}$$

$$(2.15)$$

plus the relative boundary and initial conditions there $\mathcal{V}_N(t) = span < \tilde{y}_1(t, \omega), .., \tilde{y}_N(t, \omega) >$ and $\mathcal{W}_N(t) = span < \tilde{u}_1(\mathbf{x}, t), .., \tilde{y}_N(\mathbf{x}, t) >$.

By solving the system we recover all the terms of the expansion at any time instant and we construct by this way a rank N approximate solution.

Even if the DDO decomposition does not correspond to the DO expansion in (2.1), the two approaches have strong relation. Specifically by adopting the Galerkin method, they provide the same numerical solution,

Proposition 2.3.1. *Through a Galerkin projection, the* DO *approach coincides with the* DDO *one, therefore the two methods provide the same numerical solution.*

Proof. Given the DDO solution $\tilde{u}_N(\mathbf{x}, t;\ \omega) = \tilde{\bar{u}}(\mathbf{x}, t) + \sum_{i=1}^{N} a_{ij}(t)\tilde{u}_i(\mathbf{x}, t)\tilde{y}_j(t;\ \omega)$ we define $y_i(t;\ \omega) = \sum_{i=1}^{N} a_{ij}(t)\tilde{y}_j(t;\ \omega)$.

We want to verify that $\tilde{u}_N(\mathbf{x}, t; \omega) = \tilde{\bar{u}}(\mathbf{x}, t) + \sum_{i=1}^{N} \tilde{u}_i(\mathbf{x}, t) y_i(t; \omega)$ corresponds to the DO solution u_N. First of all $\tilde{u}_N$ satisfies the DO condition. Then it is sufficient to show that $\tilde{u}_N$ is solution of the DO system.

Observe that the equation for the mean function in (2.6) coincides with the one in (2.15). For convenience we denote $\mathcal{L}^*(u(\cdot, t; \omega); \omega) = \mathcal{L}(u(\cdot, t; \omega); \omega) - \mathbb{E}[\mathcal{L}(u(\cdot, t; \omega); \omega)]$. Moreover we remind that for any stochastic function $f \in \mathrm{L}_P^2(\Omega)$ it holds:

$$\prod_{\mathcal{V}_N^\perp} \left[f(\omega) \right] = f(\omega) - \sum_{i=1}^{N} \mathbb{E}[f(\omega)y_i(\omega)]y_i(\omega) \tag{2.16}$$

By substitution we obtain:

$$
\begin{aligned}
\frac{\partial y_i(t; \omega)}{\partial t} \quad &= \sum_{j=1}^{N} \frac{da_{ij}(t)}{dt} \tilde{y}_j(t; \omega) + \sum_{j=1}^{N} a_{ij}(t) \frac{\partial \tilde{y}_j(t; \omega)}{\partial t} \\[2mm]
&= \sum_{j=1}^{N} \mathbb{E}\big[< \mathcal{L}^*(u(\cdot, t; \omega); \omega), \tilde{u}_i(\mathbf{x}, t) > \tilde{y}_j(t; \omega)\big] \tilde{y}_j(t; \omega) \\
&\qquad\qquad + \prod_{\mathcal{V}_N^\perp} \big[< \mathcal{L}^*(u(\cdot, t; \omega); \omega), \tilde{u}_i(\cdot, t) > \big] \\[2mm]
&= \sum_{j=1}^{N} \mathbb{E}\big[< \mathcal{L}^*(u(\cdot, t; \omega); \omega), \tilde{u}_i(\mathbf{x}, t) > \tilde{y}_j(t; \omega)\big] \tilde{y}_j(t; \omega) \\
&\quad + < \mathcal{L}^*(u(\cdot, t; \omega); \omega), \tilde{u}_i(\cdot, t) > - \sum_{k=1}^{N} \mathbb{E}[< \mathcal{L}^*(u(\cdot, t; \omega); \omega), \tilde{u}_i(\cdot, t) > \tilde{y}_k(t; \omega)]\tilde{y}_k(t; \omega) \\[2mm]
&= < \mathcal{L}^*(u(\cdot, t; \omega); \omega), \tilde{u}_i(\cdot, t) >
\end{aligned}
$$

$$\tag{2.17}$$

The equations for the stochastic coefficients correspond to the equations in (2.6). Furthermore by defining the covariance matrix as $C_{ij}(t) = \sum_{k=1}^{N} a_{ik}(t)a_{kj}(t)$ the system of equations for the deterministic fields $\{u_i\}_{i=1,\dots N}$ is recovered. In conclusion the DDO solution satisfies the DO system. Analogously one can easy verify that the DO solution satisfies the DDO system in (2.15), say $a(t) = C_{y_i y_j}^{1/2}(t)$. We conclude that the DDO and DO approach arrive at the same numerical solution. $\qquad\square$

2.4   An equivalent Variational Formulation

Let $\mathcal{M}_N$ be the manifold of all the functions that admit a rank N representation as in (2.1), i.e.:

$$
\mathcal{M}_N = \big\{ v(\mathbf{x}, t; \omega) \in \mathrm{L}^\infty([0, \mathrm{T}], \mathcal{H})] : \quad v(\mathbf{x}, t; \omega) = \bar{v}(\mathbf{x}, t) + \sum_{i=1}^{N} z_i(t; \omega)v_i(\mathbf{x}, t),
$$
$$
< v_i(\mathbf{x}, t), v_j(\mathbf{x}, t) >= \delta_{ij}, \mathbb{E}[z_i(\omega, t)] = 0 \big\} \tag{2.18}
$$

and let $\mathcal{T}_u \mathcal{M}_N(t)$ be the tangent space to $\mathcal{M}_N$ at $u_N(t)$. Then the DO approach corresponds to a Galerkin formulation according to which the residual of the equation (2.5) is projected onto the tangent space $\mathcal{T}_u \mathcal{M}_N$ at each time instant. Specifically the formulation reads:

. At each $t \in [0, \text{T}]$, find the approximate solution $u_N(\cdot, t, \cdot) \in \mathcal{M}_N$ with $\dfrac{\partial u_N(\cdot, t, \cdot)}{\partial t} \in \mathcal{T}_u \mathcal{M}_N(t)$ such that:

$$\mathbb{E}\big[< \frac{\partial u_N(\cdot, t, \omega)}{\partial t} - \mathcal{L}(u_N(\cdot, t, \omega); \omega), v(\cdot, \omega) > \big] = 0 \qquad \forall v \in \mathcal{T}_u \mathcal{M}_N(t) \quad (2.19)$$

This projection is equivalent to require that the components in the expansion (2.1) are the solution of the DO system in (2.6). Then DO approximate solution minimize the residual of (2.5) at any time inant. However this does not coincide necessarily with the best rank N approximation v_N, that instead satisfies:

- $v_N \in \mathcal{M}_N$,

- $\mathbb{E}\big[\|u(\cdot, t; \omega) - v_N(\cdot, t; \omega)\|_{\text{L}^2(\text{D})}\big]$ is minimized

at any $t \in [0, \text{T}]$. Observe that here the solution u is projected on the manifold $\mathcal{M}_N$, instead of the residual in the tangent manifold $\mathcal{T}_u \mathcal{M}_N$. Moreover it is equivalent to minimizing the error with respect to the total variance. Consequently the truncated KL expansion corresponds to the best rank N approximation in an L^2 sense.
On the other hand the DO approach takes inspiration from the KL expansion. It evolves the low rank solution and adapts at each time instant the spatial basis as well the stochastic variables to what best describes the structure of the solution without computing the KL decomposition at each time step. This makes the method numerically accessible and effective in terms of approximation error at any time instant for long time integration.

2.5 Approximation Proprieties

The DO method provides an approximate solution that is not necessary equal to the truncated Karhunen-Loève expansion but aims to be close to it. In order to investigate the relation between the error of the DO solution and the error of the best N rank approximation, we exploit the equivalence between the DO the DDO formulations and recall the convergence estimates provided by *Lubich et al* in [12], [11] for finite dimensional problems. In particular we report here one of the main results provided by the authors that suggest the possibility to bound the error of the DO method in terms of best approximation error under proper conditions.
By transferring the problem in finite dimensional setting, The DDO formulation is applied to an evolution matrix equations i.e. $\dot{A} = \mathcal{L}(A)$ with $A \in \mathbb{R}^{n \times m}$. The error analysis is provided by comparing the solution $Y(t)$, achieved by the dynamical low rank method, with the best N rank approximation, in the Frobenius norm. In particular if the problem $\dot{A} = \mathcal{L}(A)$ has a continuously differentiable N-rank best approximation $X(t)$ then the error for the dynamical low rank method can be bounded in terms of the best approximation error. This shows that the dynamical low rank method provides a locally quasi-optimal low rank approximation, under proper conditions.

Theorem 2.5.1. *[12] Suppose that a continuously differentiable best approaximation $X(t) \in \mathcal{M}_N$ to $A(t)$ exists for $t \in [0, \text{T}]$. Let the $N - th$ singular value of $X(t)$ has the lower bound $\sigma_N(X(t)) \geq \rho > 0$, and assume that the best-approximation error of the DDO method is bounded by $\|X(t) - A(t)\| \leq \dfrac{1}{16}\rho$ for $t \in [0, \text{T}]$. Then the approximation error with initial value $\tilde{U}(0) = X(0)$ is bounded in Frobenius norm by:*

$$\|\tilde{U}(t) - X(t)\| \leq 2\beta e^{\beta t} \int_0^t \|X(s) - A(s)\| \, ds \qquad with \beta = 8\mu\rho^{-1} \qquad (2.20)$$

for $t \in [0, \text{T}]$ and as long as the right-hand side is bounded by $\frac{1}{8}\rho$.

The method have been generalized in [10] for higher order tensors, approximated in low rank Tucker or hierarchical Tucker format.

2.6   Over-approximation and Ill-conditioned problems

We define a N rank function any stochastic field $u_N \in \mathcal{M}_N$ where N is the dimension of the manifold. Moreover we say that $u_N \in \mathcal{M}_N$ has effective rank equal to N if the covariance matrix associated to the stochastic coefficients in the decomposition (2.1) has rank equal to N. Specifically the effective rank of u_N corresponds to the rank of the covariance matrix or equivalently to the rank of the matrix $S_{ij} = a_{ij}$ in (2.14) in the DDO approach. Since the covariance matrix evolves, it follows that also the effective rank might change in time. The theoretical results illustrated in the previous section as well as the system of equations (2.6) or equivalently (2.15) concern the case in which the rank of the approximate solution is equal to N and the rank of the exact solution is larger or equal to N. We analyze now what happens when the solution is over-approximated, i.e. the exact solution has effective rank smaller than N although it is approximated by N rank functions.

Consider the DO system; the equations for the modes are coupled by the covariance matrix. When the rank of the approximate solution u_N is N, the problem is well posed, the covariance matrix can be inverted and the solution is obtained generally. Otherwise the system is overdetermined and we say that the solution is over-approximated. Under generally, we refer to ill-conditioned problems when the covariance matrix has zero eigenvalues or when the ratio between the largest and the smallest singular value is large. An obvious example of over-approximation arises when we handle stochastic dynamical systems with deterministic initial condition. In this case we aim to evolve a N rank solution even if the initial datum, which does not have any stochastic features, has effective rank zero. On the other hand that case highlights the necessity of dealing with this type of situations.

For finite dimensional problems, in [12] it is proved that, under specific assumption on the singular values of S and proper conditions of regularity for the best N-rank solution, the error of the dynamically low rank approximation is bounded also in the case

of ill-conditioning. In particular the authors proved that when there is a gap in the distribution of the singular values of S, the low rank approximation is not subjected to instability. Specifically, it concerns that case in which the singular values can be divided in two ranges $\vec{\lambda}^1 = (\lambda_1, ..., \lambda_s)$ and $\vec{\lambda}^2 = (\lambda_{s+1}, ..., \lambda_n)$ with $\min(\vec{\lambda}^1) >> \max(\vec{\lambda}^2)$ and the N-rank approximate solution is expanded as

$$Z_n = U \begin{pmatrix} S_1 & 0 \\ 0 & S_2 \end{pmatrix} V^\top = U^1 S^1 V^{1\top} + U^2 S^2 V^{2\top}$$

where, according to the DDO formulation $U \in \mathbb{R}^{q \times N}$, $V \in \mathbb{R}^{p \times N}$, $U = (U^1, U^2)$, $V = (V^1, V^2)$, have orthonormal columns and $\vec{\lambda}^i = \rho(A^i)$ with $i = 1, 2$. The theoretical results show that the set of the smallest singular values $\vec{\lambda}^2$ does not give any remarkable contribution no matter what the derivatives of V^2, U^2 are, and the N-rank solution corresponds to the s-rank one, up to small perturbations, as the matrix S^2 remains small. In line with this observation we adopt an analogous approach to deal with over-approximated problems in the DO framework. First of all we observe that any function $u_N \in \mathcal{M}_N$ can be written as:

$$u_N(\mathbf{x}, t; \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N} z_i(t; \omega) w_i(\mathbf{x}, t) \tag{2.21}$$

where, given $v_1(t), ..., v_N(t)$ eigenvectors of the covariance matrix $C_{yy}(t)$, we have:

- $w_j(\mathbf{x}, t) = \sum_{i=1}^{N} u_i(\mathbf{x}, t) v_{ji}(t)$

- $z_j(t; \omega) = \sum_{i=1}^{N} y_i(t; \omega) v_{ij}(t)$

Note that the stochastic coefficients z_i are orthogonal in $L_P^2(\Omega)$ and the transformation preserves the orthonormality of the deterministic fields.

Proposition 2.6.1. *Let $u_N(\mathbf{x}, t; \omega) \in \mathcal{M}_N$ expanded as in (2.21). Moreover assume that:*

$$u_N(\mathbf{x}, t; \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N_1(t)} z_i(t; \omega) w_i(\mathbf{x}, t) + \sum_{i=N_1(t)+1}^{N} z_i^*(t; \omega) w_i(\mathbf{x}, t) \tag{2.22}$$

where $\mathbb{E}[z_k^*(t,\,\omega)z_k^*(t,\,\omega)] = 0$ *for all* $k = N_1(t)+1,\,...,N$ *then the system in (2.6) becomes:*

$$
\begin{cases}
\dfrac{\partial \bar{u}(\mathbf{x},\,t)}{\partial t} \;=\; \mathbb{E}[\mathcal{L}(u(\cdot,t;\,\omega);\,\omega)] \\[2ex]
\dfrac{\partial w_i(\mathbf{x},\,t)}{\partial t}\lambda_i(t) \;=\; \prod_{\mathcal{W}_N(t)^\perp}\mathbb{E}[\mathcal{L}(u(\cdot,t;\,\omega);\,\omega)z_i(t;\,\omega)] & \forall i = 1,\,...,\,N_1(t) \\[2ex]
\prod_{\mathcal{W}_N(t)^\perp}\mathbb{E}[\mathcal{L}(u(\cdot,t;\,\omega);\,\omega)z_i(t;\,\omega)] \;=\; 0 & \forall i = N_1(t)+1,\,...,\,N \\[2ex]
\dfrac{\partial z_i(t;\,\omega)}{\partial t} \;=\; <\mathcal{L}(u(\cdot,t;\,\omega);\,\omega) \,-\, \mathbb{E}[\mathcal{L}(u(\cdot,t;\,\omega);\,\omega)],\,w_i(\cdot,t)> & \forall i = 1,\,...,\,N_1(t) \\[2ex]
\dfrac{\partial z_i^*(t;\,\omega)}{\partial t} \;=\; <\mathcal{L}(u(\cdot,t;\,\omega);\,\omega) \,-\, \mathbb{E}[\mathcal{L}(u(\cdot,t;\,\omega);\,\omega)],\,w_i(\cdot,t)> & \forall i = N_1(t)+1,\,...,\,N
\end{cases}
$$

(2.23)

where $\lambda_i(t) = \mathbb{E}[z_i(t,\,\omega)z_i(t,\,\omega)]$

In practice we assume that, given a bi-orthogonal representation as in (2.21), the basis functions associated to zero singular values do not evolve as the singular values remain equal to zero. The advantage of this approach consists in considering in the expansion (2.1) also the latent variables, i.e. the zero variance stochastic variables, in a way that, even if at time $\bar{t}$ they do not give any contribution, they are however allowed to evolve at $t > \bar{t}$. This means that the DO approach develops an approximate solution $u_N \in \mathcal{M}_N$ with effective rank that is bounded by N but which evolves according to the effective rank of the exact solution.

2.6.1   An illustrative example

Let us introduce an example to clarify the concept. Consider the following stochastic problem with initial deterministic condition:

$$
\begin{cases}
\dfrac{\partial u(x,t;\,\omega)}{\partial t} \,-\, \delta(\omega)\Delta u(x,t;\,\omega) \;=\; 0 & x \in (0,\,\mathrm{L}),\, t \in [0,\,\mathrm{T}],\, \omega \in \Omega \\[2ex]
u(0,t;\,\omega) \;=\; 0 & t \in [0,\,\mathrm{T}],\, \omega \in \Omega \\[1ex]
u(\mathrm{L},t;\,\omega) \;=\; 0 & t \in [0,\,\mathrm{T}],\, \omega \in \Omega \\[1ex]
u(x,0;\,\omega) \;=\; \sum_{i=1}^{N}\sin\left(\dfrac{2i\pi x}{\mathrm{L}}\right) & x \in [0,\,\mathrm{L}],\, \omega \in \Omega
\end{cases}
$$

(2.24)

The initial condition is a deterministic finite linear combination of the first N eigenfunctions of the Laplace operator. This implies that the solution evolves in the stochastic subspace spanned by the N eigenfunctions and develops a manifold of dimension N. The solution u, that at $t = 0$ doesn't have any random feature but is affected by the stochasticity of the system as soon as it evolves and its rank increases in time. On the other hand, the system is dissipative and the solution tends asymptotically to the deterministic zero solution. Therefore, the rank will tend asymptotically to zero as $t \to \infty$. To limit

the truncation error at later time, N modes are needed in the representation (2.1) since the beginning although all the coefficients have to be initialized to zero. Hence the initial covariance matrix is singular and with zero rank. Furthermore we deal with nearly singular matrices also when the random coefficients go back to zero as $t \to \infty$. The need of using a larger number of modes with respect to what the initial datum requires is emphasized if the differential operator has strong reaction terms. However, even if the initial datum involves a full rank covariance matrix, nevertheless this may becomes singular or nearly singular as time evolves, namely when one or more random coefficients become zero or they have very small variance compared to the others. The proposition (2.6.1) concerns these situations.

Chapter 3

Stochastic Linear Parabolic Equation

In this chapter we analyze problems governed by linear parabolic diffusion equations in order to see how the DO approach works. In this framework we investigate the relation between the eigenvalue problem associated to the Laplace operator and the correlation operator, by following what discussed in [34]. In particular we illustrate a spacial case in which the DO approach degenerates to the POD method using as deterministic basis functions the eigenfunctions of the Laplace operator. After discussing the implementation aspects, some simple numerical examples will be introduced to verify the consistency of the method with the analytic solutions.

3.1   Problem Setting

Consider the following stochastic linear parabolic problem:

$$
\begin{cases}
\dfrac{\partial u(\mathbf{x}, t, \omega)}{\partial t} - \nabla \cdot (a(\mathbf{x}, \omega) \nabla u(\mathbf{x}, t, \omega)) = f(\mathbf{x}, t, \omega) & \mathbf{x} \in \mathrm{D},\, t \in [0, \mathrm{T}],\, \omega \in \Omega \\
u(\sigma, t, \omega) = 0 & \sigma \in \partial \mathrm{D},\, t \in [0, \mathrm{T}],\, \omega \in \Omega \\
u(\mathbf{x}, 0, \omega) = u_0(\mathbf{x}, \omega))& \mathbf{x} \in \mathrm{D},\, \omega \in \Omega
\end{cases}
$$

$$(3.1)$$

where ∇ denotes the differential operator in the physical space. The diffusion coefficient $a : \mathrm{D} \times \Omega \to \mathbb{R}$ and the forcing term $f : \mathrm{D} \times [0,\, \mathrm{T}] \times \Omega \to \mathbb{R}$ are random functions with continuous and bounded covariance function. In order to guarantee the existence of the solution, we assume that $a(\cdot, \omega)$ is strictly positive and bounded over D for each random event $\omega \in \Omega$ i.e.:

$$
\exists a_{max}, a_{min} \in \mathbb{R}^+ : \mathrm{P}\big(\omega \in \Omega : a(\mathbf{x}, \omega) \in [a_{min}, a_{max}],\, \forall \mathbf{x} \in \overline{\mathrm{D}}\big) = 1, \qquad (3.2)
$$

which implies that a is uniformly coercive. Moreover let f be a square integrable random function for any $t \in [0, \mathrm{T}]$, i.e.: $f \in \mathrm{L}^\infty([0, \mathrm{T}], \mathcal{H})$. In [3] it has been shown, by means of energy estimates, that the weak formulation of (3.1) admits a unique solution in the

tensor space $u \in \mathrm{L}^{\infty}([0, \mathrm{T}], \mathrm{H}_0^1(\mathrm{D})) \otimes \mathrm{L}_P^2(\Omega)$.

In accordance with the DO approach we seek the approximation of u in the manifold $\mathcal{M}_N$ that minimizes the residual of (3.1) in the tangent space $\mathcal{T}_u \mathcal{M}_N$ at any time instant. This results in looking for a N rank function $u_N \in \mathrm{L}^{\infty}([0, \mathrm{T}]; \mathrm{H}_0^1(\mathrm{D})) \otimes \mathrm{L}_P^2(\Omega)$ expanded as in (2.1) in which all the terms satisfy the DO system (2.6). Specifically we assume that the approximate solution is expressed in terms of $y_1, ..., y_N \in \mathrm{L}^{\infty}([0, \mathrm{T}], \mathrm{L}_P^2(\Omega))$ and $\bar{u}, u_1, ...u_N \in \mathrm{L}^{\infty}([0, \mathrm{T}], \mathrm{H}_0^1(\mathrm{D}))$ which satisfy the DO formulation of the problem (3.1) in a weak sense.

We distinguish two types of problems: one in which all the stochasticity arises form the initial condition, being the diffusion coefficient and the forcing term deterministic, and the other in which the diffusion coefficient and/or the forcing term are random.

3.2 Diffusion equation with stochastic initial condition

In this section we consider problem (3.1) where we assume that all the stochasticity is generated by the initial datum, being the diffusion coefficient and the forcing term deterministic. For simplicity we also assume that the diffusion coefficient is constant in time. In this case the DO system yields:

$$
\begin{cases}
\dfrac{\partial \bar{u}(\mathbf{x}, t)}{\partial t} - a \Delta \bar{u}(\mathbf{x}, t) = f(\mathbf{x}, t) & \mathbf{x} \in \mathrm{D}, \, t \in [0, \mathrm{T}], \, \omega \in \Omega \\[2mm]
\sum_{i=1}^{N} \dfrac{\partial u_i(\mathbf{x}, t)}{\partial t} C_{y_i y_j}(t) = \prod_{\mathcal{W}_N(t)^{\perp}} \mathbb{E}[a \Delta u(\cdot, t, \cdot) y_j(t, \cdot)] & \forall j = 1, ...N \\[2mm]
\dfrac{\partial y_i(t; \omega)}{\partial t} = < a \Delta u(\cdot, t), \, u_i(\cdot, t) > & \forall i = 1, ...N
\end{cases}
\tag{3.3}
$$

with initial conditions given by:

$$
\begin{aligned}
\bar{u}(\mathbf{x}, 0) &= \mathbb{E}[u_0(\mathbf{x}, \omega)] & \\
u_i(\mathbf{x}, 0) &= u_{i0}(\mathbf{x}) & \forall i = 1, ..., N \\
y_i(0, \omega) &= < u_0(\cdot, \omega) - \bar{u}_0, \, u_{i0} > & \forall i = 1, ..., N
\end{aligned}
\tag{3.4}
$$

where $\{u_{i0}(\mathbf{x})\}_{i=1,...N}$ are the eigenfunctions of the correlation operator $\Gamma_{u(0)u(0)}$. The boundary conditions are given by:

$$
\begin{aligned}
\bar{u}(\sigma, t) &= 0 & \sigma \in \partial \mathrm{D} \\
u_i(\sigma, t) &= 0 & \forall i = 1, ..., N
\end{aligned}
\tag{3.5}
$$

By definition the projection operator $\prod_{\mathcal{W}_N(t)^{\perp}} \mathbb{E}[\Delta u(\cdot, t, \cdot) y_j(t, \cdot)]$ leads to:

$$
\sum_{k=1}^{N} \Delta u_k(\mathbf{x}, t) C_{y_k y_j}(t) - \sum_{r=1}^{N} \sum_{k=1}^{N} < \Delta u_k(\cdot, t), \, u_r(\cdot, t) > u_r(\mathbf{x}, t) C_{y_k y_j}(t)
\tag{3.6}
$$

where we use that $\{y_i\}_{i=1}^N$ are zero mean stochastic processes.

We are going analyze the relation between the eigenvalue problem associated to the Laplace operator and the correlation operator. W assume the diffusive coefficient equal to one and zero external force. This does not lead to any loss of generality because deterministic forcing terms influence only the mean function whose equation is decoupled from the others.

The operator $-\Delta$ is positive, self-adjoint and its inverse is compact in the Hilbert space $L^2(D)$. The spectral theory of compact operators [5] allow us to say that there exists a monotonically increasing sequence of strictly positive eigenvalues $\{\lambda_i\}_{i \in \mathbb{N}}$ and the corresponding sequence of eigenvectors $\{\phi_i\}_{i \in \mathbb{N}}$ from an orthonormal basis in $L^2(D)$. Precisely:

$$
\begin{aligned}
-\Delta\phi_i &= \lambda_i\phi_i \\
< \phi_i,\, \phi_j > &= \delta_{ij} \qquad\qquad \forall i,\, j \in \mathbb{N}
\end{aligned}
\tag{3.7}
$$

and any $v \in L^2(D)$ can be expressed as:

$$
v(\mathbf{x}) = \sum_{i=1}^\infty < v,\, \phi_i > \phi_i(\mathbf{x})
\tag{3.8}
$$

Consider now the problem (3.3). We assume that the approximate solution u_N is expanded as in (2.1) where $u_1(\cdot,t),...,u_N(\cdot,t)$ are deterministic functions, orthonormal in $L^2(D)$ at any $t \in [0, T]$. Since the eigenfunctions $\{\phi_i\}_{i \in \mathbb{N}}$ of the Laplace operator form a complete basis in $L^2(D)$ the deterministic modes can be written in terms of $\{\phi_i\}_{i \in \mathbb{N}}$, i.e.:

$$
u_i(\mathbf{x}, t) = \sum_{j=1}^\infty \tau_{j\,i}(t)\phi_j(x) \qquad\qquad \forall i = 1,...N
\tag{3.9}
$$

where $\tau_{j\,i}(t) =< u_i(\cdot,t),\, \phi_j >$. Moreover, assumed $u_i(\cdot,t) \in H_0^1$ for almost every $t \in [0, T]$, it holds:

$$
\Delta u_i(\mathbf{x}, t) = -\sum_{j=1}^\infty \lambda_j\tau_{j\,i}(t)\phi_j(x) \qquad\qquad \forall i = 1,...N
\tag{3.10}
$$

For convenience, we define the vectors of functions $\mathbf{U} = (u_1,...,u_N)^\top$, $\mathbf{Y} = (y_1,...,y_N)^\top$, $\mathbf{\Phi} = (\phi_1,...,\phi_\infty)^\top$ and the transformation matrix $\mathbf{\Upsilon}(t) \in \mathbb{R}^{N \times \infty}$ i.e. $\mathbf{\Upsilon}(t)_{ij} =< u_i(\cdot,t),\, \phi_j >$, so $\mathbf{U}(t) = \mathbf{\Upsilon}(t)\mathbf{\Phi}$. Furthermore let $\mathbf{\Lambda}$ be the diagonal matrix of the eigenvalues of the operator $-\Delta$ and $C(t) \in \mathbb{R}^{N \times N}$ the covariance matrice of $\mathbf{Y}$ at time t, i.e. $C(t)_{ij} = \mathbb{E}[y_i(\cdot,t)y_j(\cdot,t)]$.

The DO system can be re-written as:

$$
\begin{cases}
\dfrac{\partial \bar{u}(\mathbf{x}, t)}{\partial t} = \Delta\bar{u}(\mathbf{x}, t) & \mathbf{x} \in D,\, t \in [0, T],\, \omega \in \Omega \\[2ex]
C(t)\dfrac{\partial \mathbf{U}(\mathbf{x}, t)}{\partial t} = C(t)\big[\Delta\mathbf{U}(\mathbf{x}, t) - < \Delta\mathbf{U}(\cdot,t),\, \mathbf{U}^\top(\cdot,t) > \mathbf{U}(\mathbf{x}, t)\big] \\[2ex]
\dfrac{\partial \mathbf{Y}(t, \omega)}{\partial t} = < \Delta\mathbf{U}(\cdot,t),\, \mathbf{U}^\top(\cdot,t) > \mathbf{Y}(t, \omega)
\end{cases}
\tag{3.11}
$$

and by using (3.10) it yields:

$$\begin{cases} \dfrac{\partial \bar{u}(\mathbf{x},t)}{\partial t} = \Delta \bar{u}(\mathbf{x},t) & \mathbf{x} \in D,\ t \in [0,\mathrm{T}],\ \omega \in \Omega \\[3mm] \mathrm{C}(t)\dfrac{d\mathbf{\Upsilon}(t)}{dt} = \mathrm{C}(t)\big[\mathbf{\Upsilon}(t)\mathbf{\Lambda}\,\mathbf{\Upsilon}(t)^{\top}\mathbf{\Upsilon}(t) - \mathbf{\Upsilon}(t)\mathbf{\Lambda}\big] \\[3mm] \dfrac{\partial \mathbf{Y}(t,\omega)}{\partial t} = -\mathbf{\Upsilon}(t)\mathbf{\Lambda}\mathbf{\Upsilon}(t)^{\top}\mathbf{Y}(t,\omega) \end{cases} \qquad (3.12)$$

where specifically $< \Delta \mathbf{U}(\cdot,t),\ \mathbf{U}^{\top}(\cdot,t) >= -\mathbf{\Upsilon}(t)\mathbf{\Lambda} < \Phi,\ \Phi^{\top} > \mathbf{\Upsilon}(t)^{\top} = -\mathbf{\Upsilon}(t)\mathbf{\Lambda}\mathbf{\Upsilon}(t)^{\top}$ because the eigenvectors are orthonormal in $\mathrm{L}^2(\mathrm{D})$.

Special case: the DO approach degenerates to the POD method

We consider now a particular case in which the deterministic basis functions $(u_1, ..., u_N)$ are assumed to be linear combinations of N eigenfunctions of the Laplace operator and the transformation matrix $\mathbf{\Upsilon}(t)$ is then a square in $\mathbb{R}^{N \times N}$. We show that in this case the DO reduces to the PDO method.
Let the initial condition u_0 be in the manifold $\mathcal{M}_N$. We assume that the mean function is equal to zero, however the same conclusion can be achieved in the general case. According to the KL decomposition, it can be expanded in series as:

$$u_0(\mathbf{x},\omega) = \sum_{i=1}^{N} y_i(0,\omega) u_i(\mathbf{x},0) \qquad (3.13)$$

where $(u_1, ..., u_N)$ are the principal components of u_0. Now we assume that $(u_1, ..., u_N)$ are in the span of N eigenvalues of the Laplace operator, i.e.:

$$u_i(\mathbf{x},0) = \sum_{k=1}^{N} < u_i(\cdot,0),\ \phi_k > \phi_k(\mathbf{x}) \qquad\qquad i = 1, ..., N \qquad (3.14)$$

This implies that $\mathbf{\Upsilon}(0) \in \mathbb{R}^{N \times N}$, being $< u_i(\cdot,t),\ \phi_k >= 0$ for all $k > N$.
Since $\mathbf{\Upsilon}(t)$ is the transformation matrix between two orthonormal bases of the same subspace one can easy verify that it is orthogonal at any $t \in [0,\mathrm{T}]$:

$$\delta_{ij} = < u_i(\mathbf{x},t),\ u_j(\mathbf{x},t) >= \sum_{m=1}^{N}\sum_{k=1}^{N}\mathbf{\Upsilon}_{ik}(t) < \phi_k,\ \phi_m > \mathbf{\Upsilon}_{jm}(t) = \sum_{k=1}^{N}\mathbf{\Upsilon}_{ik}(t)\mathbf{\Upsilon}_{jk}(t)$$
$$(3.15)$$

Furthermore in the case we are analyzing, being $\mathbf{\Upsilon}$ square, it holds that $\mathbf{\Upsilon}(t)^{\top}\mathbf{\Upsilon}(t) = \mathbb{I}$. Now we are going to verify that

$$\begin{aligned} \mathbf{U}(\mathbf{x},t) &= \mathbf{U}(\mathbf{x},0) \\ \mathbf{Y}(t,\omega) &= \mathbf{\Upsilon}(0)e^{-\Lambda t}\mathbf{\Upsilon}(0)^{\top}\mathbf{Y}(0,\omega) \end{aligned} \qquad (3.16)$$

is solution of (3.11). First of all we observe that the condition $\mathbf{U}(\mathbf{x}, t) = \mathbf{U}(\mathbf{x}, 0)$ is equivalent to require that $\boldsymbol{\Upsilon}(t) = \boldsymbol{\Upsilon}(0)$ for any $t \in [0, \mathrm{T}]$, since $\mathbf{U}(\mathbf{x}, t) = \boldsymbol{\Upsilon}(t)\boldsymbol{\Phi}$. Then we calculate the covariance of this solution, that is:

$$
\begin{aligned}
\mathrm{C}(t) \;&=\; \boldsymbol{\Upsilon}(0)e^{-\Lambda t}\boldsymbol{\Upsilon}(0)^{\top}\mathbb{E}[\mathbf{Y}(0)\mathbf{Y}(0)^{\top}]\boldsymbol{\Upsilon}(0)e^{-\Lambda t}\boldsymbol{\Upsilon}(0)^{\top} \\
&=\; \boldsymbol{\Upsilon}(0)e^{-\Lambda t}\boldsymbol{\Upsilon}(0)^{\top}C(0)\boldsymbol{\Upsilon}(0)e^{-\Lambda t}\boldsymbol{\Upsilon}(0)^{\top}
\end{aligned}
\tag{3.17}
$$

We observe that, since $C(0)$ is assumed to be a full rank matrix and being $\boldsymbol{\Upsilon}(0)e^{-\Lambda}\boldsymbol{\Upsilon}(0)^{\top}$ strictly positive definite, the covariance matrix is strictly positive definite and then invertible at any $t \in [0, \mathrm{T}]$. Therefore, we can simplify $C(t)$ in (3.11) and equivalently in (3.12) and then we obtain:

$$
\begin{cases}
\dfrac{d\boldsymbol{\Upsilon}(0)}{dt} \;=\; \big[\boldsymbol{\Upsilon}(0)\boldsymbol{\Lambda}\,\boldsymbol{\Upsilon}(0)^{\top}\boldsymbol{\Upsilon}(0) \,-\, \boldsymbol{\Upsilon}(0)\boldsymbol{\Lambda}\big] \\[2mm]
\dfrac{\partial\mathbf{Y}(0, \omega)}{\partial t} \;=\; -\boldsymbol{\Upsilon}(0)\boldsymbol{\Lambda}\boldsymbol{\Upsilon}(0)^{\top}\mathbf{Y}(0, \omega)
\end{cases}
\tag{3.18}
$$

We use that $\boldsymbol{\Upsilon}$ is square:

$$
\boldsymbol{\Upsilon}(t)\boldsymbol{\Lambda}\,\boldsymbol{\Upsilon}(t)^{\top}\boldsymbol{\Upsilon}(t) \,-\, \boldsymbol{\Upsilon}(t)\boldsymbol{\Lambda} \;=\; \boldsymbol{\Upsilon}(t)\boldsymbol{\Lambda} \,-\, \boldsymbol{\Upsilon}(t)\boldsymbol{\Lambda} \;=\; 0
$$

and then the first equation in (3.18) is automatically satisfied. Now we pass to verify the equation for $\mathbf{Y}$. Since the transformation matrix is square and constant in time, the second equation in (3.18) can be rewritten in terms of $\boldsymbol{\Upsilon}(t)\mathbf{Y}(t, \omega)$ as:

$$
\frac{\partial\big(\boldsymbol{\Upsilon}(t)^{\top}\mathbf{Y}(t, \omega)\big)}{\partial t} \;=\; -\boldsymbol{\Lambda}\boldsymbol{\Upsilon}(t)^{\top}\mathbf{Y}(t, \omega)
\tag{3.19}
$$

with initial condition $\boldsymbol{\Upsilon}(0)^{\top}\mathbf{Y}(0, \omega)$. The solution is given by:

$$
\boldsymbol{\Upsilon}(t)^{\top}\mathbf{Y}(t, \omega) = e^{-\boldsymbol{\Lambda}t}\boldsymbol{\Upsilon}(0)^{\top}\mathbf{Y}(0, \omega)
$$

that implies $\mathbf{Y}(t, \omega) = \boldsymbol{\Upsilon}(t)e^{-\boldsymbol{\Lambda}t}\boldsymbol{\Upsilon}(0)^{\top}\mathbf{Y}(0, \omega) = \boldsymbol{\Upsilon}(0)e^{-\boldsymbol{\Lambda}t}\boldsymbol{\Upsilon}(0)^{\top}\mathbf{Y}(0, \omega)$.
We conclude that $\mathbf{U}(\mathbf{x}, t) = \mathbf{U}(\mathbf{x}, 0)$ and $\mathbf{Y}(t, \omega) = \boldsymbol{\Upsilon}(0)e^{-\boldsymbol{\Lambda}t}\boldsymbol{\Upsilon}(0)^{\top}\mathbf{Y}(0, \omega)$ is the unique solution of (3.11). This implies that the transformation matrix and consequently the deterministic modes do not evolve in time and the DO approach degenerates to the POD method according to which the solution is totally described by the evolution of the stochastic coefficients. Specifically the approximate solution u_N has the following analytic formulation:

$$
\begin{aligned}
u_N(\mathbf{x}, t, \omega) \;&=\; \mathbf{U}(\mathbf{x}, 0)^{\top}\boldsymbol{\Upsilon}(0)e^{-\boldsymbol{\Lambda}t}\boldsymbol{\Upsilon}(0)^{\top}\mathbf{Y}(0, \omega) \\
&=\; \boldsymbol{\Phi}(\mathbf{x})^{\top}e^{-\boldsymbol{\Lambda}t}\boldsymbol{\Upsilon}(0)^{\top}\mathbf{Y}(0, \omega)
\end{aligned}
\tag{3.20}
$$

We remark that this analysis doesn't concern the mean function and it holds also when the initial condition has mean different than zero since the equation for the mean, in the problem (3.3), is decoupled from the others.

3.2.1   Approximate solution and truncation error

In this section we aim to analyze the accuracy of the DO approximation, compared to the best N rank approximation, when the initial condition $u_0 \notin \mathcal{M}_N$. It implies that the initial datum is truncated and only the first N principal components of u_0, corresponding to those with largest variance, are considered. We will see how the truncation error influences the the approximate solution. In particular we start by showing a special case in which, under strong assumptions, the DO approximate solution coincide exactly with the KL expansion.

Consider an initial stochastic condition u_0 that is not in a finite dimensional linear manifold, $u_0 \notin \mathcal{M}_N$. For simplicity we assume that $\bar{u}_0(\mathbf{x}) = \mathbb{E}[u(\mathbf{x}, 0, \omega)] = 0$ that implies $\bar{u}(\mathbf{x}, t) = 0$ for any $t \in [0, \mathrm{T}]$. By following the KL approach, the initial function can be expanded as:

$$u_0(\mathbf{x}, \omega) = \sum_{i=1}^{\infty} y_{0i}(\omega)u_{0i}(\mathbf{x}) \tag{3.21}$$

where $\{u_{0i}\}_{i \in \mathbb{N}}$ are the principal components associated to the correlation operator $\Gamma_{u(0)u(0)}$ and $y_{0i}(\omega) = < u_0(\cdot, \omega), u_{0i} >$ for all $i \in \mathbb{N}$. We first assume that the principal components of the initial datum correspond exactly to the eigenfunctions of the Laplace operator, i.e. :

$$\phi_i(\mathbf{x}) = u_{0i}(\mathbf{x}) \qquad\qquad \forall i \in \mathbb{N}$$

The exact solution can be calculated analytically and it is given by:

$$u(\mathbf{x}, t, \omega) = \sum_{i=1}^{\infty} y_{0i}(\omega)e^{-\lambda_i t}u_{i0}(\mathbf{x}) \tag{3.22}$$

where $\{\lambda_i\}_{i \in \mathbb{N}}$ are the eigenvalues of the Laplace operator.

The expression (3.22) corresponds to the KL expansion of $u(\mathbf{x}, t, \cdot)$ at any $t \in [0, \mathrm{T}]$, by taking $y_i(t, \omega) = y_{0i}(\omega)e^{-\lambda_i t}$ and $u_i(\mathbf{x}, t) = u_{i0}(\mathbf{x})$, for all $i \in \mathbb{N}$. In fact the covariance operator of u reads:

$$
\begin{aligned}
v \in \mathrm{L}^2(\mathrm{D}) \to \Gamma_{u(t)u(t)}(v) \quad &= \int_{\mathrm{D}} C_{u(t)u(t)}(\mathbf{x}, \mathbf{x}')v(\mathbf{x}')\, d\mathbf{x}' \\[2mm]
&= \int_{\mathrm{D}} \mathbb{E}[\sum_{i=1}^{\infty} y_{0i}e^{-\lambda_i t}u_{i0}(\mathbf{x}) \sum_{k=1}^{\infty} y_{0k}e^{-\lambda_k t}u_{k0}(\mathbf{x}')]v(\mathbf{x}')\, d\mathbf{x}' \\[2mm]
&= \int_{\mathrm{D}} \sum_{i=1}^{\infty} e^{-2\lambda_i t}\mathbb{E}[y_i(t, \cdot)y_i(t, \cdot)]u_{i0}(\mathbf{x})u_{i0}(\mathbf{x}')v(\mathbf{x}')\, d\mathbf{x}'
\end{aligned}
$$
$$\tag{3.23}$$

where Λ is the diagonal matrix of the eigenvalues of the Laplace operator. We used the fact that, according to the KL decomposition, the initial stochastic coefficients $\{y_{0i}\}_{i \in \mathbb{N}}$ are uncorrelated. It follows that the principal components of u coincide with $\{u_{0i}\}_{i \in \mathbb{N}}$ at any time instant and the associated stochastic coefficients in the KL expansion are given by:

$$y_i(t, \omega) = < u(\cdot, t, \omega), u_{0i} > = y_{0i}(\omega)e^{-\lambda_i t} \qquad\qquad i \in \mathbb{N} \tag{3.24}$$

thanks to the $L^2(D)$-orthonormality of $\{u_{0i}\}_{i \in \mathbb{N}}$.

We calculate now the DO approximate solution in $\mathcal{M}_N$. First of all the initial datum is truncated:

$$u_{0N}(\mathbf{x}, \omega) = \sum_{i=1}^{N} y_{0i}(\omega) u_{0i}(\mathbf{x}) = \mathbf{U}_0(\mathbf{x}) \mathbf{Y}_0(\omega). \tag{3.25}$$

Then by recalling our assumption that the deterministic basis corresponds to a set of N eigenfunctions of the Laplace operator, we are back to the case previously analyzed. The method indeed doesn't see the initial approximation, it degenerates to the POD method and develops, analogously to what seen before, an approximate solution u_N given by:

$$u_N(\mathbf{x}, t, \omega) = \sum_{i=1}^{N} y_{0i}(\omega) e^{-\lambda_i t} u_{0i}(\mathbf{x}) \tag{3.26}$$

By comparing the DO solution with the analytic solution we see that the method at this level doesn't introduce any other source of error except the initial truncation error. By denoting with $\epsilon(t)$ the error in norm $L^2(D) \otimes L^2_P(\Omega)$ at time t, this can be estimated as:

$$\epsilon(t) = \mathbb{E}\big[\|u(\cdot, t, \cdot) - u_N(\cdot, t, \cdot)\|^2_{L^2(D)}\big] = \sum_{i=N+1}^{\infty} \mathbb{E}[y_{0i}^2] e^{-2\lambda_i t} \tag{3.27}$$

This shows that the error is bounded by the initial truncation error and it goes to zero when N goes to infinity. Namely the DO solution converges to the exact solution when N goes to infinity with rate of convergence driven by the rate of decay of the eigenvalues of the covariance operator. We can conclude that, under the assumption that the principal components of the initial datum correspond to the eigenfunctions of the Laplace operator, the DO solution corresponds to the best N-rank approximation i.e. the N truncated KL expansion at any time instant.

However the assumption that we have done is very strong. We replace it by assuming the first N initial principal components to be linear combinations of N eigenfunctions of the Laplace operator. Specifically let $u_0(x, \omega)$ be the initial condition expanded as in (3.21) with:

$$\begin{aligned} u_{0i} &\in span < \phi_1, ..., \phi_N > & i = 1, ..., N \\ u_{0i} &\in L^2(D) & i = N+1, ..., \infty \end{aligned} \tag{3.28}$$

that implies $\mathbf{U}(0) = \boldsymbol{\Upsilon}(0)\boldsymbol{\Phi}$ where $\boldsymbol{\Upsilon}(0)_{ij} = 0$ for $i \leq N \wedge j > N$. Equivalently it holds:

$$\begin{aligned} u_{0i} &= \sum_{j=1}^{N} \boldsymbol{\Upsilon}(0)_{ij} \phi_j & i = 1, ..., N \\ u_{0i} &= \sum_{j=1}^{\infty} \boldsymbol{\Upsilon}(0)_{ij} \phi_j & i = N+1, ..., \infty \end{aligned} \tag{3.29}$$

The initial function u_0 is truncated as in (3.25). Next we denote with $\boldsymbol{\Upsilon}^N(t)$ the transformation matrix of dimension $N \times N$ such that $\boldsymbol{\Upsilon}^N(t)_{ij} = \boldsymbol{\Upsilon}(\mathbf{t})_{ij}$ for all $i, j = 1, ..., N$ and with $\mathbf{U}^N(0)$, $\mathbf{Y}^N(0)$, $\boldsymbol{\Phi}^N$ the vectors of functions $(u_{01}, ..., u_{0N})^\top$, $(y_{01}, ..., y_{0N})^\top$ and $(\phi_1, .., .\phi_N)^\top$ respectively, so that, under the assumption (3.28) the approximated initial

datum can be rewritten as $u_N = \mathbf{U}^{N\top}\mathbf{Y}^N(0) = (\mathbf{\Upsilon}^N(0)\mathbf{\Phi}^N)^\top \mathbf{Y}^N(0)$.

Moreover we denote with $\mathbf{\Upsilon}^*(t)$ the transformation matrix such that for all $i, j = 1, ..., \infty$ $\mathbf{\Upsilon}^*(t)_{ij} = \mathbf{\Upsilon}(t)_{N+i,j}$ and with $\mathbf{U}^*(0)$, $\mathbf{Y}^*(0)$ the vectors functions $(u_{0,N+1}, ..., u_{0,\infty})^\top$ and $(y_{0,N+1}, ..., \phi_{0,\infty})^\top$.

Then the exact initial condition can be rewritten as:

$$u_0(\mathbf{x}, \omega) = (\mathbf{\Upsilon}^N(0)\mathbf{\Phi}^N)^\top \mathbf{Y}^N(0) + (\mathbf{\Upsilon}^*(0)\mathbf{\Phi})^\top \mathbf{Y}^*(0) \qquad (3.30)$$

We recall that, if the initial datum is a linear combination of N eigenfunctions of the Laplace operator, then the DO method degenerates to the POD one and the rank N approximate solution corresponds to the exact solution. Moreover we observe that the Laplace operator is linear so that the problem (3.1) with initial condition u_0 (3.30) can be reformulated as the sum of 2 analogous problems with initial data $(\mathbf{\Upsilon}^N(0)\mathbf{\Phi}^N)^\top \mathbf{Y}^N(0)$ and $(\mathbf{\Upsilon}^*(0)\mathbf{\Phi})^\top \mathbf{Y}^*(0)$ respectively. The solution of the first problem corresponds to the DO approximate solution of (3.1) while the second problem concerns the time evolution of the truncation error. Namely if we define the function $e = u - u_N$, this is solution of the problem:

$$\begin{cases} \dfrac{\partial e(\mathbf{x}, t; \omega)}{\partial t} - \Delta e(\mathbf{x}, t; \omega) = 0 & \mathbf{x} \in \mathrm{D}, \ t \in [0, \mathrm{T}], \ \omega \in \Omega \\ e(\sigma, t; \omega) = 0 & \sigma \in \partial\mathrm{D} \\ e(\mathbf{x}, 0; \omega) = (\mathbf{\Upsilon}^*(0)\mathbf{\Phi})^\top(\mathbf{x})\mathbf{Y}^*(0, \omega) \end{cases}$$
$$(3.31)$$

The solution of (3.31) can be calculated analytically and leads to:

$$e(\mathbf{x}, t; \omega) = \mathbf{\Phi}^\top(\mathbf{x})\mathbf{\Upsilon}^{*\top}(0)\mathbf{\Upsilon}(0)e^{-\Lambda t}\mathbf{\Upsilon}^{*\top}(0)\mathbf{Y}^*(0, \omega) \qquad (3.32)$$

where Λ is the matrix of eigenvalues of the Laplace operator. By denoting with $\epsilon(t)$ the square error in norm $\mathrm{L}^2(\mathrm{D}) \otimes \mathrm{L}^2_P(\Omega)$ at time t, it corresponds to the total variance of $e(t)$, i.e. $\epsilon(t) = \mathbb{E}[\|u(\cdot, t, \cdot) - u_N(\cdot, t, \cdot)\|^2_{\mathrm{L}^2(\mathrm{D})}] = \mathbb{E}[\|e(\cdot, t, \cdot)\|^2_{\mathrm{L}^2(\mathrm{D})}]$ and the following bound holds:

$$\epsilon(t) = \mathbb{E}[\|e(\cdot, t, \cdot)\|^2_{\mathrm{L}^2(\mathrm{D})} \leq \epsilon(0)e^{-2\lambda_1 t} \qquad (3.33)$$

where $\lambda_1 > 0$ is the smallest eigenvalues of the Laplace operator.

An Illustrative Example

We illustrate a trivial example that emphasizes the analytical results:

$$\begin{cases} \dfrac{\partial u(x, t; \omega)}{\partial t} - \dfrac{\partial^2 u(x, t; \omega)}{\partial x^2} = 0 & x \in (0, 2\pi), \ t \in [0, \mathrm{T}], \ \omega \in \Omega \\ u(0, t; \omega) = u(2\pi, t; \omega) = 0 & t \in [0, \mathrm{T}], \ \omega \in \Omega \\ u(x, 0; \omega) = z_1(\omega)\dfrac{1}{\sqrt{\pi}}\sin(x) + z_2(\omega)\dfrac{1}{\sqrt{\pi}}\sin(2x) & x \in (0, 2\pi), \ \omega \in \Omega \end{cases}$$
$$(3.34)$$

where z_1, z_2 are independent uniform random variables with zero mean and variance $\mathbb{E}[z_1^2] = 1$, $\mathbb{E}[z_2^2] = 2$. The exact solution can be calculated analytically and it reads:

$$u(\mathbf{x}, t, \omega) = z_1(\omega)e^{-t}\frac{1}{\sqrt{\pi}}\sin(x) + z_2(\omega)e^{-4t}\frac{1}{\sqrt{\pi}}\sin(2x) \qquad x \in [0, 2\pi],\ t \in [0, \mathrm{T}],\ \omega \in \Omega$$

(3.35)

and the total variance is given by $\mathbb{V}ar[u(\mathbf{x}, t; \cdot)] = \mathbb{E}[z_1^2]e^{-2t} + \mathbb{E}[z_2^2]e^{-8t}$.
The initial condition is a rank 2 function with the principal components that correspond to the first two eigenfunctions of the Laplace operator. It follows that the expansion of the initial datum (3.34) corresponds to the KL expansion and the exact solution evolves in the manifold $\mathcal{M}_2$ at any time instant. By applying the DO method with $N = 2$, no truncation error is introduced at the first step and the DO method degenerates to the POD method. At the continuous level both the DO and the KL approach provide the exact solution.
Consider now that the solution is approximated in $\mathcal{M}_1$. The initial function is approximated according to the KL decomposition by $u_1(x, \omega) = z_2(\omega)\frac{1}{\sqrt{\pi}}\sin(2x)$, which is the term with largest variance, and the DO method develops the following approximate solution

$$u_1^{DO}(x, t, \omega) = z_2(\omega)e^{-4t}\frac{1}{\sqrt{\pi}}\sin(2x) \qquad x \in [0, 2\pi],\ t \in [0, \mathrm{T}],\ \omega \in \Omega \qquad (3.36)$$

while the KL approximate solution is:

$$u_1^{KL}(x, t, \omega) = \begin{cases} z_2(\omega)e^{-4t}\dfrac{1}{\sqrt{\pi}}\sin(2x) & \text{for } t \in [0, \mathrm{T}] : \mathbb{E}[z_1^2]e^{-2t} \leq \mathbb{E}[z_2^2]e^{-8t} \\[2em] z_1(\omega)e^{-t}\dfrac{1}{\sqrt{\pi}}\sin(x) & \text{for } t \in [0, \mathrm{T}] : \mathbb{E}[z_1^2]e^{-2t} > \mathbb{E}[z_2^2]e^{-8t} \end{cases}$$

(3.37)

Figure 3.1 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, i.e. the 1-truncated KL expansion (right).
This example highlights the meaning of the estimate (3.33). The error of the DO method is bounded by the truncation error and goes to zero with rate of decay that depends on the smallest eigenvalue of the Laplace operator:

$$\epsilon(t)_{DO} \sim \mathbb{E}[z_1^2]e^{-2t}$$

while the error of the best approximation is:

$$\epsilon(t)_{KL} \sim \min\left(\mathbb{E}[z_1^2]e^{-2t},\ \mathbb{E}[z_2^2]e^{-8t}\right)$$

which is proportional to $\mathbb{E}[z_2^2]e^{-8t}$ for $t >> 0$.
We underline that this example concerns a very particular case, since the eigenfunctions of the Laplace operator correspond to the principal components of the initial condition, but it aims to emphasize the relation between the best N rank approximation and the DO approximate solution with respect to the truncation error.
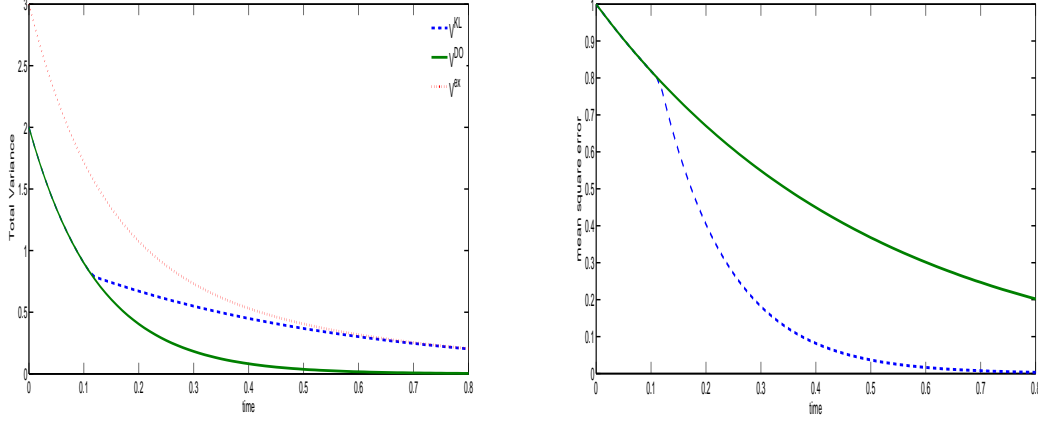
Figure 3.1: On the left: Evolution of the total variance $\mathbb{V}ar(t)$ of the KL and DO approximate solution with $N = 1$ as well as the exact solution. On the right: Time evolution of the mean square error $\epsilon(t)$ of the DO method with $N = 1$ and the best approximation.

3.2.2 Weak formulation and Numerical approximation

The DO approach consists in seeking the approximate solution $u_N \in \mathcal{M}_N$ of u that minimizes at any time instant the residual of the equation (3.1) in $\mathcal{T}_{u(t)}\mathcal{M}_N$, i.e. the tangent space to $\mathcal{M}_N$ in $u(t)$. This is equivalent to looking for a function u_N of the form $u_N(\mathbf{x}, t, \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N} u_i(\mathbf{x}, t)y_i(t, \omega)$ where the terms of the expansion satisfy the DO system:

$$\begin{cases} \dfrac{\partial \bar{u}(\mathbf{x}, t)}{\partial t} - \Delta \bar{u}(\mathbf{x}, t) = 0 & \mathbf{x} \in \mathrm{D}, \, t \in [0, \mathrm{T}], \, \omega \in \Omega \\[2ex] \sum_{i=1}^{N} \dfrac{\partial u_i(\mathbf{x}, t)}{\partial t} C_{y_i, y_j}(t) = \prod_{\mathcal{W}_N(t)^\perp} \mathbb{E}[\Delta u(\mathbf{x}, t, \cdot)y_j(t, \cdot)] & \forall j = 1, ..., N \\[2ex] \dfrac{\partial y_i(t, \omega)}{\partial t} = <\Delta u(\cdot, t, \omega) - \mathbb{E}[\Delta u(\cdot, t, \omega)], \, u_i(\cdot, t)> & \forall i = 1, ..., N \end{cases}$$

(3.38)

with the following boundary conditions:

$\bar{u}(\sigma, t) = 0 \qquad \sigma \in \partial \mathrm{D}, \, t \in [0, \mathrm{T}]$

$u_i(\sigma, t) = 0 \qquad \forall i = 1, ..., N$

and with initial conditions given by:

$\bar{u}_0(\mathbf{x}) = \mathbb{E}[u_0(\mathbf{x}, \omega)]$ for all $\mathbf{x} \in \mathrm{D}$,

$\{u_{0i}(\mathbf{x})\}_{i=1,...N}$ the first N eigenfunctions of the correlation operator $\Gamma_{u(0)u(0)}$,

$y_{i0}(\omega) = <u_0(\cdot, \omega), \, u_{0i}>$ with $\omega \in \Omega$ and for any $i = 1, ..., N$.

We remind that $\mathcal{W}_N(t)$ is the subspace spanned by the deterministic basis $\{u_1, ..., u_N\}$ at time t and the projection operator onto the orthogonal to $\mathcal{W}_N(t)$ in (3.38) reads:

$$\Pi_{\mathcal{W}_N^\perp} \Delta u_i(\mathbf{x}, t) = \Delta u_i(\mathbf{x}, t) - \sum_{k=1}^N <\Delta u_i(\cdot, t), u_k(\cdot, t)> u_k(\mathbf{x}, t) \qquad i = 1, ..., N \quad (3.39)$$

We denote with $\mathbf{u}$ and $\mathbf{y}$ the vectors of functions such that $\mathbf{u}(\mathbf{x}, t) = \big(u_1(\mathbf{x}, t), ..., u_N(\mathbf{x}, t) \big)$ and $\mathbf{y}(\omega, t) = \big(y_1(\omega, t), ..., y_N(\omega, t) \big)$. Define the vectorial projection operator as $\mathbf{\Pi} : \mathbf{v} \to (\Pi(v_1), ..., \Pi(v_N))$ for any $\mathbf{v}$ in $[\mathrm{L}^2(\mathrm{D})]^N$ as:

$$\mathbf{\Pi}_{\mathcal{W}_N^\perp} \Delta \mathbf{u}(\mathbf{x}, t) = \Delta \mathbf{u}(\mathbf{x}, t) - \mathbf{u}(\mathbf{x}, t) <\Delta \mathbf{u}(\cdot, t)^\top, \mathbf{u}(\cdot, t)> \qquad (3.40)$$

Finally the weak DO formulation for the problem (3.1) reads:

. *for any $t \in [0, \mathrm{T}]$, find $\bar{u}(\cdot, t) \in \mathrm{H}_0^1(\mathrm{D})$, $\mathbf{u}(\cdot, t) \in [\mathrm{H}_0^1(\mathrm{D})]^N$ and $\mathbf{y}(t, \cdot) \in [\mathrm{L}^2(\Omega)]^N$ such that:*

$$\begin{cases} <\dfrac{\partial \bar{u}(\cdot, t)}{\partial t}, \psi_i> \ + \ <\nabla \bar{u}(\cdot, t), \nabla \psi_i> = 0 \\[2em] <\dfrac{\partial \mathbf{u}(\cdot, t)}{\partial t}, \psi_k> C(t) \ + \ \mathbf{p}(\mathbf{u}(\cdot, t), \mathbf{u}(\cdot, t), \psi_k) C(t) \ = \ 0 \\[2em] \dfrac{\partial \mathbf{y}(t, \omega)}{\partial t} \ + \ \mathbf{y}(t, \omega) <\nabla \mathbf{u}^\top(\cdot, t), \nabla \mathbf{u}(\cdot, t)> = 0 \end{cases} \qquad (3.41)$$

for all ψ_i, $\psi_j \in \mathrm{H}_0^1(\mathrm{D})$ and for a.e. $\omega \in \Omega$,

where $\mathbf{p}(\cdot, \cdot, \cdot)$ is defined as:

$$\begin{aligned} \mathbf{p} : (\mathbf{u}, \mathbf{v}, w) \to \ &- <\mathbf{\Pi}_{<\mathbf{W}_N^\top>} \Delta \mathbf{v}, w> \\[1em] &= <\nabla \mathbf{v}, \nabla w> \ - \ <w, \mathbf{u}> <\nabla \mathbf{v}, \nabla \mathbf{u}> \end{aligned} \qquad (3.42)$$

where $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w} \in [\mathrm{H}_0^1(\Omega)]^N$ and $<\mathbf{u}_i, \mathbf{u}_j> = \delta_{ij}$. We remark that according to the DO representation the stochastic components are separated from the functions defined in the physical space. Specifically in the DO system (3.41) the first two sets of equations depend on the the deterministic variable $\mathbf{x}$ while the last one is defined in the probability space. Thanks to this, deterministic and stochastic functions can be discretized independently and with different strategies. However, the system (3.41) remains coupled at any time instant. In particular we choose the Finite Element method to discretize the deterministic functions and the Stochastic Collocation to solve the equations in ω.

3.2.3   Spatial Discretization

The physical space is discretized by using the linear Finite Element method. Let $\mathcal{T}_h$ be the triangulation defined in the spatial domain D being h the mesh spacing parameter

and N_h the number of degrees of freedom that, by using linear elements, corresponds to the vertice in the triangulation. We define $V_h \subset H_0^1(D)$ the finite element space of the continuous piecewise linear functions defined in $\mathcal{T}_h$. Any function $u(\mathbf{x}) \in H_0^1(D)$ is approximated in V_h as follows:

$$u(x) \approx u_h(\mathbf{x}) = \sum_{j=1}^{N_h} u_j \rho_j(\mathbf{x}) \qquad (3.43)$$

where $u_j = u_h(\mathbf{x}_j)$, for $j = 1, ..., N_h$ are the nodal values of u_h and $\{\rho_1(\mathbf{x}), ..., \rho_{N_h}(\mathbf{x})\}$ are the Lagrange basis functions of V_h defined on the vertices of the triangulation.

Any time dependent function $u \in L^\infty([0, \text{T}], H_0^1)$ is approximated with a formulation analogous to (3.43), where the the nodal values are replaced by time dependent functions $u_j = u_h(\mathbf{x}_j, t)$.

The semi-discrete formulation for the deterministic part of (3.41) reads: for any $t \in [0, \text{T}]$, find $\bar{u}_h(\cdot, t) \in V_h$, $\mathbf{u}_h(\cdot, t) \in [V_h]^N$ such that:

$$< \frac{\partial \bar{u}_h(\cdot, t)}{\partial t}, \rho_k > + < \nabla \bar{u}_h(\cdot, t), \nabla \rho_k > = 0 \qquad\qquad k = 1, ..., N_h$$

$$< \frac{\partial \mathbf{u}_h(\cdot, t)}{\partial t}, \rho_k > C(t) + \mathbf{p}(\mathbf{u}_h(\cdot, t), \mathbf{u}_h(\cdot, t), \rho_k) C(t) = 0 \qquad\qquad k = 1, ..., N_h$$

$$(3.44)$$

Thanks to the linearity of the Laplace operator, in the case of deterministic diffusion term, the equation for the mean is decoupled from the other N equations.

The time derivative is discretized by using the semi-implicit Euler method with time step Δt. Denote with u^n the solution at time $t = n\Delta t$. The fully discretized formulation is: for $n = 0, 1, ..., N_T$ with $N_T = \lfloor \text{T}/\Delta t \rfloor$ find $\bar{u}_h^{n+1} \in V_h$, $\mathbf{u}_h^{n+1} \in [V_h]^N$ such that:

$$< \bar{u}_h^{n+1}, \rho_k > + \Delta t < \nabla \bar{u}_h^{n+1}, \nabla \rho_k > = < \bar{u}_h^{n+1}, \rho_k >$$

$$< \mathbf{u}_h^{n+1}, \rho_k > C^n + \Delta t \mathbf{p}(\mathbf{u}_h^n(\cdot, t), \mathbf{u}_h^{n+1}(\cdot, t), \rho_k) C^n = < \mathbf{u}_h^n, \rho_k > C^n$$

$$(3.45)$$

for $n = 1, ...N_T$. Both the covariance matrix and the projection operator are treated explicitly in order to decouple the deterministic set of equations from the stochastic system. Even if the subspace $\mathcal{W}_N$, generated by the deterministic basis, is time dependent we chose to consider it freezed at the previous time step in the resolution of (3.44) in order to reduce the computational effort and decouple the deterministic equations. Dealing with a totally coupled system as in (3.45) may indeed require an excessive computational cost especially with large physical domains and multidimensional stochastic space.

Stochastic Discretization

We chose to solve the stochastic equations by using the Stochastic Collocation method. Assume that the probability space is parametrized by a vector $\vec{\xi}$ of S stochastic variables

$\vec{\xi} = (\xi_1, ..., \xi_S)$, let $f(\vec{\xi})$ be the joint probability density function and let $\mathbf{\Gamma}$ be the support of $\vec{\xi}$. According to the distribution of $\vec{\xi}$ we select a set of collocation points $\{\vec{\xi}_i \in \mathbf{\Gamma}\}$. The stochastic equations are collocated in each collocation point and the approximate solution $y_n(\vec{\xi})$ is computed by a suitable interpolation of the results.

Suppose that the probability space is mono-dimensional, $S = 1$, then the stochastic processes $y_1, ..., y_N \in \mathrm{L}^\infty([0, \mathrm{T}], \mathrm{L}^2_P(\Omega))$ are approximated by:

$$y_i(t, \xi(\omega)) \approx y_{iw}(t, \xi(\omega)) = \sum_{k=1}^{N_y} y_i(t, \xi_k) \mathcal{L}_k(\omega) \tag{3.46}$$

where N_y is the number of collocation points and $\{\mathcal{L}_k\}_{k=1}^{N_y}$ is the sequence of Lagrange polynomials of degree $N_y - 1$ associated to the collocation points.

In the problem (3.41) we deal with a system of N stochastic ordinary differential equations where the time derivative is discretized by the implicit Euler method. At any time step $t^n = n\Delta t$ with $t^n \in [0, \mathrm{T}]$ the discretized system is collocated in each collocation point $\{\vec{\xi}_k \in \mathbf{\Gamma}, \ k = 1, ..., N_y\}$ of the stochastic grid in order to recover all the coefficients $\{y_1(t^{n+1}, \xi_k), ..., y_N(t^{n+1}, \xi_k)\}_{k=1}^{N_y}$. If the differential operator $\mathcal{L}$ is linear and deterministic, this leads to N_y decoupled systems of dimension $N \times N$:

$$\mathbf{y}^{n+1}(\xi_k) + \Delta t < \nabla\mathbf{u}^{n+1}, \nabla\mathbf{u}^{n+1} > \mathbf{y}^{n+1}(\xi_k) = \mathbf{y}^n(\xi_k) \tag{3.47}$$

for any $k = 1, ..., N_y$ and at any time step $t^n = n\Delta t$ with $t^n \in [0, \mathrm{T}]$. The spatial inner product represents the projection of the stochastic response in the subspace $\mathcal{W}_N$. Since we solve at each time step first for the deterministic modes and then for the stochastic variables (Gauss-Seidel-type approach), this projection can already be done on the updated deterministic modes at t^{n+1}.

The covariance matrix, which needs to be computed at each time step in order to solve the deterministic equations in (3.45), is estimated through the quadrature formula corresponding to the collocation points, i.e.:

$$\mathbb{C}^n = \mathbb{E}[\mathbf{y}^{n\top}\mathbf{y}^n] \cong \sum_{k=1}^{N_y} \mathbf{y}^{\top n}(\xi_k)\mathbf{y}^n(\xi_k) w_k \tag{3.48}$$

where $w_1, ..., w_{N_y}$ are the weights associated to each point of the stochastic grid. We remind that $\mathbf{y}$ are supposed to be zero mean stochastic process.

The method can be generalized to multidimensional stochastic spaces. In the case of full tensor stochastic grid the formulation is exactly the same, where the stochastic variables are assumed to be real valued functions of the vector $\vec{\xi}$. The equations are collocated in each point of the full tensor grid and once the coefficients $\{y_1(t^{n+1}, \xi_k), ..., y_N(t^{n+1}, \xi_k)\}_{k=1}^{N_y}$ are recovered at each time step, $\mathbf{y}$ is interpolated by using the tensor product of the one dimensional Lagrange polynomials. Remarkable computational advantages can be achieved by using sparse grids. See [7], [18], [21] for details. However we underline that the sparse grid approximation is interpolatory only if the collocation points are nested.

3.2.4 Algebraic Formulation

First of all we define the following matrices:

- $\bar{U}_j = \bar{u}_h^n \in \mathbb{R}^{N_h}$,

- $U^n = u_{i\,h}^n \in \mathbb{R}^{N_h \times N}$,

- $Y^n = y_{i\,h}^n \in \mathbb{R}^{N \times N_y}$,

- $\mathbb{C}^n \in \mathbb{R}^{N \times N}$,

- $\mathbb{M}$, $\mathbb{K}$, $\mathbb{I}$ the mass, the stiffness and the identity matrix respectively.

then the algebraic formulation of the discretized DO system in (3.38) reads:

$$
\begin{cases}
\bar{U}^{n+1} + \Delta t \mathbb{K}\bar{U}^{n+1} = \bar{U}^n \\
U^{n+1}\mathbb{C}^n + \Delta t(\mathbb{I} - \mathbb{M}U^n U^{n\top})\mathbb{K}U^{n+1}\mathbb{C}^n = U^n\mathbb{C}^n \\
Y^{n+1} + \Delta t U^{n+1\top}\mathbb{K}U^{n+1}Y^{n+1} = Y^n
\end{cases} \tag{3.49}
$$

Say $\mathbf{R}(\mathbf{x})$ the vector of the basis functions of the Finite Element space, $\mathbf{R}(\mathbf{x}) = (\phi_1(\mathbf{x}), ..., \phi_{N_h}(\mathbf{x}))$, and $\mathbf{L}(\vec{\xi})$ the vector of the Lagrange polynomials into the collocation points, $\mathbf{L}(\vec{\xi}) = (L_1(\vec{\xi}), ..., L_{N_y}(\vec{\xi}))$, then the discretized approximate solution u_N can be formulated as $u_N(x, t^n, \xi) = \mathbf{R}(\mathbf{x})\bar{U}^n + \mathbf{R}(\mathbf{x})U^n Y^n \mathbf{L}^\top(\vec{\xi})$. Observe that we never store nor require the explicit "full tensor" $u_N(\mathbf{x}_i, t^n, \xi_j)\, i = 1, ..., N_h\, j = 1, ..., N_y$ and the evolution of the approximate solution is totally described by the N terms of the DO expansion.

Orthogonalization in the probability space

We consider here the second set of equations in (3.45). If consists in a system of N deterministic equations that are coupled because of the covariance matrix that multiply $\mathbf{u}$ on the right side. A trivial option to decouple the equations consists in multiplying both sides by the inverse of the covariance matrix. Unfortunately nothing ensures that this is possible. The covariance matrix indeed evolves in time and it can become singular (or nearly singular). We have seen that deterministic initial conditions provide singular covariance matrices but also dissipative processes develop nearly singular matrices when the process tends to the deterministic steady state. Another possibility consists in using the pseudo-inverse. This choice provides stability to the system but on the other hand prevents the rank from increasing. The eigenfields associated to zero eigenvalues are indeed set to zero and the associated stochastic fields are not allowed to increase anymore. The strategy we adopted is based on re-orthogonalizing the random coefficients at each time step. We remark indeed that the system does not preserve the un-correlation of the stochastic coefficients in general, being a condition not required in the DO approach.

The covariance matrix is by definition symmetric and positive semi-definite. It follows that at any time instant there exists a set of N eigenvalues $\{\lambda_k(t)\}_{k=1}^N$ and N eigenvectors $\{v_k(t)\}_{k=1}^N$ orthogonal with respect to the euclidean norm. Therefore at any time instant

there exists a transformation according to which the stochastic field $u_N \in \mathcal{M}_N$ can be written as:

$$u_N(\mathbf{x}, t; \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N} z_i(t; \omega) w_i(\mathbf{x}, t) \qquad (3.50)$$

where:

- $w_j(\mathbf{x}, t) = \sum_{i=1}^{N} u_i(\mathbf{x}, t) v_{ij}(t) \, \forall j = 1, ..., N$

- $z_j(t; \omega) = \sum_{i=1}^{N} y_i(t; \omega) v_{ji}(t) \, \forall j = 1, ..., N$

In particular the stochastic coefficients $\{z_i\}_{i=1}^{N}$ are orthogonal in $L_P^2(\Omega)$, i.e. $\mathbb{E}[z_i(t) z_j(t)] = \lambda_i(t) \delta_{ij}$. Moreover the transformation preserves the orthonormality of the deterministic fields since the matrix $\{v_{ij}\}$ is orthogonal. Specifically the covariance matrix of the uncorrelated stochastic variables $\{z_i\}_{i=1}^{N}$ corresponds to the diagonal matrix of the eigenvalues of $C(t)$. We use this observation to decouple the deterministic system in (3.45).

At the discrete level the covariance matrix, that is treated explicitly and freezed at the previous time step for the resolution of the deterministic system, is diagonalized and the system is solved with respect to the functions $\{w_i\}_{i=1}^{N}$. Let $\mathbb{V}^n$ be the matrix of the eigenvectors of $\mathbb{C}^n$, in algebraic form the system can be reformulated as follows:

$$W^{n+1}\mathbb{D}^n + \Delta t(\mathbb{I} - \mathbb{M}U^n U^{n\top})\mathbb{K}W^{n+1}\mathbb{D}^n = W^n \mathbb{D}^n \qquad (3.51)$$

where $W^n = U^n \mathbb{V}^n$, $W^{n+1} = U^{n+1}\mathbb{V}^n$ and $\mathbb{D}$ is diagonal. This strategy decouples the system and in addition it permits to deal with singular covariance matrices. In view of the observation (2.23) the deterministic fields associated to zero variance stochastic coefficients are unchanged. According to the representation (3.50) we denote with W_i and Y_i the ith mode and stochastic coefficient respectively, associated to the eigenvalue λ_i, for $i = 1, ..., N$. Finally the DO system in algebraic form reads:

$$\begin{cases} \bar{U}^{n+1} + \Delta t \mathbb{K}\bar{U}^{n+1} = \bar{U}^n \\ W_i^{n+1} + \Delta t(I - \mathbb{M}U^n U^{n\top})\mathbb{K}W_i^{n+1} = W_i^n & \lambda_i^n > 0 \\ W_i^{n+1} = W_i^n & \lambda_i^n \le 0 \\ Y^{n+1} + \Delta t U^{n+1\top}\mathbb{K}U^{n+1}Y^{n+1} = Y^n \end{cases} \qquad (3.52)$$

Implementation Details

The computational code used for the numerical tests shown in sections 3.2.5, 3.3.1, 4.4.2, 4.5 is realized in Matlab and implemented for one and two dimensional physical domains. In the second case the spatial grid, the mass and stiffness matrices are generated using the code FreeFem++ (see www.freefem.org) and imported in Matlab. Approximation in the stochastic variables have been obtained by tensorial stochastic grids on Gauss points. The linear systems in (3.52) are solve with the Matlab command $back - slash$ or with $gmres$ in case of 2 dimensional spatial domains. The covariance matrix is diagonalized with the command eig. As described in the previous section, we assume that only the

modes associated to eigenvalues strictly larger than zero evolve. For computational reasons we need to set a threshold with respect to which the eigenvalues are considered non zero. In order to guarantee more stability to the problem the threshold is weighted with respect to the largest eigenvalue:

$$\begin{aligned}
\lambda_i^n > \epsilon \cdot \max_{j=1,...,N}(\lambda_j^n) &\implies W_i^n \text{ evolves} \\
\lambda_i^n < \epsilon \cdot \max_{j=1,...,N}(\lambda_j^n) &\implies W_i^n \text{ left unchanged}
\end{aligned} \tag{3.53}$$

In the numerical examples that follow the threshold set has been $\epsilon = 10^{-15}$.

In conclusion the DO method consists, at any time iteration, in $N + 1$ equations of dimension $N_h \times N_h$ plus N_y equations of dimension $N \times N$, where N_h, N_y are the number of the physical degrees of freedom and of stochastic collocation points, respectively. We underline that the computational cost is reduced by the diagonalization of the covariance matrix that leads to actually solve only a number of deterministic systems corresponding to the rank of u_N intead of N.

3.2.5 Numerical Examples

Test Case 1: sinusoidal basis functions

Consider the following mono-dimensional problem:

$$\begin{cases}
\dfrac{\partial u(x,t;\,\omega)}{\partial t} - \Delta u(x,t;\,\omega) = 0 & x \in (0,\,10),\, t \in \mathrm{T},\, \omega \in \Omega \\
u(0,t;\,\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\
u(10,t;\,\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\
u(x,0;\,\omega) = z(\omega)\sqrt{\tfrac{1}{5}}\sin\left(\tfrac{\pi x}{5}\right) & x \in (0,\,10),\, \omega \in \Omega
\end{cases} \tag{3.54}$$

Here $z(\omega)$ is a uniform random variable with zero mean and variance $1/3$ so that the initial datum is a zero mean stochastic field, while the differential operator is deterministic.

According to the DO approach we seek an approximate solution $u_N \in \mathcal{M}_N$, that satisfies the DO system associated to the problem (3.54). We aim to verify if and how u_N changes with respect to the dimension of the manifold $\mathcal{M}_N$ where the solution is approximated. For this purpose, in what follows, the number of modes N is considered between 1 and 10.

According to the Dirichlet boundary conditions, we choose to initialize the modes to orthonormal sinusoidal functions in $L^2(\mathrm{D})$ where D is the interval [0, 10]:

$$u_i(x,0) = \sqrt{\frac{1}{5}}\sin\left(\frac{i\pi x}{5}\right) \qquad\qquad i = 1,...,N \tag{3.55}$$

Then the initial condition can be rewritten as:

$$u(x,0;\,\omega) = \sum_{i=1}^{N} y_i(0,\omega)u_i(x,0) \tag{3.56}$$

where the stochastic coefficents are initialized as follows:

- $y_1(0,\omega) = z(\omega)$,

- $y_i(0,\omega) = 0$, $\forall i = 2,...,N$.

In particular the covariance matrix at $t = 0$ is singular for any $N > 1$ since only one random variable has variance larger than zero. Observe that the example we are investigating corresponds to the case analyzed in the section 3.2 where we supposed the principal components of the initial datum equal to the eigenfunctions of the Laplace operator. The numerical tests confirm the analytical results; the DO method degenerates to the POD method. One can indeed verify that the exact solution, that is given by:

$$u_{ex}(x,t;\omega) = z(\omega)e^{\frac{-\pi^2 t}{25}}\sqrt{\frac{1}{5}}\sin\left(\frac{i\pi x}{5}\right) = z(\omega)e^{\frac{-\pi^2 t}{25}}u_1(x,0) \qquad (3.57)$$

lives in a manifold of dimension 1 and its total variance is given by:
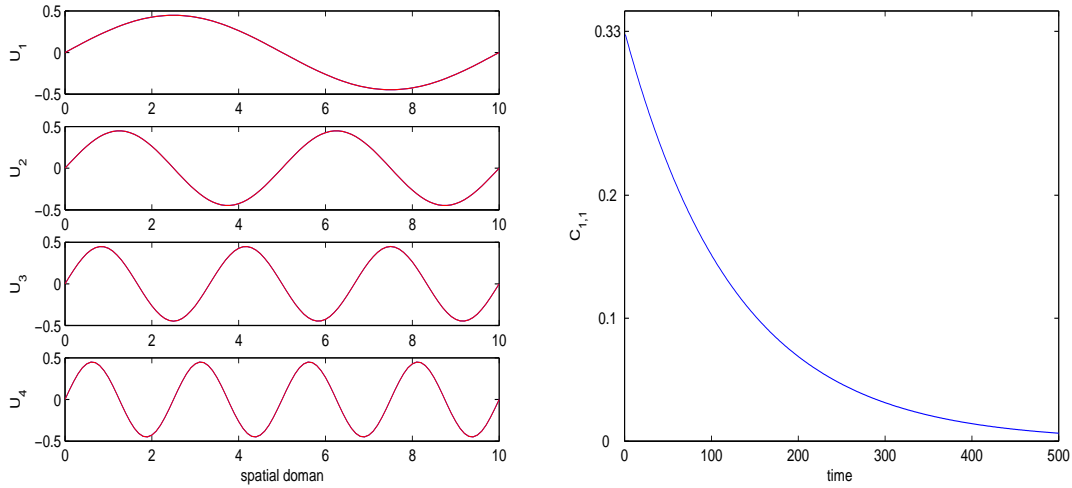
Figure 3.2: On the left: The modes at time $T = 2$ with $N = 4$, $\Delta t = 10^{-2}$, spatial discretization $h = 0.1$, $N_y = 9$. On the right: Time evolution of the variance of the stochastic process Y_1.

$$\mathbb{V}ar(t) = \mathbb{E}[z(\omega)^2]e^{\frac{-2\pi^2 t}{25}} \qquad (3.58)$$

For any N analyzed the modes do not evolve in time , see Figure (3.2) (left). Furthermore, since the method in this specific case does not introduce any truncation error with respect to the initial datum, the DO solution corresponds to the KL expansion at any time step. In particular the process is totally described by the evolution of the first stochastic coefficient, see Figure (3.2) (right). For $N > 1$ any y_i with $i = 2,...,N$ remains identically equal to zero. The total variance of the solution is then identified by the variance of y_1 that decays to zero with constant rate proportional to the first eigenvalue of the Laplace operator. Consequently the rank of the covariance matrix is constantly equal to one

until all the stochasticity of the solution is dissipated, and than goes to zero (which will happen however only for $t \to \infty$). Moreover this example allows us to verify the behavior of the method in the case of over-approximation, (i.e. a number N of modes larger then the effective rank of the solution). Specifically for this example this occurs for $N > 1$. For any N the method provides a numerical solution, that potentially belongs to $\mathcal{M}_N$ but that has effective rank 1, consistently with the exact solution. For what concerns the system of deterministic PDEs in (3.41), being the covariance matrix already diagonal at each time step, the algorithm solves only the linear system associated to the first mode.

Test Case 2: hierarchical basis functions

In this section we want to investigate a more general case in which the deterministic basis functions do not correspond to the eigenfunctions of the Laplace operator and the initial datum is not in a finite dimensional space spanned by N eigenfunctions. We consider a problem analogous to (3.54) but with initial condition given by:

$$\begin{cases} \dfrac{\partial u(x,t;\,\omega)}{\partial t} - \Delta u(x,t;\,\omega) = 0 & x \in (0,\,8),\, t \in \mathrm{T},\, \omega \in \Omega \\ u(0,t;\,\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\ u(8,t;\,\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\ u(x,0;\,\omega) = u_0(x;\,\omega) & x \in (0,\,8),\, \omega \in \Omega \end{cases} \tag{3.59}$$

Here the initial condition u_0 is a linear function of $z(\omega)$, that is a uniformly distributed random variable with zero mean and variance $1/3$. We initialized the deterministic basis functions to a sequence of hierarchical functions, see Figure 3.3, and assume that the initial condition is expanded as:

$$u(x,0;\,\omega) = \sum_{i=1}^{N} y_i(0,\omega) u_i(x,0) \tag{3.60}$$

where the random coefficients are:

- $y_1(0,\omega) = z(\omega)$,

- $y_i(0,\omega) = 0, \; \forall i = 2,...,N.$

Here N, that is the number of modes, is between 1 and 15. We remark that in order to apply the DO method the modes have to be orthonormal in $\mathrm{L}^2(\mathrm{D})$, and consequently the hierarchical basis functions (Figure 3.3) need to be re-orthonormalized. From a computational point of view the orthogonalization is achieved by using the QR decomposition that consists in factorizing a generic matrix $A \in \mathbb{R}^{m \times n}$, with $m \geq n$, in a orthogonal matrix Q of dimension $m \times m$ times an upper triangular matrix $R \in \mathbb{R}^{m \times n}$. Specifically the initial datum needs to be reformulated as follows:

$$u(x,0;\,\omega) = \sum_{i=1}^{N} \tilde{y}_i(0,\omega) \tilde{u}_i(x,0) \tag{3.61}$$
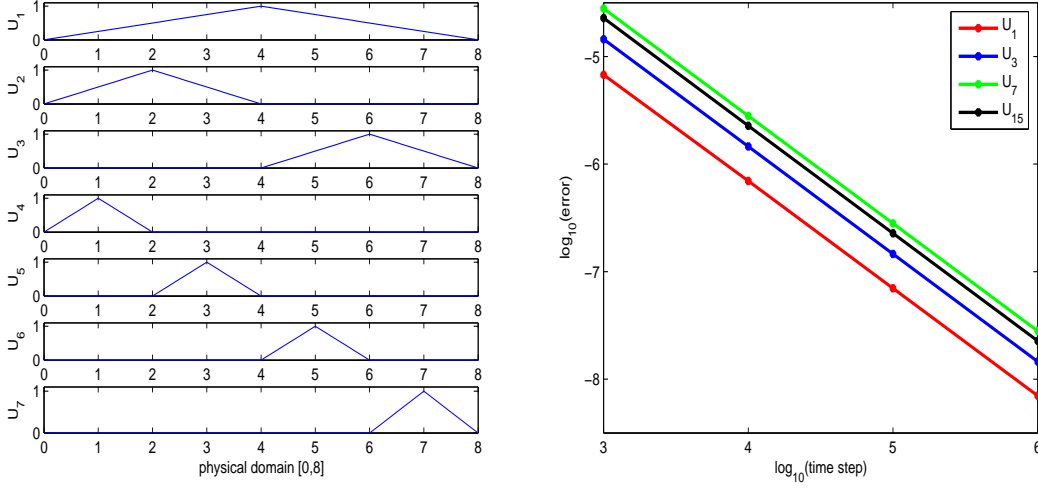
Figure 3.3: On the left: The hierarchical bases with $N = 6$. On the right: The error ϵ w.r.t. the time step.

where the basis functions are orthonormal in $\mathrm{L}^2(\mathrm{D})$, i.e. $< \tilde{u}_i(\cdot, 0), \tilde{u}_j(\cdot, 0) >= \delta_{ij}$. Since the QR decomposition results in an orthogonal matrix Q with respect to the euclidean norm, the factorization is applied to the matrix $\mathbb{M}^{1/2}U$ where we remind that $\mathbb{M}$ is the mass matrix of the Finite Element space and $U \in \mathbb{R}^{N_h \times N}$ is defined as $U_{ij} = u_j(x_i)$, and the orthonormal set of basis functions is identified by $\tilde{U} = \mathbb{M}^{-1/2}Q$. The orthonormality is easy to verify:

$$\tilde{U}^\top \mathbb{M} \tilde{U} = Q^\top \mathbb{M}^{-1/2} \mathbb{M} \mathbb{M}^{-1/2} Q = \mathbb{I}. \tag{3.62}$$

In order to recover a decomposition equivalent to (3.60) also the stochastic coefficients need to be updated. To summarize:

- $[Q, R] = qr(\mathbb{M}^{1/2}U)$,

- $\tilde{U} = \mathbb{M}^{-1/2}Q$,

- $\tilde{Y} = RY$.

Observe that the finite dimensional space spanned by the new basis functions is exactly the same as the one described by the hierarchical basis in Figure 3.3 (left). We apply the DO method to problem (3.59) starting from an initial datum expanded according to (3.61).

Thanks to the linearity of the Laplace operator and the structure of the initial condition, that is a 1-rank function, the exact solution evolves in a manifold of dimension 1 at any time instant, however with a deterministic subspace that changes in time. Consequently, according to the DO approach, the approximate solution is expected to be described by modes that evolve in time. Moreover, contrary to the example 1 the method is expected to introduce truncation error that depends on the number of the modes and that is
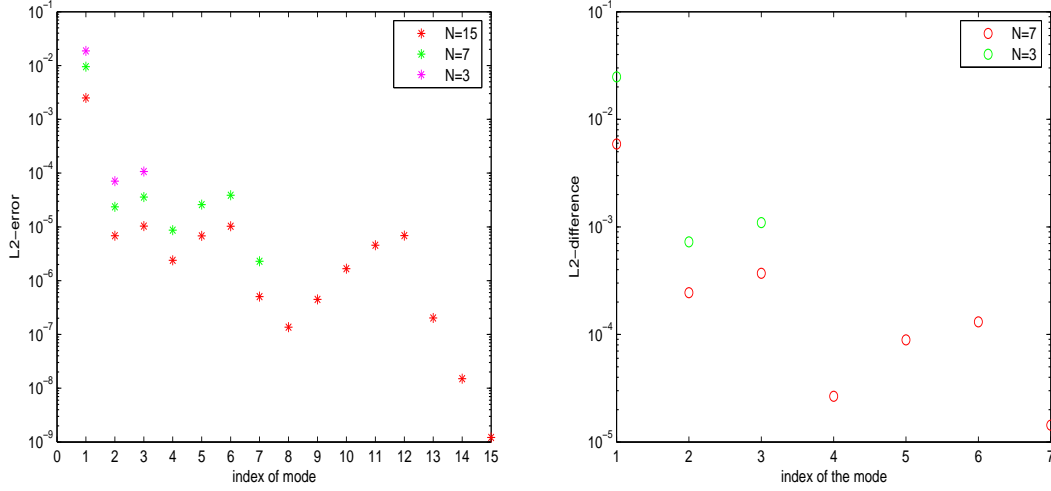
Figure 3.4: Norm γ at time $t = 10$ and $\Delta t = 10^{-3}$ (on the left), $\Delta t = 10^{-2}$ (on the right) and different number of modes.

influenced by the time step, since the system of $PDEs$ in (3.41) is solved by freezing the covariance matrix in order to decouple the deterministic equation from the stochastic ones. The numerical tests confirm the previous observations. The deterministic basis functions change in time and we quantified the evolution by computing the following difference in L^2(D)-norm:

$$\gamma_i(t) = \parallel u_i(\cdot, 0) - u_i(\cdot, t) \parallel_L^2 (\mathrm{D}) \qquad\qquad i = 1, ...N \qquad\qquad (3.63)$$

The results are displayed in Figure 3.4 where to different colors correspond to different values of N. We observe that the the process is mainly described by the evolution of the first stochastic coefficient but, contrary to example 1, the other random variables do not remain identically equal to zero. Specifically, their variance increases as the variance of the first random variable decreases, Figure 3.5 (Left). However we remark that, consistently to the theoretical observations, the numerical solution "lives" in a manifolds of dimension 1 provided by the rank of the covariance matrix that is constantly equal to one. We quantified the error of the approximate solution in norm L^2(D)$\otimes$L$_P^2(\Omega)$ at fixed time:

$$\epsilon = \left(\mathbb{E}[\| u_{ex}(x, T, \omega) - u_{DO}(x, T, \omega)_{L^2}^2] \right)^{\frac{1}{2}} \qquad\qquad (3.64)$$

where $u_{ex}(x, t, \omega)$ is the reference solution, computed with the Stochastic Collocation method by using a highly accurate sparse grid in order to guarantee a numerical solution very close to the exact one. As shown in Figure 3.3 (right) the error is proportional to the time step with order 1 and goes to zero when Δt tends to zero. This shows that the truncation error introduced in the stochastic space is negligible compared to the time discretization error.
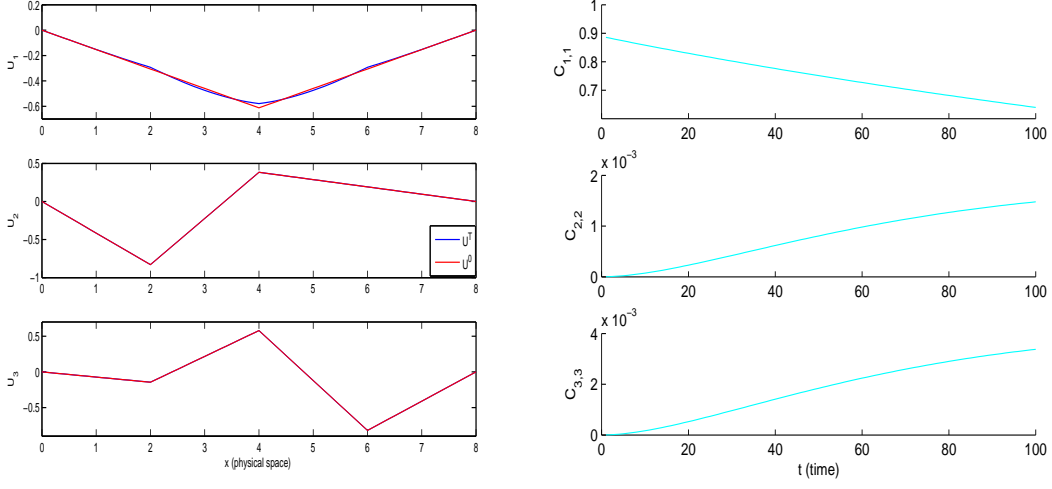
Figure 3.5: On the left: Evolution of the modes with $N = 3$, $\Delta t = 10^{-2}$, spatial discretization $h = 0.1$, $N_y = 9$. On the right: Time evolution of the variance.

Test Case 3: non linear reaction term

We compare now the results obtained in Test cases 1 and 2 in which the problem is governed by a parabolic PDE with non linear reacton term. Specifically in this example we consider

$$
\begin{cases}
\dfrac{\partial u(x,t;\,\omega)}{\partial t} - \Delta u(x,t;\,\omega) = F(u(x,t;\omega)) & x \in [0,\,10],\ t \in \mathrm{T},\ \omega \in \Omega \\[2mm]
\dfrac{\partial u}{\partial x}(0,t;\,\omega) = 0 & t \in \mathrm{T},\ \omega \in \Omega \\[2mm]
\dfrac{\partial u}{\partial x}(10,t;\,\omega) = 0 & t \in \mathrm{T},\ \omega \in \Omega \\[2mm]
u(x,0;\,\omega) = \dfrac{2}{5} + z(\omega)\sqrt{\tfrac{1}{5}}\cos\left(\tfrac{\pi x}{5}\right) & x \in [0,\,10],\ \omega \in \Omega
\end{cases}
$$

$$(3.65)$$

where $F(u) = \beta u(u-1)(\alpha - u)$ with $\alpha \in (0,1)$, $\beta > 0$, and $z(\omega)$ is a uniform random variable with zero mean and variance $\sigma^2 = 4/15$. Details on the numerical approximation of (3.65) will be given in the next chapter, section 4.3.2. The initial condition is a rank 1 stochastic field and the exact solution u is in a one-dimensional manifold, since the stochastic space has dimension 1 (only one random variable is involved in (3.65)). However this manifold is not linear. It follows that the DO approximate solution, that is sought is a linear manifold of dimension N, might require $N > 1$ modes to well describe the exact solution. In order to investigate the accuracy of the approximation based on the dimension of the linear manifold, we numerically solved the problem for different values of N. The initial condition can be expanded in series in accordance with the KL

decomposition as:

$$u(x, t_0, \omega) = \bar{u}(x, t_0) + \sum_{k=1}^{N} u_k(x, t_0) y_k(t_0, \omega)$$

where

- $\bar{u}(x, t_0) = \dfrac{2}{5}$,

- $u_k(x, t_0) = \sqrt{\dfrac{1}{5}} cos\big((k-1)\pi \dfrac{x}{5}\big)$, for all $k = 1, ..., N$

- $y_2(t_0, \omega) = z(\omega)$,

- $y_k(t_0, \omega) = 0 \ \forall k = 1, \ k = 3, ..., N$

where the deterministic basis functions associated to zero variance stochastic variables are arbitrarily initialized to cosinus functions. The rank of the covariance matrix is initially equal to one, since only one coefficient has variance different than zero. Numerical tests show that the rank increases in time, meaning that the solution is approximated in a linear manifold of dimension $N > 1$. On the other hand, as shown in Figure 3.8(left) the basis functions evolve in time, in order to adapt to the solution. The non linear reaction term makes the solution to evolve in strongly non linear manifold. Moreover this manifold evolves in time that implies that more and more "directions" are needed in time to describe it. On one side the DO approximation requires $N > 1$ modes to span linearly the solution, but on the other hand adapts the linear "directions" in time, in order not to continue to add modes as the manifold of the solution evolves. Moreover we analyzed the error of the DO approximate solution based on the number of modes and the discretization time step. The error is computed in norm $L^2(D) \otimes L^2_P(D)$ with respect to a numerical solution computed with the Stochastic Collocation method with a highly accurate sparse grid. Figure 3.8(right) shows that the error decreases by adding modes, and for $N > 1$ it decreasing by reducing the time discretization step size Δt. This means that the error in the stochastic space becomes negligible with respect to the time discretization error by incrementing the dimension of the linear manifold where the solution is approximated, where it seems to dominate the time-discretization error for $N \leq 4$.

3.3   Stochastic Diffusion Coefficient

We consider now the parabolic equation in (3.1) with stochastic diffusion coefficient $a \in L^\infty_P(\Omega)$ and deterministic forcing term. We assume satisfied the conditions that provide the existence of a unique solution u in $L^\infty([0, T]; H^1_0(D)) \otimes L^2_P(\Omega)$. In particular let $a(\omega)$ be a stochastic field in $L^\infty_P(\Omega)$ uniformly distributed with mean $\mu > 0$ and variance σ^2, with $\mu > \sigma$. We write $a(\omega)$ as:

$$a(\omega) = \mu + \sigma z(\omega) \qquad\qquad z(\omega) \sim \mathcal{U}(-1, 1) \qquad\qquad (3.66)$$

Figure 3.6: On the left: Modes at time $t = 0$ (blu) and time $t = 0.7$ (green), with $N = 4$ $\Delta t = 10^{-2}$, spatial discretization $h = 0.1$, $N_y = 7$ collocation points. On the right: Mean square error of the DO solution with $N = 2, 4, 10$ w.r.t. the time step.

then the problem is formulated as follows:

$$
\begin{cases}
\dfrac{\partial u(\mathbf{x}, t, \omega)}{\partial t} - \big[\mu + \sigma z(\omega)\big]\Delta u(\mathbf{x}, t, \omega) = f(\mathbf{x}, t) & \mathbf{x} \in \mathrm{D},\, t \in [0, \mathrm{T}],\, \omega \in \Omega \\[2mm]
u(\sigma, t, \omega) = 0 & \sigma \in \partial\mathrm{D},\, t \in [0, \mathrm{T}],\, \omega \in \Omega \\[2mm]
u(\mathbf{x}, 0; \omega) = u_0(\mathbf{x}, \omega) & \mathbf{x} \in \mathrm{D},\, \omega \in \Omega
\end{cases}
$$
$$(3.67)$$

According to the DO approach, we seek an approximate solution $u_N \in \mathcal{M}_N$, i.e. expanded as in (2.1), whose components $y_1, ..., y_n \in \mathrm{L}^\infty([0, \mathrm{T}], \mathrm{L}^2_P(\Omega))$ and $\bar{u}, u_1, ..., u_N \in \mathrm{L}^\infty([0, \mathrm{T}], \mathrm{H}^1_0(\mathrm{D}))$ satisfy the DO system (2.6) in weak sense. Denote with $\mathbf{u}$ and $\mathbf{y}$ the vectors of functions such that $\mathbf{u}(\mathbf{x}, t) = \big(u_1(\mathbf{x}, t), ..., u_N(\mathbf{x}, t)\big)$ and $\mathbf{y}(\omega, t) = \big(y_1(\omega, t), ..., y_N(\omega, t)\big)$ then the system reads:

$$
\begin{cases}
\dfrac{\partial \bar{u}(\mathbf{x}, t)}{\partial t} - \mu\,\Delta\bar{u} - \sigma\Delta\mathbf{u}(\mathbf{x}, t)C_{yz}(t) = f(\mathbf{x}, t) \\[3mm]
\dfrac{\partial \mathbf{u}(\mathbf{x}, t)}{\partial t}C_{yy}(t) = \prod_{\mathcal{W}_N(t)^\perp}[\Delta\mathbf{u}(\mathbf{x}, t)(\mu C_{yy}(t) + \sigma C_{yyz}(t)) + \sigma\Delta\bar{u}C_{yz}^\top(t)] \\[3mm]
\dfrac{\partial \mathbf{y}(t, \omega)}{\partial t} = [(\mu + \sigma z(\omega))\mathbf{y}(t, \omega) - \sigma C_{yz}^\top(t)] <\Delta\mathbf{u}^\top(\cdot, t),\, \mathbf{u}(\cdot, t) > \\[3mm]
\qquad\qquad\qquad\qquad\qquad\qquad + \sigma z(\omega) <\Delta\bar{u}(\cdot, t),\, \mathbf{u}(\cdot, t) >
\end{cases}
$$
$$(3.68)$$

with Dirichlet boundary conditions and initial condition given by:

$$\bar{u}(\sigma, t) = 0,\ \forall \sigma \in \partial\mathrm{D},\, t \in [0, \mathrm{T}]$$

$\mathbf{u}(\sigma, t) = 0 \; \forall \sigma \in \partial \mathrm{D}, \; t \in [0, \mathrm{T}]$

$\bar{u}_0(\mathbf{x}) = \mathbb{E}[u_0(\mathbf{x}, \omega)]$ for all $\mathbf{x} \in \mathrm{D}$,

$\mathbf{u}_0(\mathbf{x})$ given by the first N eigenfunctions of the correlation operator $\Gamma_{u(0)u(0)}$,

$\mathbf{y}_0(\omega) = < u_0(\cdot, \omega), \mathbf{u}_0 >$ with $\omega \in \Omega$.

and where we have defined:

- $C_{yz}(t) = \mathbb{E}[z\mathbf{y}^\top(t, \cdot)]$,

- $C_{yy}(t) = \mathbb{E}[\mathbf{y}^\top(t, \cdot)\mathbf{y}(t, \cdot)]$,

- $C_{yyz}(t) = \mathbb{E}[z\mathbf{y}^\top(t, \cdot)\mathbf{y}(t, \cdot)]$

The weak formulation yields:

. *for any $t \in [0, \mathrm{T}]$, find $\bar{u}(\cdot, t) \in \mathrm{H}_0^1(\mathrm{D})$, $\mathbf{u}(\cdot, t) \in [\mathrm{H}_0^1(\mathrm{D})]^N$ and $\mathbf{y}(t, \cdot) \in [\mathrm{L}_P^2(\Omega)]^N$ such that:*

$$
\begin{cases}
< \dfrac{\partial \bar{u}(\cdot, t)}{\partial t}, \psi_i > + \mu < \nabla \bar{u}(\cdot, t), \nabla \psi_i > + \sigma < \nabla \mathbf{u}(\cdot, t), \nabla \psi_i > C_{yz}(t) = f(\mathbf{x}, t) \\[2mm]
< \dfrac{\partial \mathbf{u}(\cdot, t)}{\partial t}, \psi_k > C_{yy}(t) + \mathbf{p}(\mathbf{u}(\cdot, t), \mathbf{u}(\cdot, t), \psi_k)[\mu C_{yy}(t) + \sigma C_{yyz}(t)] \\[2mm]
\qquad\qquad\qquad\qquad\qquad + \sigma \mathbf{p}(\mathbf{u}(\cdot, t), \bar{u}(\cdot, t), \psi_k) C_{yz}^\top(t) = 0 \\[2mm]
\dfrac{\partial \mathbf{y}(t, \omega)}{\partial t} - [(\mu + \sigma z(\omega)) \mathbf{y}(t, \omega) - \sigma C_{yz}^\top(t)] < \nabla \mathbf{u}^\top(\cdot, t), \nabla \mathbf{u}(\cdot, t) > \\[2mm]
\qquad\qquad\qquad\qquad\qquad - \sigma z(\omega) < \nabla \bar{u}(\cdot, t), \nabla \mathbf{u}(\cdot, t) > = 0
\end{cases}
$$
$$(3.69)$$

for all $\psi_i, \psi_k \in \mathrm{H}_0^1(\mathrm{D})$ and for a.e. $\omega \in \Omega$; where $\mathbf{p}(\cdot, \cdot, \cdot)$ is defined as in (3.42).

Similarly to what described in the section 3.2.2, the physical space is discretized with the Finite Element method, while the stochastic differential equations are solved by the Stochastic Collocation method. The time derivative is discretized by the semi-implicit Euler method and the covariance matrix is treated explicitly in order to decouple the equations defined in the physical domain from those defined in the probability space. Moreover the projection operator is evaluated at the previous time step to recover the linearity of the problem. Specifically, by adopting the same notation as in section 3.2.4, the discretized problem can be written in algebraic form as follows:

$$
\begin{cases}
\mathbb{M}\bar{U}^{n+1} + \Delta t \mu \mathbb{K} \bar{U}^{n+1} + \Delta t \sigma \mathbb{K} U^{n+1} \mathbb{C}_{yz}^n = \mathbb{M}\bar{U}^n + \Delta t F^n \\[1mm]
\mathbb{M} U^{n+1} \mathbb{C}^n + \Delta t P^n \mathbb{K} U^{n+1}(\mu \mathbb{C}^n + \sigma \mathbb{C}_{yyz}^n) + \sigma \Delta t P^n \mathbb{K} \bar{U}^{n+1} \mathbb{C}_{yz}^n = \mathbb{M} U^n \mathbb{C}^n \\[1mm]
Y^{n+1} + \Delta t (\mu + \sigma Z) U^{n+1\top} \mathbb{K} U^{n+1} Y^{n+1} = Y^n \\[1mm]
\qquad\qquad + \mu \Delta t U^{n+1\top} \mathbb{K} U^{n+1} \mathbb{C}_{yz}^n - \sigma \Delta t \bar{U}^{n+1\top} \mathbb{K} U^{n+1} Z
\end{cases}
$$
$$(3.70)$$

where in particular Z is the vector of the values of z in the collocation points, $\mathbb{Q}$ is a matrix of dimension $N \times N$ defined as $\mathbb{C}_{yyz}^n = \mathbb{E}[(\mathbf{y}^n)^\top \mathbf{y}^n z]$, $\mathbb{C}_{yz}$ is the column vector $\mathbb{E}[(\mathbf{y}^n)^\top z]$ and P^n is the discrete projection operator in the subspace $\mathcal{W}_N(t^n)$, i.e. $P = (\mathbb{I} - \mathbb{M}U^n(U^n)^\top)$.

We remark that, contrary to the case in which the diffusion term is a deterministic real value, here the equations for the mean function and the modes are all coupled. In particular the equation for the mean filed $\bar{u}$ is coupled to the equations for the other spatial modes.
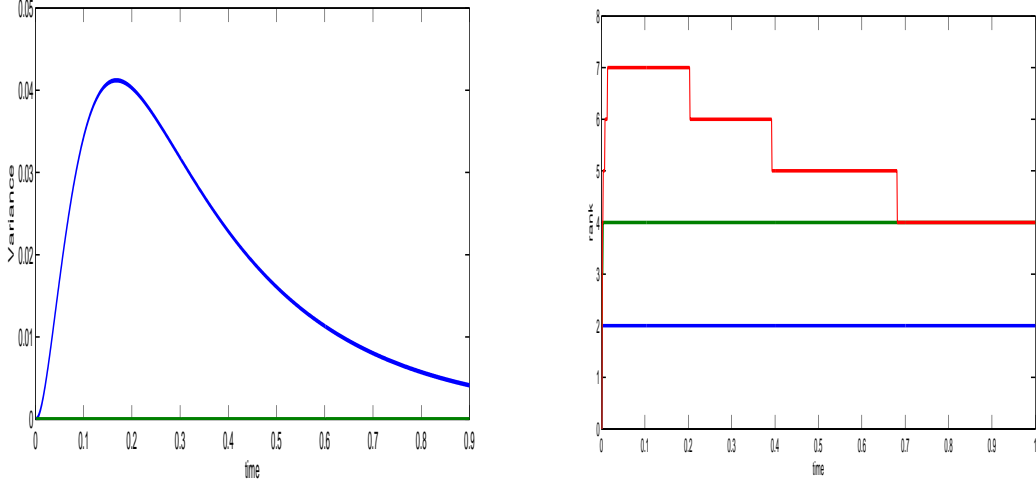

Figure 3.7: On the left: Numerical test 3.3.1 **special initial condition**: Time evolution of the variance of the stochastic coefficients with $N = 4$ $\Delta t = 10^{-2}$, spatial discretization $h = 0.1$, $N_y = 9$ collocation points. On the right: Numerical test 3.3.1 **general initial condition**: Time evolution of the rank of the covariance matrix associated to the DO solution with $N = 2, 4, 8$, $N_y = 9$ collocation points.

3.3.1   Numerical Tests

Special initial condition

Consider the problem governed by the following stochastic *PDE*:

$$\begin{cases} \dfrac{\partial u(x,t;\omega)}{\partial t} - \beta(\omega)\Delta u(x,t;\omega) = 0 & x \in (0,\,10),\, t \in \mathrm{T},\, \omega \in \Omega \\ u(0,t;\,\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\ u(10,t;\,\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\ u(x,0;\,\omega) = u_0(x) & x \in (0,\,10),\, \omega \in \Omega \end{cases}$$

$$(3.71)$$

where $\beta(\omega)$ is a uniform random variable $\mathcal{U}(\mu, \sigma^2)$ with $\mu > 0$. Let $\beta(\omega)$ be reformulated as $\mu + \sigma z(\omega)$ with $z \sim \mathcal{U}[-1, 1]$. We consider first a particular initial condition that is
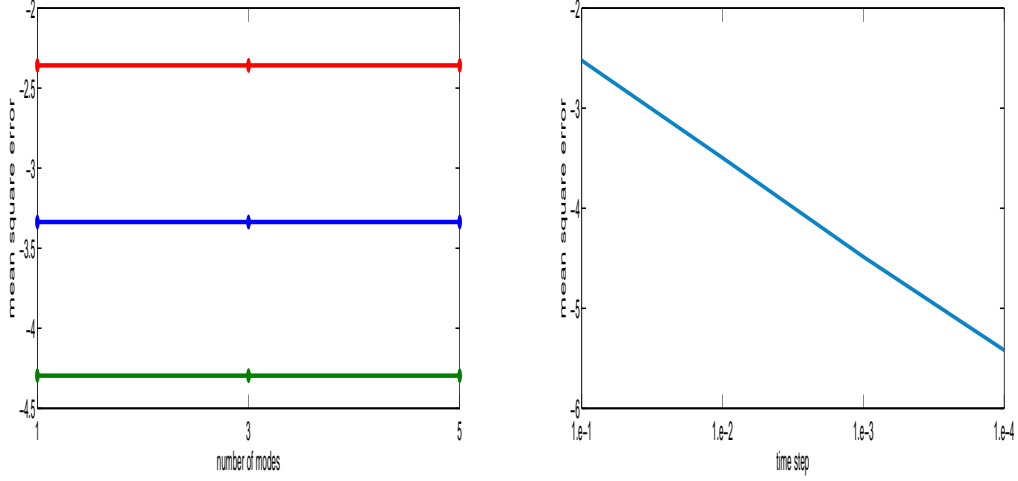
Figure 3.8: On the left: The mean square error of the DO approximate solution with $\Delta t = 10^{-1}$ (red), $\Delta t = 10^{-2}$ (blu), $\Delta t = 10^{-3}$ (green) $N_y = 7$ collocation points. On the right: Mean square error of the DO approximate solution w.r.t. to the time step, $N_y = 7$, $N = 1$.

assumed to coincide with an eigenfunctions of the Laplace operator. Specifically it is defined as:

$$u_0(x) \;=\; \sqrt{\frac{1}{5}}\sin\left(\frac{\pi x}{5}\right) \tag{3.72}$$

Even if the initial condition is deterministic the solution is immediately affected by the stochasticity of the system at $t > 0$ and evolves in a 1 dimensional manifold generated by u_0. It reads:

$$u_{ex}(x,t;\omega) \;=\; e^{-\beta(\omega)\frac{\pi^2}{25}t}\sqrt{\frac{1}{5}}\sin\left(\frac{\pi x}{5}\right) \tag{3.73}$$

and in particular the exact mean function and the total variance are given by:

$$\bar{u}_{ex}(x,t) = \frac{25}{2\sigma^2\pi^2 t}e^{-(\mu+\sigma^2)\frac{\pi^2}{25}t}\left(e^{\sigma^2\frac{2\pi^2}{25}t} - 1\right)\sqrt{\frac{2}{10}}\sin\left(\frac{2}{10}\pi x\right)$$

$$\mathbb{V}ar_{ex}(t) = \frac{25}{4\sigma^2\pi^2 t}e^{-(\mu+\sigma^2)\frac{2\pi^2}{25}t}\left(e^{\sigma^2\frac{4\pi^2}{25}t}\left(1 - \frac{25}{\sigma^2\pi^2 t}\right) - 1 - \frac{25}{\sigma^2\pi^2 t} + \frac{50}{\sigma^2\pi^2 t}e^{\sigma^2\frac{2\pi^2}{25}t}\right) \tag{3.74}$$

The analytic solution suggests that the DO method degenerates to the POD method. First of all, according to the DO expansion, the initial datum is reformulated as in (2.1) so that:

- $\bar{u}(x,0) = u_0(x)$,

- $u_1(x,0),...,u_N(x,0)$ correspond to the first N eigenfunctions of the Laplace operator,

- $y_1(0, \omega), ..., y_N(0, \omega)$ are identically equal to zero.

and the DO method leads to a system as in (3.69). Before discussing the numerical results we observe that the analytical solution in (3.73) can be rewritten as:

$$u_{ex}(x, t; \omega) = \bar{u}_{ex}(x, t) + y_1(t; \omega)u_1(x, 0) \qquad (3.75)$$

that leads us to expect only the first stochastic coefficient to evolve. This is confirmed by the numerical results which can be summarized as follows:

- The modes do not evolve. For what concerns the system of PDEs, at each time iteration only 2 equations are actually solved: the one for the mean function and the one for the first mode because this is the only one filed associated to a non-zero eigenvalue.

- All the stochastic evolution is described by the first random coefficient while the others remain equal to zero, independently of the number of modes N. The variance of y_1, initially zero, grows up as soon as the solution evolves and then it is dissipated and goes to zero as the solution tends to zero, Figure: 3.7 (left);

- the rank of the covariance matrix is equal to zero at the first time iteration since the initial condition is deterministic and then is steadily equal to one because the solution is affected by the randomness of the operator as soon as it evolves. When the solution goes to zero all the stochasticity is dissipated, the solution tends to a deterministic function and the covariance matrix returns to be identically equal to zero.

We conclude that the manifold of the solution, which has dimension equal to 1 but that does not evolve linearly in time (as one can analytically verify in (3.73)), can be approximated by the rank 1 DO approximate solution, which instead describes a linear manifold of dimesnion one. Figure 3.8 (left) indeed shows that the error of the DO approximate solution, in mean square sense, does not depend on the number of modes and the order of convergence is established by the time discretization step size, see Figure 3.8 (right).

Special initial condition in a 2D spatial domain

Now we are going to verify if the results of the previous section are influenced by the dimension of the physical space. We consider a problem analogous to (3.71) in a bi-dimensional spatial domain $D = [0, 1]^2$. Assume that the initial condition is:

$$u_{0\mathbf{i}}(\mathbf{x}) = \sqrt{2}\sin(\pi x_1)\sin(\pi x_2)\sum_{\mathbf{i}=i_1,i_2}^{N} y_{\mathbf{i0}}(\omega)\sqrt{2}\sin(i_1\pi x_1)\sin(i_2\pi x_2), \qquad (3.76)$$

where $\mathbf{i}$ is a multi-index, N is the number of the deterministic basis functions and all the stochastic coefficients are initialized to zero. Analogously to the mono-dimensional
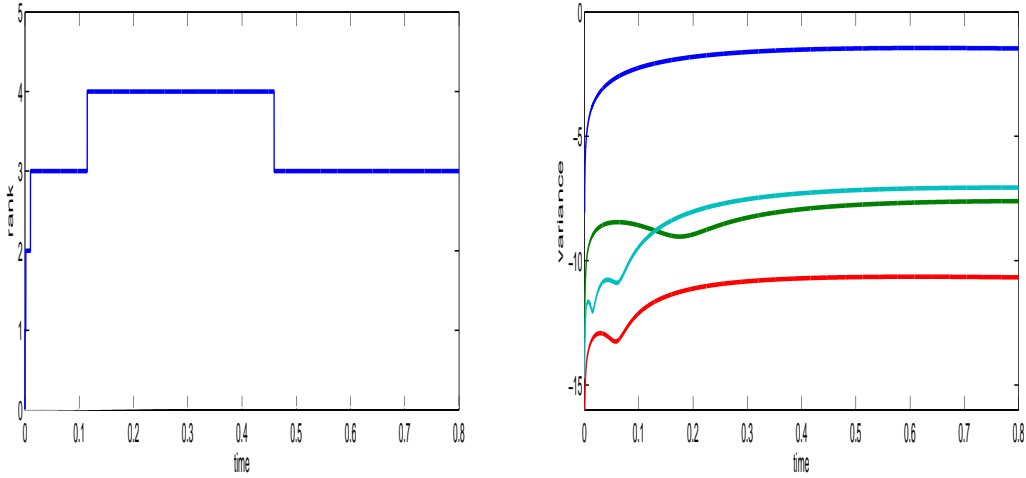
Figure 3.9: On the left: Time evolution of the rank of the covariance matrix with $N = 4$, $\Delta t = 10^{-2}$, spatial discretization $h = 0.05$, $N_y = 5$ collocation points. On the right: Time evolution of the variance of the stochastic coefficient of the DO approximate solution with $N = 4$, $\Delta t = 10^{-2}$, $N_y = 5$ collocation points (log. scale).

problem, the solution is in a manifold of dimension 1, since only one random variable is involved which however is non linear. We computed the DO approximate solution with N between 1,...,10. Figure 3.9 (left) shows that the rank of the covariance matrix in this case increases in time. On the other hand Figure 3.9 (right) displays that there is a gap between the variance of the random coefficients and only one of them develops remarkable variance. This means that the solution can be approximated with only one mode by dropping the stochastic coefficients with negligible variance. This is confirmed in Figure 3.10 (left) which shows that the mean square error does not depend on the number of modes, or rather the error in the stochastic space is negligible compared to the spatial and temporal discretization error. These considerations concern the approximate solution computed with 5 collocation points, moreover we aim to verify if this parameter influences the approximation. Figure 3.10 (right) shows that the error increases when reducing the number of collocation points and may dominate the time discretization error for small Δt. However it does not change by adding modes, Figure 3.10 (left).

General initial condition

We consider again the problem (3.71) but with a more general initial condition. Specifically we chose:

$$u_0(x) = \frac{1}{100}x(x - 10)^2 \tag{3.77}$$

Observe that the initial datum is deterministic but it can not be expressed in terms of a finite number of eigenfunctions of the Laplace operator. According to the DO expansion, the initial datum is reformulated as in (2.1) with:
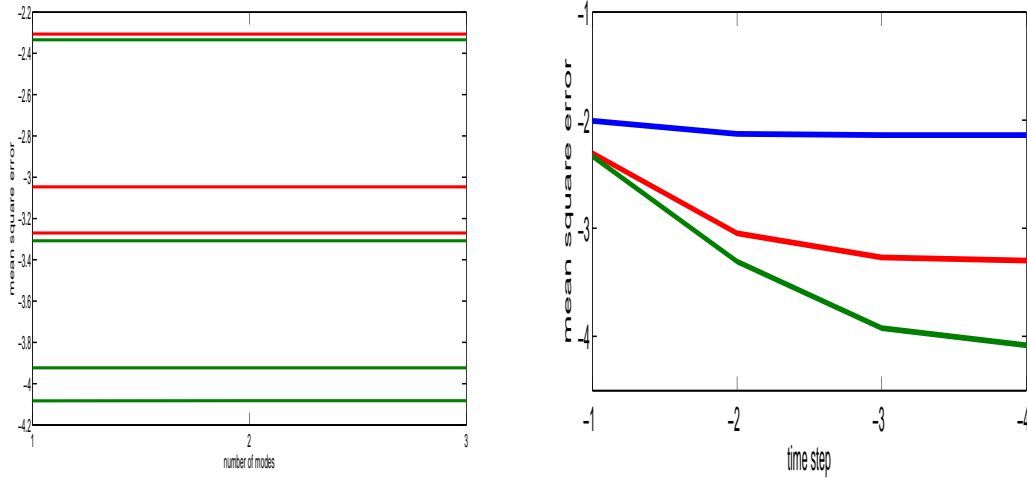
Figure 3.10: On the left: Error of the DO approximate solution w.r.t the time step and with number of collocation points $N_y = 2$(green), $N_y = 3$ (red), $N_y = 5$(green). On the right: Error of the DO approximate solution with number of collocation points $N_y = 3$ (red), $N_y = 5$(green) and with $\Delta t = 10^{-1}$, $\Delta t = 10^{-2}$, $\Delta t = 10^{-3}$.(log-log scale)

- $\bar{u}(x,0) = u_0(x)$,

- $u_1(x,0), ..., u_N(x,0)$ corresponding to the first N eigenfunctions of the Laplace operator,

- $y_1(0,\omega), ..., y_N(0,\omega)$ are identically equal to zero.

and the DO system is defined as in (3.69). In particular the covariance matrix is identically equal to zero at the first time iteration, being the initial condition deterministic. Contrary to case of deterministic operator and stochastic data analyzed in section 3.2, the stochastic diffusion term generates a non linearity in the stochastic space. Because of this the solution of (3.71) evolves in a non linear manifold. In addition the manifold evolves in time, as u is solution of a time-dependent problem. However the dimension remains equal to 1, since only one random variable is involved in the differential operator and no stochasticity comes from the initial datum. The DO approach provides a linear approximation of the solution in which the effective dimension coincides with the rank of the covariance matrix associated to the random coefficient. In view of this it is important to understand how the rank evolves in time with respect to the number of modes and collocation points, because this tells us the dimension of the linear manifold where the solution can be approximated. Numerical tests confirm that the rank of the covariance matrix grows up at the second time iteration in order to generate a stochastic subspace able to describe the process evolution. However we see that the rank remain bounded. It increases up to a maximum values and then it decreases to zero when the solution goes asymptotically to the deterministic function zero. The maximum value achieved obviously depends on the number N of basis functions selected initially, as well as on the
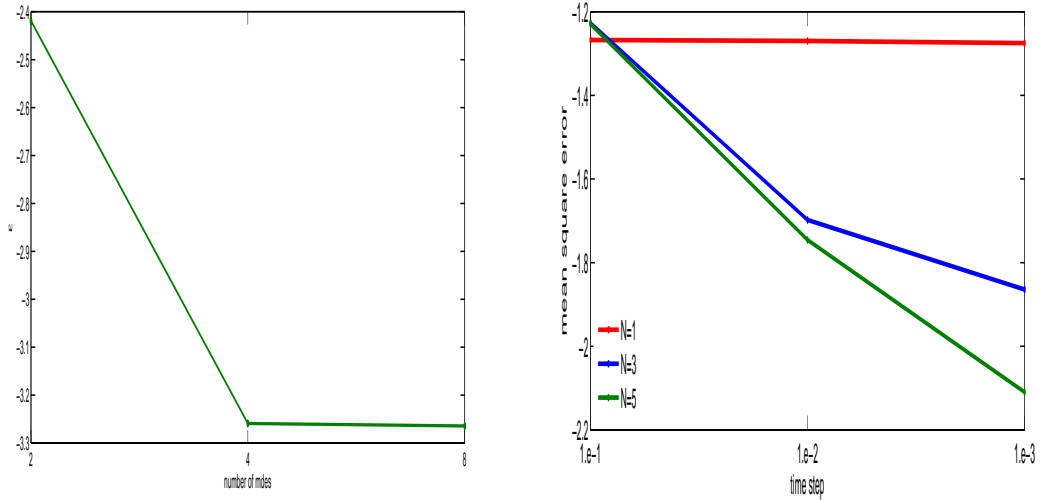
Figure 3.11: On the left: Approximation error $\epsilon(t)$ of the DO solution with $N_y = 9$ compared to the solution of the Stochastic Collocation method with $N_y = 20$, w.r.t. N, at $t = 0.7$. $\Delta t = 10^{-2}$, spatial discretization $h = 0.1$. On the right: Error of the DO solution in mean square sense, w.r.t the time step and with $N = 1, 3, 5$, $N_y = 9$ and spatial discretization $h = 0.1$. (log.scale)

number of collocation points used to solve the stochastic system, specifically:

$$0 \leq rank(\mathbb{C}) \leq min(N, N_y) \tag{3.78}$$

As shown in Figure 3.7 (right), in the case we are analyzing the rank reaches the saturation level for $N = 7$. It means that it does not increase any further, even if one increases the number of the collocation points and basis functions. This tells us that the manifold of the solution, which, we remark, evolves non-linearly in time, can be approximated by 7 modes. They evolve in time by spanning the new "directions" along which the solution evolves, and no any other mode give contribution to the approximation. We verify the consistency of the analysis concerning the rank of the covariance matrix by computing the error of the DO approximation in the stochastic space. This is estimated by comparing the DO approximate solution to the solution u^{sc} of the Stochastic Collocation method with highly accurate sparse grid. In Figure 3.11 (left) the error $\epsilon(t) = \mathbb{E}[\|u_N(\cdot, t, \cdot) - u_N(\cdot, t, \cdot)\|_L^2(\mathrm{D})]$ at $t = 0.7$. The results confirm that no improvement are achieved by using $N > 4$, in accordance with the rank of the covariance matrix at that time step, see Figure 3.7 (right). However it is important to understand how the accuracy of the approximation degrades if we uses a number of modes N lower than the saturation level of the covariance matrix. In fact the goal of the DO approach consists in approximating the solution by using few basis functions possibly and in light of that we aim to reduce the dimension of the approximation by dropping out all the components which do not give remarkable contribution. In Figure (3.11) (left) we compute the approximation error in norm $\mathrm{L}^2(\mathrm{D}) \times \mathrm{L}_P^2(\Omega)$ of the DO solution with different number of modes and with different time step. We observe that the error in the stochastic space
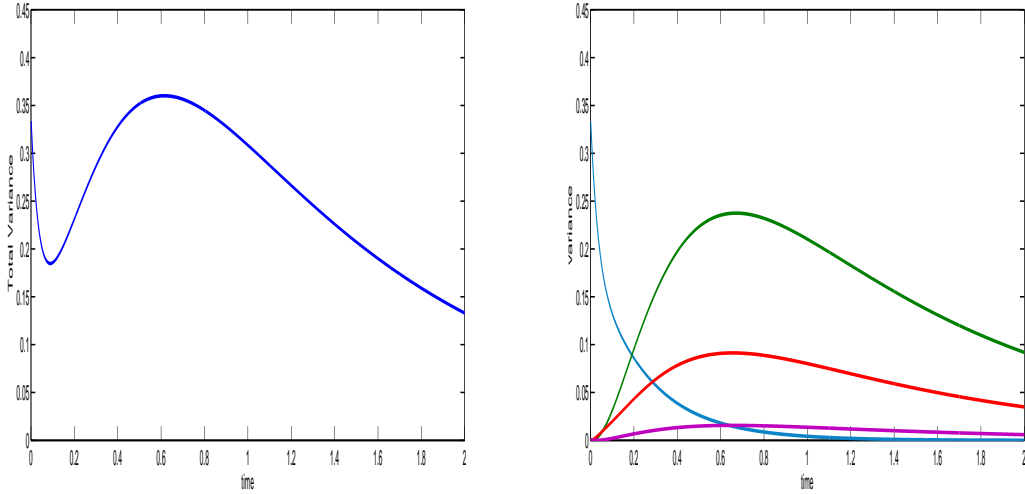
Figure 3.12: On the left: Time evolution of the total variance of the exact solution. On the right: Time evolution of the variance of the stochastic coefficients in the DO expansion for the approximate solution with $N = 4$.

dominate the time discretization error with $N = 1$ and then decreases by adding modes up to the saturation level.

Bi-dimensional stochastic space

We consider now the case in which both the diffusion term and the initial condition are stochastic variables. In particular the problem reads:

$$\begin{cases} \dfrac{\partial u(x,t;\omega)}{\partial t} - \beta(\omega)\Delta u(x,t;\omega) = 0 & x \in (0,\,10),\, t \in \mathrm{T},\, \omega \in \Omega \\ u(0,t;\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\ u(10,t;\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\ u(x,0;\omega) = u_0(x) + z(\omega)\sqrt{\dfrac{1}{5}}\sin\left(\dfrac{\pi x}{5}\right) & x \in (0,\,10),\, \omega \in \Omega \end{cases}$$

$$(3.79)$$

with $u_0(x) = \frac{1}{100}x(x-10)^2$ and where z, β are independent uniform random variables, $z(\omega) \sim \mathcal{U}(\mu_2, \sigma_2^2)$ and $\beta(\omega) \sim \mathcal{U}(\mu_1, \sigma_1^2)$, with $\mu_1 > 0$. Since the random variables are independent, the stochastic space and consequently the manifold where the solution "lives" have dimension 2. The DO approximate solution is then expected to have rank at least 2. Moreover the manifold of the exact solution is not linear. In Figure 3.14(left) one can see that the rank of the covariance matrix associated to the DO solution increases up to 8, when $N \geq 8$. We observe that this is an upper bound, which means that the rank does not go over 8 independently of N and the number of the collocation points. Furthermore Figure 3.12(right) shows that only few stochastic variables have remarkable variance, which means that the solution can be approximated in a linear manifold of low
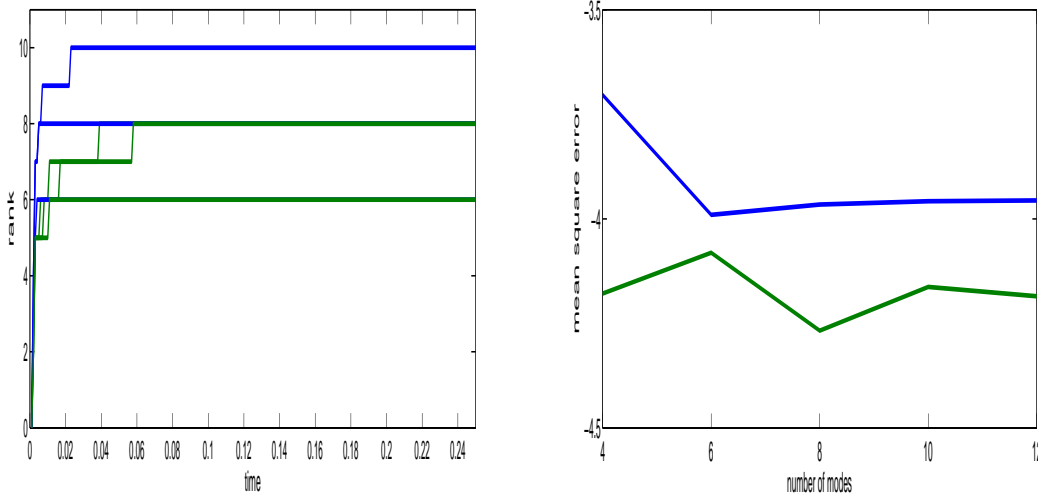
Figure 3.13: On the left: Time evolution of the rank of the DO approximate solution with $N = 4, 6, 8, 10$ and number of collocation points $N_y = 5^2$ (blu) and $N_y = 3^2$ (green). On the right: Error of the DO approximate solution computed with a number of collocation points $N_y = 5^2$ (blu) and $N_y = 3^2$ (green), compared to the solution of the Stochastic Collocation method with $N_y = 15^2$ in mean square sense.

dimension with good accuracy, as one can see in Figure 3.14(right). The error decreases according to the time step, which implies that the error in the stochastic space is negligible compared to the time discretization error for $N \geq 4$, in accordance to the time evolution of the variance of the stochastic variables in Figure 3.12(right).

Reaction term with stochastic coefficient

We conclude this section with a more challenging example in which both the coefficients of the diffusion and reaction terms are stochastic variables:

$$\begin{cases} \dfrac{\partial u(x,t;\,\omega)}{\partial t} - \beta(\omega)\Delta u(x,t;\,\omega) = \delta(\omega)F(u(x,t;\omega)) & x \in (0,\,10),\, t \in \mathrm{T},\, \omega \in \Omega \\ \dfrac{\partial u}{\partial x}(0,t;\,\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\ \dfrac{\partial u}{\partial x}(10,t;\,\omega) = 0 & t \in \mathrm{T},\, \omega \in \Omega \\ u(x,0;\,\omega) = \begin{cases} 1 & x \leq 5 \\ 0 & x > 5 \end{cases} & \omega \in \Omega \end{cases}$$

$$(3.80)$$

where $F(u) = u(u-1)(\alpha-u)$ with $\alpha \in (0,1)$, $\beta(\omega)$ and $\delta(\omega)$ are two uniform independent random variables. The solution is then described by a bi-dimensional manifold that is strongly not linearly, since the reaction term is a cubic polynomial. In the previous example we have seen that by increasing the number of modes, and equivalently the dimension of the linear manifold where we approximate the solution, we can improve the accuracy
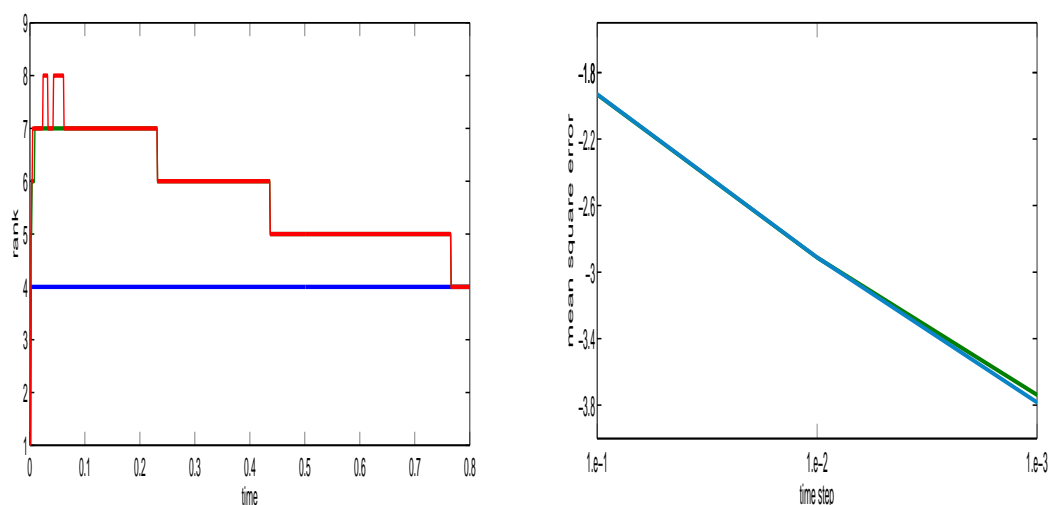
Figure 3.14: On the left: Time evolution of the rank of the DO approximate solution with $N = 4, 8, 12$, $\Delta t = 10^{-3}$, number of collocation points $N_y = 15$. On the right: Error of the DO approximate solution in mean square sense, w.r.t the time step and with $N = 4, 5$, number of collocation points $N_y = 5^2$

of the approximation, up to the saturation level of the covariance matrix. However the number of collocation points represents an other important parameter that influences the approximation, since the stochastic coefficients and, consequently the approximate solution, are approximated in a polynomial space using the evaluations in the collocation points. Figure 3.13(left) shows that the increasing trend of the rank of the covariance matrix is indeed influenced by the number of collocation points, and consequently also the accuracy of the approximate solution. We compared the solution of the DO and Stochastic Collocation method, this one computed with a highly accurate sparse grid, in order to quantify the influence of this parameter. Figure 3.13(right) shoes the error, in mean square sense, of two DO approximate solutions, computed with a stochastic tensor grid with respectively 3 and 5 collocation point per axis, compared to the solution of the Stochastic Collocation method that uses 15 points. One can see that the error of the DO approximate solution decreases by using a more accurate stochastic grid. This can be explained by reminding that the DO approximate solution tends to coincide to the solution of the Stochastic Collocation method by increasing N up to the number of collocation points. Then with a large number of modes the convergence rate depends on the number of collocation points in the same way as that of the Stochastic Collocation method.

Chapter 4

Stochastic Reaction-Diffusion Equations: application to the electrocardiology

In this chapter we focus on parabolic differential equations with non linear reaction term describing the electric signal in biological tissues. After discussing the probabilistic approach, we are going to verify the effectiveness of the DO method to this type of equations.

4.1 Cardiac Electrical Activity and Mathematical Models

The heart is a muscular organ that acts as a pump. The flow of ions across the cell membranes causes electrical impulses that give rise to perpetuating waves of excitation. The wave spreads through the whole heart and enables the impulse to travel from a cell to another. This excitation state and its spread is what coordinates and feeds the contractions of the cardiac cells. From a macroscopic point of view, this is essentially what happens when blood is pumped to the body. However this process depends on several parameters and it is correlated to many other sub-process. This makes the problem quite complex to modelize.
Cardiac cells have two features linked each other: they have a contractile ability and they are excitable. The action of the mechanical function is caused by electrical signals that propagate in the tissue while the propagation is allowed by the excitability of the cells. The stimulation arises in the sinoatrial node where the pacemecker cells generate the electric pulse that determines the heart beat. When an excitable cell is activated the membrane potential of that cell generates the so-called *action potential*. It is caused by a potential difference that gives rise to transfer of ionic charges. When the local depolarization reaches a certain threshold the action potential starts and the impulse is transmitted to neighboring cells. For details [29].
The Hodgkin Huxley and subsequently many other models have been developed to de-

scribe the action potential of a single cell. They consist on biophysically-based model and reproduce the action potential by modeling the underlying sub-cellular processes. An alternative to this complex approach is provided by non-biophysical models, among which the most known is probably the FitzHugh-Nagumo one. These simplified models aim at describing the "qualitative" features of the action potential without attempting to address the underlying bio-physiological processes. For details [28].

4.2   Traveling waves

A traveling wave is a solution that travels at constant speed with fixed shape. We recall two types of traveling waves in excitable systems. The first one, called traveling front, is characterized by two steady levels: some low value in front of the wave and some higher value behind the wave. On the contrary, the other one can be described as a curve that begins and end at the same value. It means that a recovery phase, which follows the excitation, takes the wave back to the initial state. This is called traveling pulse.
In other words a traveling front acts like a zipper switching from resting to exciting state. If the recovery variable can force back the solution to the steady state we have the traveling pulse.
We focus on the traveling front without considering the recovery variable, or equivalently by assuming it fixed to the steady state. The evolution of a traveling front is described by the bistable equation, so called because it has two stable rest points. It is related to the $FitzHugh - Nagumo$ model, without recovery, described in the next section.

4.2.1   Travelling fronts: Bistable equation

The Bistable equation is a spacial case of Cable equation and it consists in a parabolic PDE, with non linear reaction term, i.e.:

$$\frac{\partial u}{\partial t} - \Delta u = f(u) \tag{4.1}$$

where $f(u)$ is assumed to be a cubic polynomial. We assume $f(u)$ having the zeros at 0, 1 and α, with $\alpha \in (0,1)$. The first two zeros are stable which means that $u = 0$ and $u = 1$ are the steady equilibriums of the PDE. The other zero α is instead repulsive. The dynamics of the solution is described by the transition between the two steady states. This feature makes u a travelling front. The reaction term can be written in the following form:

$$f(u) = Au(u-1)(\alpha - u) \qquad \alpha \in (0,1) \tag{4.2}$$

where A is a constant that determines the speed of the wave.
We have seen that the excitable dynamics comes from the reaction term and in particular for large A the reaction dominates the diffusion. This generates dynamics characterized by sharp fronts.
Analytic solution can be obtained only for particular initial conditions. This makes the wave propagation in the $FitzHugh - Nagumo$ model not completely understood

yet, especially with multidimensional spatial domain. On the other hand the numerical approach can achieve good results even if small discretization time step and specific numerical treatment are often required to handle with the reaction term which, beside generating sharp slops and fast dynamics, is not linear.

We start the analysis from the mono-dimensional case for which an analytic solution can be derived. This enables us to understand how the parameters influence the dynamic and which implications we should expect by considering them as stochastic variables. Furthermore it give us the opportunity to test the quality of the numerical results.

Let us consider the problem in a mono-dimensional domain:

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f(u) \tag{4.3}$$

Since the traveling front is a wave that travels with constant speed c, we seek a solution of the form:

$$u(x,t) = v(x + ct) \tag{4.4}$$

Denoting with ξ the new variable $\xi = x + ct$, the *PDE* 4.3 becomes:

$$cv'' - v' = f(v) \tag{4.5}$$

After solving the previous ordinary differential equation, for details ([29]), we conclude that the problem 4.3 with initial condition $u(x,0) = \frac{1}{2} + \frac{1}{2}\tanh\left(\frac{\sqrt{A}}{2\sqrt{2}}x\right)$ have the following analytic solution:

$$u(x,t) = \frac{1}{2} + \frac{1}{2}\tanh\left(\frac{\sqrt{A}}{2\sqrt{2}}(x + ct)\right) \tag{4.6}$$

where the speed c is given by:

$$c = \sqrt{\frac{A}{2}}(1 - 2\alpha) \tag{4.7}$$

Observe that the speed of the propagation depends on α, that is the repulsive zero of the reaction function $f(u)$. In particular the speed decreases as α tends to 0.5, value for which the direction of the wave propagation changes.

Stochastic approach

From a biological point of view the PDE in (4.1) models the ionic current through the cellular membranes and the inter-cellular space and provides a macroscopic description of the action potential avoiding to directly involve the related sub-cellular processes. It represents an alternative to the biophysically based models which detail several cellular interactions by adding more and more functions. The constant A represents the excitation rate and α is the normalized threshold potential value. They depend on several variables among which the membrane capacitance, the membrane resistance, cytoplasmic resistance, cell diameter and clearly the ionic channel conductances. All these parameters

are largely uncertain and such uncertainty should be properly included in the deterministic model. The fitting of parameters requires sophisticated anatomical, physiological, biological and clinical experimental programs that not only are difficult to achieve but are also very prone to noises. In addition the parameters depend on each individual and they may change in time, as consequence of many situations among which diseases, stress, diet and so on. By considering stochastic parameters we can achieve comprehensive analysis which incorporate the uncertainty that is intrinsically part of the problem as well that which comes from the measurement.

For what concerns the bistable equation, the problem can be formulated as follows:

$$\begin{cases} \dfrac{\partial u}{\partial t} - \Delta u = A(\omega)u(u-1)(\alpha(\omega) - u) \\ u_{|t_0} = u_0(\mathbf{x}, \omega) \end{cases} \tag{4.8}$$

where the solution $u(\mathbf{x}, t, \omega)$ is a stochastic process and the parameters, the initial condition or both of them are stochastic.

4.3   Bistable Equation: DO approach

In this section we apply the DO approach to the stochastic bistable equation. After provided the DO formulation of the problem and the computational details, we discuss the numerical results by distinguish two typologies of problem: in the first the stochasticity is intrinsically part of the operator in the governing equations, in the second the randomness is totally generated by the initial condition. We aim to investigate if and in which cases the low rank approximation is a suitable approach to approximate excitable systems as in (4.8), and how the source of uncertainty affects the answer.

4.3.1   DO formulation

We consider the stochastic problem governed by $SPDE$ in (4.8) with Neumann boundary conditions. We remind that the DO approach computes an approximate solution in $\mathcal{M}_N$, the subspace of all the N rank stochastic fields, by projecting at each time instant the residual of the equation (4.8) onto $\mathcal{T}_{u(t)}\mathcal{M}_N$ that is the tangent space to $\mathcal{M}_N$ at $u_N(t)$. In the specific case of the stochastic bistable equation the DO method results in solving the following system:

$$\begin{cases} \dfrac{\partial \bar{u}(\mathbf{x}, t)}{\partial t} - \Delta \bar{u}(\mathbf{x}, t) = \mathbb{E}[f(u(\mathbf{x}, t; \omega); \omega)] \qquad\qquad \mathbf{x} \in \mathrm{D},\, t \in [0, \mathrm{T}],\, \omega \in \Omega \\[2ex] \sum_{i=1}^{N} \dfrac{\partial u_i(\mathbf{x}, t)}{\partial t} C_{y_i y_j}(t) = \prod_{\mathcal{W}_N^{\perp}} \sum_{k=1}^{N} \left[\Delta u_k(\mathbf{x}, t) C_{y_k y_j}(t) + \mathbb{E}[f(u(\mathbf{x}, t; \omega); \omega) y_j(t; \omega)] \right], \\[1ex] \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall\, j = 1, ... N \\[1ex] \dfrac{dy_i(t, \omega)}{dt} = \; < \sum_{k=1}^{N} \Delta u_k(\mathbf{x}, t) y_k(t, \omega) + f(u(\mathbf{x}, t; \omega); \omega) - \mathbb{E}[f(u(\mathbf{x}, t; \omega); \omega)],\, u_i(\mathbf{x}, t) > \\[1ex] \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall\, i = 1, ..., N \end{cases}$$

$$\tag{4.9}$$

with the following boundary conditions:

$$\frac{\partial \bar{u}}{\partial n}(\sigma, t) = 0 \qquad \sigma \in \partial D,\ t \in [0, T]$$
$$\frac{\partial u_i}{\partial n}(\sigma, t) = 0 \qquad \forall i = 1, ..., N$$

where n denotes the normal to the boundary ∂D, and with initial conditions given by:

- $\bar{u}_0(\mathbf{x}) = \mathbb{E}[u_0(\mathbf{x}, \omega)]$ for all $\mathbf{x} \in D$,

- $\{u_{0i}(\mathbf{x})\}_{i=1,...N}$ that are the first N eigenfunctions of the correlation operator $C_{u(0)u(0)}$,

- $y_{i0}(\omega) = <u_0(\cdot, \omega),\ u_{0i}>$ with $\omega \in \Omega$ and for any $i = 1, ...N$.

System (4.9) consists in $N + 1$ deterministic $PDEs$ coupled to N stochastic $ODEs$ and the approximate solution is recovered as:

$$u_N(\mathbf{x}, t;\ \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N} y_i(t;\ \omega) u_i(\mathbf{x}, t) \qquad (4.10)$$

being N the dimension of the manifold in which the solution u of (4.8) is approximated. We assume $\bar{u},\ u_1, ..., u_N \in \mathrm{L}^\infty([0,\ \mathrm{T}],\ \mathrm{H}^1(D)$ and $y_1, ..., y_N \in \mathrm{L}^\infty([0,\ \mathrm{T}],\ \mathrm{L}_P^2(\Omega)$. Denoted with $\mathbf{u}$ and $\mathbf{y}$ the vector of functions such that $\mathbf{u}(\mathbf{x}, t) = \big(u_1(\mathbf{x}, t), ..., u_N(\mathbf{x}, t)\big)$ and $\mathbf{y}(\omega, t) = \big(y_1(\omega, t), ..., y_N(\omega, t)\big)$ the weak formulation of (4.9) reads: for any $t \in [0,\ \mathrm{T}]$, find $\bar{u}(\cdot, t) \in \mathrm{H}^1(D)$, $\mathbf{u}(\cdot, t) \in [\mathrm{H}^1(D)]^N$ and $\mathbf{y}(t, \cdot) \in [\mathrm{L}^2(\Omega)]^N$ such that:

$$\begin{cases} < \dfrac{\partial \bar{u}(\cdot,\ t)}{\partial t}, \psi > + <\nabla \bar{u}(\cdot, t), \nabla \psi> = <\mathbb{E}[f(u(\cdot, t, \cdot))],\ \psi> \\[4mm] < \dfrac{\partial \mathbf{u}(\cdot,\ t)}{\partial t}, \psi > C(t) + \mathbf{p}_1(\mathbf{u}(\cdot, t), \mathbf{u}(\cdot, t), \psi) C(t) = \mathbf{p}_2(\mathbf{u}(\cdot, t), \mathbb{E}[f(u(\cdot, t, \cdot))^\top \mathbf{y}], \psi) \\[4mm] \dfrac{\partial \mathbf{y}(t, \omega)}{\partial t} + \mathbf{y}(t, \omega) <\nabla \mathbf{u}(\cdot, t), \nabla \mathbf{u}(\cdot, t)> = <f(u(\cdot, t, \cdot)) - \mathbb{E}[f(u(\cdot, t, \cdot))],\ \mathbf{u}(\cdot, t)> \end{cases}$$
$$(4.11)$$

for all $\psi \in \mathrm{H}^1(D)$ and where $\mathbf{p}_1(\cdot, \cdot, \cdot)$, $\mathbf{p}_2(\cdot, \cdot, \cdot)$ is defined as:

$$\mathbf{p}_1 : (\mathbf{u}, \mathbf{v}, w) \rightarrow - <\mathbf{\Pi}_{<\mathbf{u}>^\top} \Delta \mathbf{v},\ w>$$
$$\mathbf{p}_1(\mathbf{u}, \mathbf{v}, w) = <\nabla \mathbf{v}, \nabla w> - <w, \mathbf{u}><\nabla \mathbf{v}, \nabla \mathbf{u}> \qquad (4.12)$$

for any $\mathbf{u},\ \mathbf{v},\ \mathbf{w} \in [\mathrm{H}^1(\Omega)]^N$ and $<\mathbf{u}_i,\ \mathbf{u}_j> = \delta_{ij}$.

$$\mathbf{p}_2 : (\mathbf{u}, \mathbf{v}, w) \rightarrow <\mathbf{\Pi}_{<\mathbf{u}>^\top} \mathbf{v},\ w>$$
$$\mathbf{p}_2(\mathbf{u}, \mathbf{v}, w) = <\mathbf{v}, w> - <w, \mathbf{u}><\mathbf{v}, \mathbf{u}> \qquad (4.13)$$

for any $\mathbf{u}, \mathbf{v}, \mathbf{w} \in [\mathrm{L}^2(\Omega)]^N$ and $< \mathbf{u}_i, \mathbf{u}_j >= \delta_{ij}$. Even if at the continuous level all the equations in $(4DOeq)$ are coupled each other, they can be divided in two subsystem, one deterministic and one stochastic and two independent discretization strategies can be adopted in the physical and probability space.

4.3.2   Numerical Approximation

Similarly to what described in Section 3.2.2 the deterministic PDEs are solved by using the Galerkin method with linear finite element discretization while the Stochastic Collocation method is used to solve the stochastic ODEs. According to the weak formulation (4.10) at any t the basis functions are discretized in the finite dimensional space $\mathrm{W}_h \subset \mathrm{H}^1(\mathrm{D})$ of continuous piecewise linear functions defined in the triangulation $\mathcal{T}_h$ of the physical domain. The stochastic coefficients are instead computed as a global polynomial approximation upon the solutions obtained by collocating the governing equations in each collocation point. The details of the two method are described in the section 3.2.2. The time derivative is discretized with the Euler method. In particular the diffusion terms are always treat implicitly while the reaction term, that is non linear, explicitly. Once again the covariance matrix $C(t)$ is freezed at the previous time step when solving the deterministic equations, the same applies to the projection operator. All these choices are motived by the purpose of keeping the deterministic equations decoupled from the stochastic equations in order to take the computational cost of the DO method low. A fully coupled system for problems as in (4.10) indeed require a high computational effort. By using the same notation introduced in the Chapter 3, we pass directly to the algebraic form of (4.10):

$$
\begin{cases}
\mathbb{M}\bar{U}^{n+1} + \Delta t \mathbb{K}\bar{U}^{n+1} = \mathbb{M}\bar{U}^n + \Delta t \mathbb{M}\bar{F}^n \\[2mm]
\mathbb{M}U^{n+1}\mathbb{C}^n + \Delta t(I - \mathbb{M}U^n U^{n\top})\mathbb{K}U^{n+1}\mathbb{C}^n = \mathbb{M}U^n\mathbb{C}^n + \Delta t(\mathbb{I} - \mathbb{M}U^n U^{n\top})\mathbb{M}\overline{FY}^n \\[2mm]
Y^{n+1} + \Delta t U^{n+1\top}\mathbb{K}U^{n+1}Y^{n+1} = Y^n + \Delta t U^{n+1\top}\mathbb{M}(F^n - \bar{F}^n)
\end{cases}
$$

$$(4.14)$$

where $\bar{F}$ is the column vector of the nodal values of $\hat{\mathbb{E}}[f(u)]$ at time t^n, i.e. $\bar{F}^n = \hat{\mathbb{E}}[f(u_h)]$ and $F \in \mathbb{R}^{N_h \times N_y}$ and $\overline{FY}^n_{ij} = \mathbb{R}^{N_h \times N}$ are the matrices defined as $F^n_{ij} = f(u_h(\mathbf{x}_i, t^n, \xi_j))$ and $\overline{FY}^n_{ij} = \hat{\mathbb{E}}[f(u_h(\mathbf{x}_i, t^n, \cdot)y_j(t^n, \cdot)]$ respectively. The symbol $\hat{\mathbb{E}}[\cdot]$ denotes the approximated expected value estimated through quadrature formula corresponding to the collocation points.

We observe that the equation for the mean function is decoupled from the others. On the contrary the second set of equations are coupled each other through the covariance matrix that is possibly singular and then not invertible. The strategy we adopted to overcome the problem consists in diagonalizing the covariance matrix. In other words the expansion in (4.10) is re-orthogonalized in $\mathrm{L}^2(\Omega)$ before solving the $PDEs$ for the deterministic basis functions. By definition the covariance matrix is symmetric and positive semi-definite. It follows that at any time instant there exists a set of N eigenval-

ues $\{\lambda_k(t)\}_{k=1}^N$ and N eigenvector $\{v_k(t)\}_{k=1}^N$ orthogonal with respect to the euclidean norm.Therefore at any time instant there exists a transformation according to which the stochastic field $u_N \in \mathcal{M}_N$ can be expanded in orthogonal basis on the stochastic space, i.e.:

$$u_N(\mathbf{x}, t; \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^N z_i(t; \omega) w_i(\mathbf{x}, t) \tag{4.15}$$

with:

- $w_j(\mathbf{x}, t) = \sum_{i=1}^N u_j(\mathbf{x}, t) v_{ij}(t)$

- $z_j(t; \omega) = \sum_{i=1}^N y_i(t; \omega) v_{ji}(t)$

In particular the covariance matrix associated to the stochastic coefficients in (4.30) corresponds to the diagonal matrix of the eigenvalues of C. However we stress that the orthogonality of the random variables is not required by the DO approach and above all it is not preserved in time. Indeed the approximation of the initial datum, according to the KL expansion, provides a double orthogonal decomposition, but that feature is not preserved except in the case in which the principal components of u_0 coincide with the eigenvalues of the operator $\mathcal{L}$. At each time iteration we diagonalize the covariance matrix and we solve the deterministic system of $PDEs$ in to the unknowns $w_1, ..., w_N$, by considering the eigenvectors $v_1, ..., v_N$ freezed at the previous time step. Specifically, defined V and D the matrices of eigenvectors and eigenvalues of C, it holds:

$$\mathbb{M}U^{n+1}\mathbb{V}^n\mathbb{D}^n + \Delta t(I - \mathbb{M}U^nU^{n\top})\mathbb{K}U^{n+1}\mathbb{V}^n\mathbb{D}^n$$
$$= \mathbb{M}U^n\mathbb{V}^n\mathbb{D}^n + \Delta t(\mathbb{I} - \mathbb{M}U^nU^{n\top})\mathbb{M}\mathbb{E}[F^nY^{n\top}\mathbb{V}^n] \tag{4.16}$$

By assuming the eigenvectors fixed in time at each iteration, (4.16) can be written in terms of the alternative orthogonal representation as:

$$\mathbb{M}W^{n+1}\mathbb{D}^n + \Delta t(I - \mathbb{M}U^nU^{n\top})\mathbb{K}W^{n+1}\mathbb{D}^n$$
$$= \mathbb{M}W^n\mathbb{D}^n + \Delta t(\mathbb{I} - \mathbb{M}U^nU^{n\top})\mathbb{M}\mathbb{E}[F^nZ^{n\top}] \tag{4.17}$$

where $W^* = U^*\mathbb{V}^n$ and $Z^n = \mathbb{V}^{n\top}Y^n$.

Now, in view of the proposition (2.6.1) the deterministic fields associated to zero variance stochastic coefficients are left unchanged. Observe that this treatment is consistent with the problem because on the right side we recover $\mathbb{E}[F^nZ^{n\top}]$, i.e. the correlation between the reaction term and the uncorrelated stochastic variables, both of them treated explicitly. In particular the correlation is null when the stochastic variable has zero variance.

In conclusion the DO system reads:

$$\mathbb{M}\bar{U}^{n+1} + \Delta t \mathbb{K}\bar{U}^{n+1} = \mathbb{M}\bar{U}^n + \Delta t \mathbb{M}\bar{F}^n$$

$$\mathbb{M}W_i^{n+1} + \Delta t (I - \mathbb{M}U^n U^{n\top})\mathbb{K}W_i^{n+1} = \mathbb{M}\,W_i^n + \frac{1}{\lambda_i}\Delta t (\mathbb{I} - \mathbb{M}U^n U^{n\top})\mathbb{M}\mathbb{E}[F^n Z_i^{n\top}]$$
$$\text{if } \lambda_i^n > 0$$

$$U_i^{n+1} = U_i^n$$
$$\text{if} \lambda_i^n < 0$$

$$Y^{n+1} + \Delta t U^{n+1\top}\mathbb{K}U^{n+1}Y^{n+1} = Y^n + \Delta t U^{n+1\top}\mathbb{K}U^{n+1}(F^n - \bar{F}^n)$$

$$(4.18)$$

4.3.3 Implementation details

The DO approach explicitly requires to the deterministic basis functions to be or-thonormal in $L^2(D)$. Can be easily verified that the condition is preserved at the continuous level. On the other hand this is not guaranteed from a numerical point of view. The problems analyzed in this section are characterized by fast dynamics that consequently affects the covariance matrix and its eigenvalues. In order to overcome the problem we chose to re-orthonormalize the deterministic basis functions at each time iteration, once solved the system (4.16). The procedure adopted is analogous to what described in the subsection 3.2.5. We underline that the deterministic basis functions are orthogonalized before solving the equations for the stochastic coefficients, since we adopt a Gauss Seidel type approach. This constraint explicitly imposed at each time step as well the diago-nalization of the equations for the deterministic basis functions, finalized in particular to deal with singular covariance matrix, justifies our choice in the time discretization of using a 1 step method instead of a multi step one. Possible numerical scheme to preserve the orthogonality are proposed in [36].

4.4 Bistable equation with stochastic threshold potential

In this section we consider a mono-domain formulation of the bistable equation, where the spatial domain is assumed to coincide with one myocardial cell with no connection between the intracellular domain and any surrounding media. From the mathematical point of view this means that we impose homogeneous boundary conditions type Neu-mann on the surface of cell to prevent current flow out the domain. We analyze the case in which the threshold potential is assumed to be a stochastic variable and the problem is modeled by a time dependent stochastic PDE, corresponding to the bistable equation, with deterministic initial conditions. Say the reaction term a cubic polynomial $f(u,\omega) = Au(\alpha(\omega) - u)(u - 1)$ and $\alpha(\omega)$, the instable zero of f, a stochastic variable, the problem reads:

$$\begin{cases} \dfrac{\partial u(\mathbf{x}, t, \omega)}{\partial t} - \Delta u(\mathbf{x}, t, \omega) = f(u(\mathbf{x}, t, \omega), \omega) & \mathbf{x} \in D,\, t \in [0,\, T],\, \omega \in \Omega \\ u(\mathbf{x}, 0, \omega) = u_0(\mathbf{x}) & \\ \dfrac{\partial u}{\partial \mathbf{n}}(\sigma, t, \omega) = 0 & \sigma \in \partial D \end{cases} \tag{4.19}$$

where n is is the unit normal vector to the boundary. In order to understand how the stochasticity of the parameter α influences the system, we focus first on the the mono-dimensional problem mentioned in section 4.2.1, for which we recovered an analytic solution. Then we discuss the numerical results of the DO method, applied to problem (4.20). We start by describing the qualitative features and then we analyze the accuracy of the DO approximate solution, compared to the one of the Stochastic Collocation method and the best N rank approximation.

4.4.1   Modeling problem

We start by considering the mono-dimensional problem:

$$\begin{cases} \dfrac{\partial u(x,t,\omega)}{\partial t} - \dfrac{\partial^2 u(x,t,\omega)}{\partial^2 x} = f(u(x,t,\omega),\omega) \qquad x \in (-\infty,\,\infty),\, t \in [0,\,\mathrm{T}],\, \omega \in \Omega \\ u(x,0,\omega) = \frac{1}{2} + \frac{1}{2}\tanh\big(\dfrac{\sqrt{A}}{2\sqrt{2}}x\big) \end{cases}$$

(4.20)

where the reaction function is a stochastic field defined as $f(u(x,t;\,\omega),\omega) = Au(\alpha(\omega) - u)(u - 1)$. The excitation rate A and the initial datum are assumed to be deterministic and the stochasticity of the system is uniquely generated by the random variable α. In particular we suppose $\alpha(\omega) \in \mathrm{L}^\infty(\Omega)$ and bounded between 0 and 1. According to (4.7) the propagation speed of the traveling front depends on the threshold potential value α and then it is as well a random variable:

$$c \in \mathrm{L}_P^\infty(\Omega) \qquad \text{s. t.} \qquad c(\omega) = \sqrt{\frac{A}{2}}(1 - 2\alpha(\omega)) \qquad (4.21)$$

Similarly to the deterministic case, the analytic solution of problem (4.20) is given by:

$$u(x,t;\,\omega) = \frac{1}{2} + \frac{1}{2}\tanh\left(\frac{\sqrt{A}}{2\sqrt{2}}(x + c(\omega)t)\right) \qquad x \in (-\infty,\,\infty),\, t \in [0,\,\mathrm{T}],\, \omega \in \Omega \quad (4.22)$$

and it is a traveling front with random propagation speed. Since the range of the parameter α has to be bounded between zero and one, we choose to model it as a uniform random variable. We observe that $\alpha = 0.5$ is a "critic" point since it is the values for which the direction of the front changes. For values of α bigger than 0.5 the solution converges to the steady state $u = 0$ while for outcomes smaller than 0.5 it tends to the higher steady level. The value $\alpha = 0.5$ is instead a point of zero probability for which the solution doesn't evolve. It means that if we consider the sign of $c(\omega)$ as function defined in the stochastic space, then $\alpha = 0.5$ is a discontinuity point. In particular it represents a discontinuity point in the stochastic space for the solution u at t that tends to infinity. In fact for vales of α lower that 0.5, u tends asymptotically to the higher steady equilibrium $u = 1$, otherwise it tends to 0. In view of applying the DO approach, we remind that the Stochastic Collocation method is often not suitable to describe discontinuous random fields. A good possibility to overcame the problem consists on decomposing the

stochastic domain in the two intervals where the solution is continuous and then sepa-
rately solve the equations for each interval.

We describe here only the case in which all the possible outcomes of α are smaller then
0.5, the opposite case gives the same results for what concerns our purposes. Specifically
we consider $\alpha(\omega) = 0.2(1 + z(\omega))$ where z is an uniform random variable in $[-1, 1]$.

For computational reason we need to consider a finite physical domain. We observe that
for fixed t it holds:

$$\lim_{x \to \infty} u(x, t, \omega) = 1 \qquad\qquad \lim_{x \to -\infty} u(x, t, \omega) = 0 \qquad \forall \omega \in \Omega \qquad (4.23)$$

Moreover for big values of A the solution $u(x, t, \omega)$ is characterized by a sharp front
defined in a small spatial interval, outside of which the function approaches rapidly the
steady states zero or one. We analyze therefore the problem (4.20) from the compu-
tational point of view by considering Neumann homogeneous boundary conditions in a
finite interval $[-d, d]$ with $d > 0$. Specifically the problem reads:

$$\begin{cases} \dfrac{\partial u(x, t, \omega)}{\partial t} - \dfrac{\partial^2 u(x, t, \omega)}{\partial^2 x} = f(u(x, t, \omega), \omega) & x \in (-d, d), \, t \in [0, \, \mathrm{T}], \, \omega \in \Omega \\ \dfrac{\partial u}{\partial x}(d, t, \omega) = 0 & \\ \dfrac{\partial u}{\partial x}(-d, t, \omega) = 0 & \\ u(x, 0; \omega) = \frac{1}{2} + \frac{1}{2} \tanh\left(\dfrac{\sqrt{A}}{2\sqrt{2}} x\right) & x \in [-d, \, d], \, \omega \in \Omega \end{cases}$$
$$(4.24)$$

that is consistent with the original problem, as the wave travels within the interval. We
will use this result to verify the accuracy of the DO approximate solution in section 4.4.2

4.4.2   Numerical Results

Initialization of the deterministic basis functions

In order to apply the DO method the initial condition has to be expanded as in
(4.10). For stochastic initial condition the initial datum is expanded by following the
KL decomposition and approximated in $\mathcal{M}_N$ by the eigenfunctions of the correlation
operator which are associated to larger variance. The deterministic basis function are
then initialized to the first N principal components of the initial datum. For deterministic
initial condition instead it is necessary to adopt an other different strategy since the initial
function does not have any component in the stochastic space and "a priori" there is not
any privileged direction. However for consistence with the problem, at time $t = 0$ the
mean value has to coincide with the deterministic initial datum while the stochastic
coefficients have to be initialized to zero. We observe that the term

$$\sum_{i=1}^{N} y_i(t, \omega) u_i(\mathrm{x}, t)$$

does not give any contribution at the $t = 0$ since the stochastic coefficients are identically equal to zero. Then the deterministic basis $u_1, ..., u_N$ can be chosen to correspond to any sequence of N orthonormal functions in $L^2(D)$. Given the homogeneous Neumann boundary conditions, one possibility consists in using cosine functions.

We call "latent" a basis function associated to a stochastic coefficient with zero variance while we say that a basis function is "activate" when the associated random variable develops variance larger than zero. At fixed time t, only the "activate" variables influence the approximation of the solution. They evolve in time to adapt to the structure of the problem while the other are left unchanged. However the adaptation of the basis functions is subjected to the error due to the time discretization. In particular the evolution of the modes, determined by the equations in (4.18), depends on the eigenvalues of the covariance matrix that is treated explicitly as well as the projection operator. However numerical tests confirm that the error in the adaptation of the modes decreases according to the time step and it is negligible compared to the approximation error in the stochastic space for small N. Another practical option to initialize the terms of the DO expansion (4.10) consists in adding additional variance to the initial datum. We observe that at the first iteration the modes do not evolve since the covariance matrix is identically equal to zero. By introducing an additional variance, that is small enough to generate a negligible error, we can overcome the problem. From the computational point of view, say ρ the threshold over which the variance of the stochastic variables is considered not zero, one or more stochastic coefficients are initialized to an arbitrary random variable with order of magnitude equal to ρ. In what follows we adopted the first approach.

Qualitative analysis

Before going into details about the accuracy of the DO approximation we give an example that highlights the mean features of the method.

The DO approximate solution consists in a linear combination of deterministic modes and stochastic coefficients. Unlike the classical spectral approaches introduced in section 1.3, nor polynomial or any fixed structures are imposed "a priori". Both the modes and the stochastic coefficients are computed "on fly", that means at each time iteration, in order to capture the structure of the problem. In this way few modes aim at globally approximate the main feature of the solution. In addiction, the DO expansion is a suitable representation of stochastic fields for what concerns the numerical "Uncertainty Quantification", context in which the goal is usually to compute statistics of the solution, in particular mean and variance. By following the DO approach the mean field is treated separately from the other modes and it is directly calculated by the method at each time step. The linear combination of the modes, with the stochastic coefficients, describes instead the variability of the process in the stochastic space and in particular the sum of the variance of the single stochastic variables corresponds to the total variance of the approximate solution. In this way we actually have a comprehensive description of the solution, as it is emphasized by the numerical test which we are going to describe.
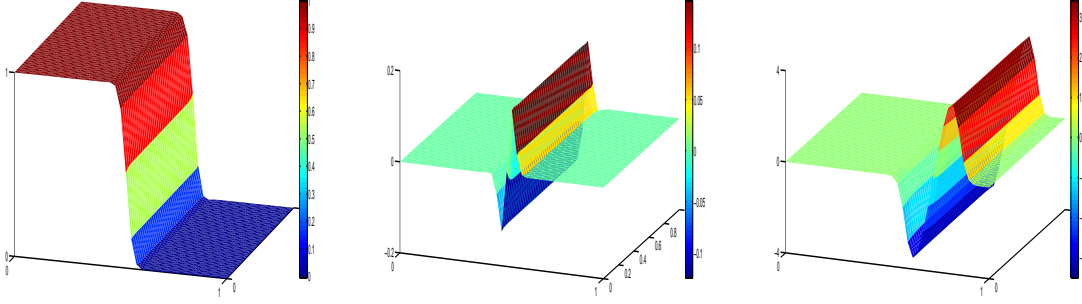
Figure 4.1: The mean field at $t = 0.05$ (left) and the standard deviation at time at $t = 0.05$ (middle) and at $t = 0.5$ (right) of the solution computed with the Stochastic Collocation method with highly accurate sparse grid.

Consider the stochastic dynamical system governed by the following $SPDE$:

$$
\begin{cases}
\dfrac{\partial u(\mathbf{x}, t, \omega)}{\partial t} - \delta \Delta u(\mathbf{x}, t, \omega) = f(u(\mathbf{x}, t, \omega)) & \mathbf{x} \in \mathrm{D} = [0, 1]^2, \, t \in [0, \mathrm{T}], \, \omega \in \Omega \\[2mm]
\dfrac{\partial u}{\partial \mathbf{n}}(\sigma, t, \omega) = 0 & \sigma \in \partial \mathrm{D} \\[2mm]
u(\mathbf{x}, 0; \omega) = \begin{cases} 1 & \text{if } x_1 \leq 0.5 \\ 0 & \text{if } x_1 > 0.5 \end{cases} &
\end{cases}
$$

$$(4.25)$$

where $f(u) = 100u(u - 1)(\alpha(\omega) - u)$, $\alpha(\omega)$ is an uniform random variable with mean $\mu = 0.2$ and variance $\sigma^2 = 0.013$ and the diffusion coefficient is $\delta = 0.01$. The solution is a stochastic field which tends asymptotically to the deterministic function $u = 1$ as t goes to infinity and it consists in a sheaf of traveling fronts with stochastic propagation speed in (4.21). Figure 4.1 shows the mean field (left) and the standard deviation (right) of the numerical solution computed with the Stochastic Collocation method with a highly accurate sparse grid. The DO solution can be computed as described in section 4.3.1. The initial mean function corresponds to the initial datum which is deterministic and the modes are arbitrarily initialized to a sequence of N orthonormal basis functions in $[0, 1]^2$ with zero stochastic coefficients. In this example we choose the cosine functions: $u_i(x_1, x_2) = \sqrt{2} \cos(i\pi x_1) cos(j\pi x_2)$, for $i, j = 1, ..., \sqrt{N}$. Figure 4.2 shows that the mean functions is a traveling front that actually describes the propagation of the solution. Moreover the modes evolve in time and properly adapt to describe the variability of the propagation speed. We observe that at any time instant the physical domain can be divided in three parts and we describe each of them by qualitatively comparing the exact solution, or rather the reference solution computed with the Stochastic Collocation method with a highly accurate sparse grid, and the DO approximate solution. Figure 4.2 shows the mean function and while in Figure 4.4 we present the first two modes of the DO approximate solution at different time steps.

- Part 1: the solution is already at the higher equilibrium level, $u = 1$. Here u is equal to a deterministic value for almost all $\omega \in \Omega$ and then the variance field is
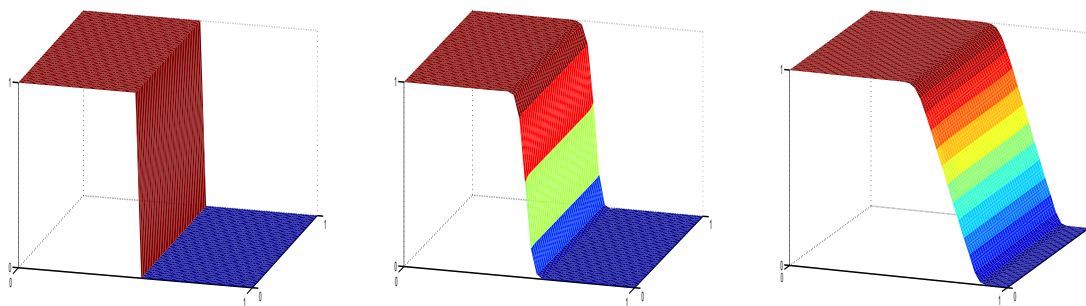
Figure 4.2: Mean function of the DO approximate solution at $t = 0$ (left), $t = 0.05$ (middle) and $t = 0.5$ (right), with $N = 6$, $N_y = 7$, $\Delta t = 0.001$

equal to 0, as shown in (4.1). In accordance with this fact, all the "activated" modes are equal to zero. We recall that at the fixed time $\bar{t}$ only the modes associated to stochastic coefficients with variance larger than zero evolve, the other ones are left unchanged and do not give any contribution to the solution at $\bar{t}$ (however they might evolve at $t > \bar{t}$). The mean function of DO approximate solution is properly equal to 1 and it is the only one term that gives remarkable contribution to the approximation.

- Part 2: the portion of the domain that corresponds to the curve of the stochastic traveling front. Here the stochasticity of the process is concentrated, the standard deviation is different from zero and the mean function represents the mean shape. The DO approximate solution is able to describe both the mean field and its variability; the mean function is close to the exact one and the "activate" modes, especially the ones that are associated to stochastic variables with large variance, adapt to the same shape of standard deviation.

- Part 3: the portion of the domain which has not yet been reached by the traveling front. The solution here is equal to the deterministic function $u = 0$ and both the standard deviation and the "activate" modes are constantly equal to zero. The mean function is zero as well and coincides with the exact one.

The same observation can be done at each time step, and this shows that the DO approximate solution is consistent with the qualitative features of the exact solution. The modes, which promptly adapt since the first time step, evolve in time by following the traveling front as well as the mean function. This shows that the DO method actually captures the structure of the process without any "a priori" information and properly describes the qualitative features of both the mean and the standard deviation field.

"A posteriori" estimates

In order to understand the dynamics of the solution in the stochastic space and the suitability of the low rank approach, we analyze the evolution in time of the covariance
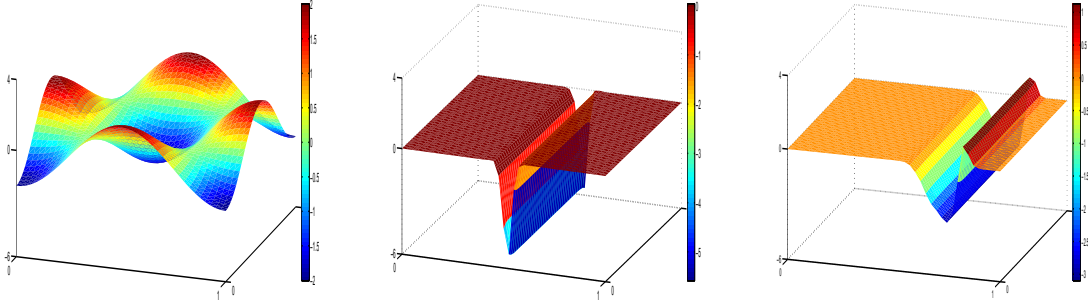
Figure 4.3: First mode of the DO approximate solution at $t = 0$ (left), $t = 0.05$ (middle) and $t = 0.5$ (right), with $N = 6$, $N_y = 7$, $\Delta t = 0.001$
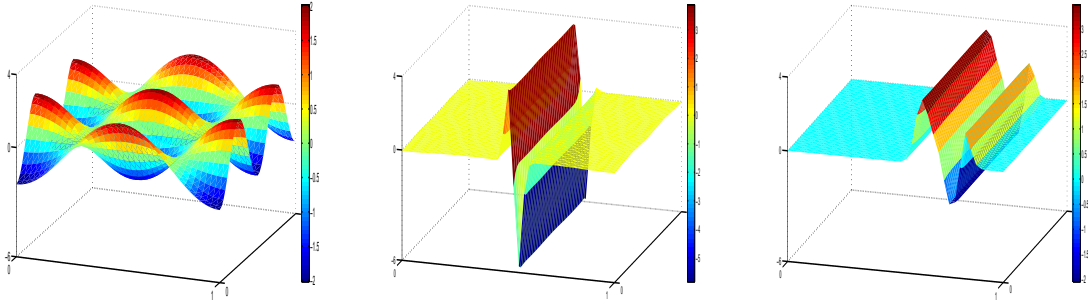

Figure 4.4: Second mode of the DO approximate solution at $t = 0$ (left) $t = 0.05$ (middle) and $t = 0.5$ (right), with $N = 6$, $N_y = 7$, $\Delta t = 0.001$,

matrix and in particular the rank, which corresponds to the effective rank of the approximate solution, and the eigenvalues, for different values of N.

Let us consider problem (4.24), the stochastic space has dimension equal to one since the stochasticity is uniquely determined by the random variable α. Thus the exact solution evolves in a one-dimensional manifold, which however is non linear, as shown by the analytic solution in (4.22). The traveling front is deterministic at $t = 0$, it propagates with the stochastic speed in (4.21) and then tends asymptotically to the deterministic value that corresponds to the steady equilibrium (in this case $u = 1$). Consequently, we expect that the rank of the covariance matrix, initially equal to zero, would increase and then go back to zero. It easy to verify that, at any time instant, the total variance of the approximate solution corresponds to the sum of the variance of the stochastic coefficients, or equivalently to the sum of the eigenvalues of $C(t)$.

$$\mathbb{V}ar[\|u_N(\cdot, t, \cdot)\|_{L^2(\mathrm{D})}] = \sum_{i=1}^{N} \mathbb{V}ar[y_i(t, \cdot)] = \sum_{i=1}^{N} \lambda_i(t)$$

Concerning the covariance matrix, the dynamic of the rank depends on both the number of modes and the number of the collocation points. It is obviously bounded by N,
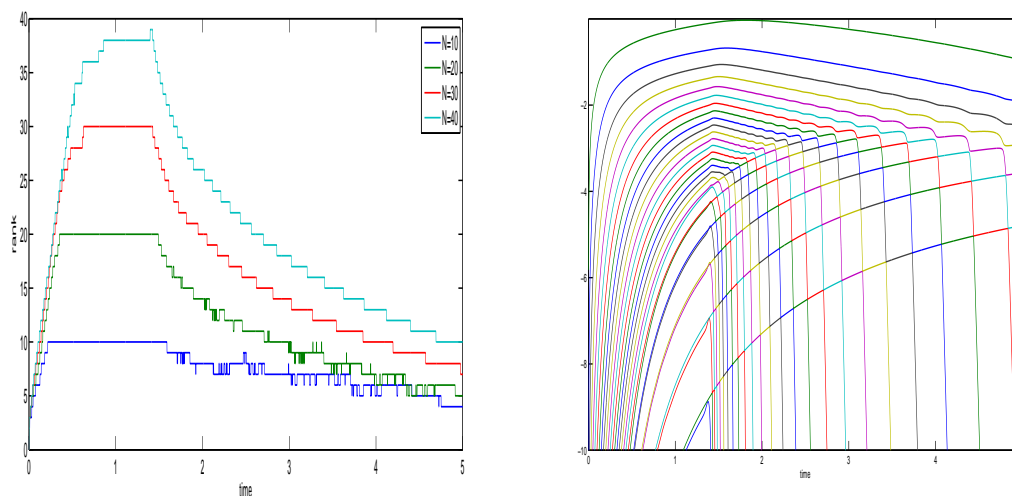
Figure 4.5: On the left: The rank evolution with $N = 10, 20, 30, 40$ and corresponding number of collocation points $N_y = N$. Excitation rate $A = 100$. On the right: Time evolution of the eigenvalues, in logarithmic scale with $N = 30, A = 10$.

the dimension of the matrix, and by N_y, the number of collocation points. We want to verify wether there is any upper bound, beyond which the rank does not increase any further, independently of N and N_y. For this purpose it is reasonable to use $N_y = N$. The numerical results show that the rank tends to reach the saturation level, that is the maximum level permitted by the parameters N and N_y. Only in the case of $N \geq 40$ the rank did not reach the saturation and increased up to 39 during the whole simulation, as shown in Figure (4.5), (left). Moreover we observed that the evolution of the rank of the covariance matrix is influenced by the excitation rate A. For consistency to biological problems we focus on values of $A \geq 100$. One can see in (4.21) that the speed of the traveling front depends on the excitation rate. In particular the larger A, the larger the variance of the propagation speed and the predominance of the reaction term are. Consequently more and more directions are needed to well describe the solution. On the contrary, for smaller values of A, e.g. $A \approx 10$, we get smoother solutions in the stochastic space, that are well described in a low dimensional manifold. In such a case the upper bound reached by the rank of the covariance matrix is relatively low, compared to the case that has been previously analyzed and does not saturate for $N \geq 30$, as shown in figure (4.6), (left).

Associated to the analysis of the effective rank of the approximate solution, we studied the time evolution of the eigenvalues of the covariance matrix. According to the observation (4.30), the eigenvalues coincide with the variance of the re-orthogonalized stochastic variables. Say u_N the DO approximate solution of rank N and $\epsilon(t)$ the approximation error in mean square sense at time $t \in [0, T]$, $\epsilon(t)$ depends on the variance of stochastic
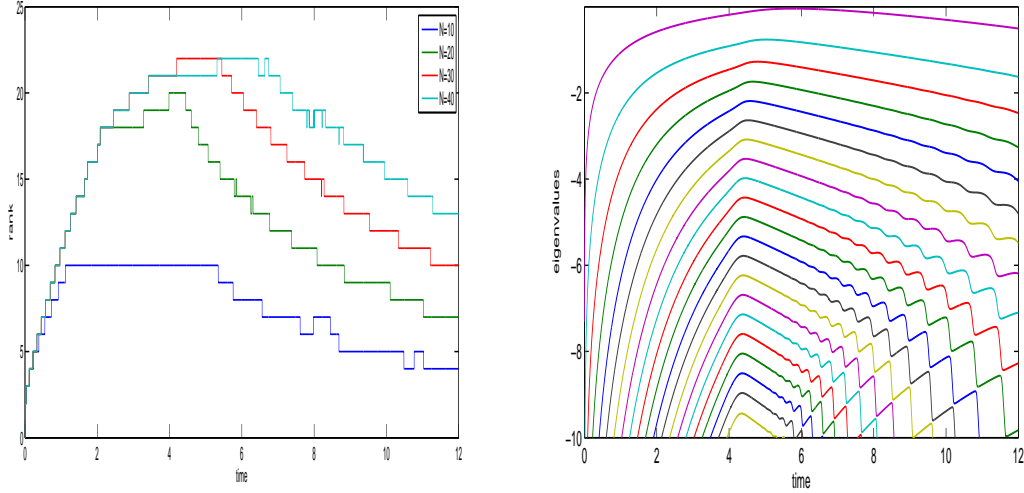
Figure 4.6: On the left: The rank evolution with $N = 10, 20, 30, 40$ and corresponding number of collocation points $N_y = N$. Excitation rate $A = 10$. On the right: Time evolution of the eigenvalues, in logarithmic scale with $N = 30$. Excitation rate $A = 10$.

variables not included in the approximation and it can be estimated as:

$$\epsilon(t) \approx \sum_{i=N+1}^{\infty} \mathbb{V}ar[y_i(t, \cdot)]$$

. In order to minimize the error in the mean square sense, we should include at any time step the N basis functions associated to the N orthogonalized stochastic coefficients with largest variance. This can be achieved only by computing the KL decomposition at any time step since it is not possible to "a priori" predict the principal components of the solution. The DO approach avoids to compute the KL decomposition at any time step, however the approximate solution which we obtain does not necessary correspond to the best N rank approximation. The analysis of the evolution in time of the eigenvalues of the covariance matrix provides an "a posteriori" estimate of the approximation error. With this aim in mind we analyze Figure (4.5) (right) in order to understand:

- if there is a gap in the distribution of the eigenvalues and how many of them develop remarkable values.

- how and when the eigenvalues increase and decay.

Thanks to the analysis of the rank of the covariance matrix, we already know that many eigenvalues are different from zero during the whole process, up to 40 for time $t < 2$. Furthermore now we observe that many of them increase up to 10^{-4} which means that the solution can not be approximate with high accuracy by only few modes. However this is due to the intrinsic dynamic of the solution and it concerns the truncated KL
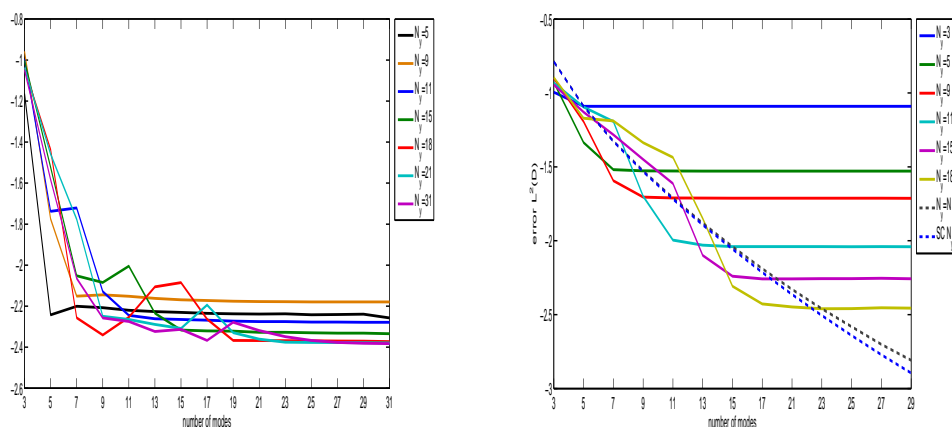
Figure 4.7: On the left: Error for the mean function of the DO approximate solution w.r.t. the exact solution in norm L^2(D) with different numbers of collocation points and modes. On the right: Error for the mean function of the DO approximate solution w.r.t. the solution of the Stochastic collocation method with highly sparse grid. In dotted line (red) $N_y = N$. In dotted line (blu) the error of the Stochastic Collocation method with the same number of collocation points.

decomposition as well (the dynamical of the variance of the stochastic variables associated to the KL decomposition is very close to Figure (4.5) (right)). The remarkable problem concerns the increasing rate of the eigenvalues. We can see in Figure (4.5) (right) that many of them rise up during the whole time interval [0, 0.7] and reach values larger than 10^{-4} for time $t > 1.5$. At the same time other eigenvalues quickly decay to zero. Then the N principal components of the solution at time $t > 1.5$ do not correspond to the evolution of the N principal components at time $t < 1.5$ since some of them are associated to stochastic processes with variance which quickly decays for $t > 1.5$. In other words, the manifold of the best rank N solution is not described along the trajectory of the initial N principal components during the whole evolution of the process. Then if we apply the DO method with $N << 39$ number of modes we are going to consider only the stochastic processes which first develop variance larger than zero, up to the saturation level of the covariance matrix. However we omit the stochastic processes whose variance increases when the covariance matrix has already reached the saturation level and these ones are going to develop a variance that is larger than 10^{-4}.

Error analysis

In this section we quantify the accuracy of the DO method for what concerns problem 4.24 by computing the error of the DO approximate solution with respect to:

- the exact solution, in order to verify the quality of the approximate solution by considering all the approximation parameters,

- the numerical solution of the Stochastic Collocation method, computed with a highly accurate sparse grid, in order to analyze the error in the stochastic space,

- the best rank N approximate solution with the aim of testing the low rank approach.

First of all, we analyze the error of the DO approximate solution compared to the analytical solution in (4.22). We consider small time interval such that the wave travels within the spatial domain, for consistency with (4.22). We computed the following error in $L^2(\mathrm{D})$-norm:

$$\epsilon_u(t) = \|u_{ex}(\cdot, t) - \bar{u}_N(\cdot, t)\|_{L^2(\mathrm{D})} \tag{4.26}$$

where $\bar{u}_N$ is the mean function of the DO approximate solution with N number of modes. Figure 4.7(left) shows the error $\epsilon_u(t)$, at fixed time t, with different number of modes and collocation points. First of all we observe that for small values of N, e.g. $N \sim 3$, the truncation error is large (10^{-1}) and dominates the spatial and time discretization error. This is in accordance with the "a posteriori" analysis obtained in Section 4.4.2. Furthermore the plot confirms that the accuracy of the solution depends on the number of modes N as well as on the stochastic collocation points N_y and reasonably there is no improvement in the quality of the approximation for $N > N_y$. However we observe that the truncation error decays quickly by adding modes when $N \sim 3$, but is negligible for only large values of N and N_y.

Figure 4.7(left) shows the error computed with respect to the numerical solution of the Stochastic Collocation method and using a highly accurate sparse grid in order to analyze only the error due to the approximation in the stochastic space. Once again we see that the error is quite large for small values of N. In addition, we computed the error of the DO solution when the number of collocation points is equal to the number of modes. Figure 4.7(left) confirms that the convergence rate of the DO approximate solution tends to coincide with the convergence rate of the Stochastic collocation method, and decays by increasing the number of collocation points.

In conclusion, it seems that the DO approach is not an effective method for this kind of problem when one wants to achieve high accuracy. However, in oder to understand wether the problem 4.24 can be suitably approximated by low rank approaches we compute the KL decomposition of the solution at any time step. Furthermore we compare the error of the truncated N- rank KL expansion, which represents the best rank-N approximation in mean square sense, with the error of the DO method, with different values of N. The aim is to verify how much larger is the error of the DO approximate solution with respect to the optimal error. Specifically we first compute a reference solution through the Stochastic Collocation method (with highly accurate sparse grid) and then the KL expansion. Subsequently, we compute the best rank N approximation at any time step. We used the same spatial and temporal discretization parameters to compute the solutions with both the Stochastic Collocation and the DO method, in order to compare only the error in the stochastic space. The error computed is defined as:

$$\epsilon(t) = \mathbb{E}[\|u_{sc}(\cdot, t, \cdot) - u_N(\cdot, t, \cdot)\|^2_{L^2(\mathrm{D})}] \tag{4.27}$$
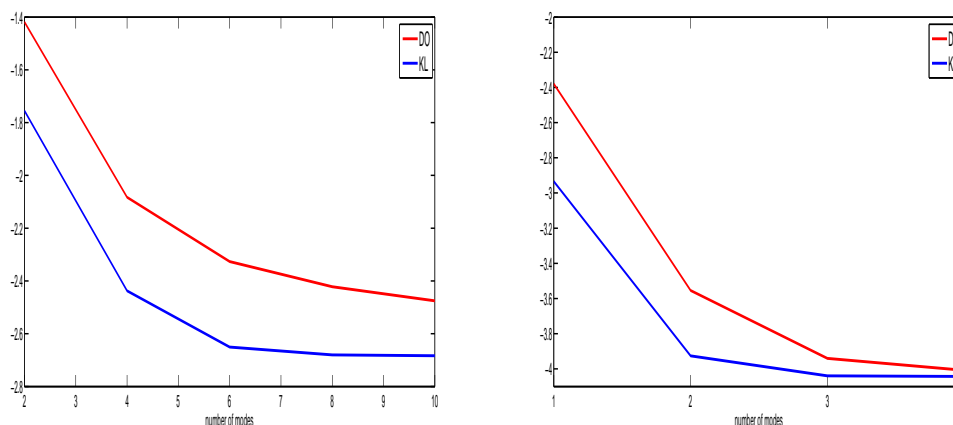
Figure 4.8: Error w.r.t. the total variance (in log scale) of the DO approximate solution (red) and the best N-rank approximation (blu), with respect to N at fixed time. Excitation rate $A = 100$ on the left, $A = 10$ on the right.

where u_{sc} is the reference solution and u_N denotes the rank N solution (KL or DO). Figure (4.9) (right) shows the error ϵ of the KL and DO approximate solution with respect to N, at time t fixed and with excitation rate $A = 100$. We observe that the error of DO approximate solution is proportional to the best approximation error, but the proportional constant does not decrease substantially by increasing N. However the error of the best N rank approximation is quite large for small values of N, which attests the difficulty to apply the low rank approach to this kind of problems. On the other hand better results are obtained for problems with slower dynamic. We repeat the same analysis for problem in 4.24 with excitation rate $A = 10$. Figure (4.7) (left) shows that the best rank N approximation as well the DO approximate solution achieve higher level of accuracy and with few modes.

4.5 Stochastic initial condition

In this section we numerically verify the suitability of the DO approach for problems governed by the deterministic bistable equation, with initial stochastic condition. We analyze the dynamics of the eigenvalues of the covariance matrix and we compare the error of the DO approximate solution to the error of the best N rank approximation.
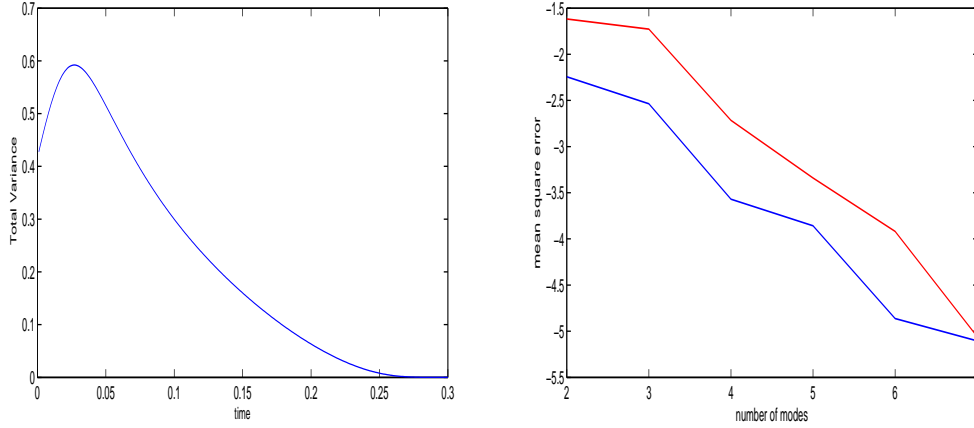
Figure 4.9: On the Left: Evolution of the total variance of the solution. On the Right: The mean square error (in log scale) of the DO approximate solution (red) compared to the best N-rank approximation (blu), with respect to N at fixed time. Excitation rate $A = 100$

Specifically we consider the following problem

$$
\begin{cases}
\dfrac{\partial u}{\partial t}(x, t, \omega) - \dfrac{\partial^2 u}{\partial x^2}(x, t, \omega) = f(u(x, t, \omega)) & x \in [0,\, 10],\, t \in [0,\, \mathrm{T}],\, \omega \in \Omega \\[2mm]
\dfrac{\partial u}{\partial x}(0, t, \omega) = 0 & t \in [0,\, \mathrm{T}],\, \omega \in \Omega \\[2mm]
\dfrac{\partial u}{\partial x}(10, t, \omega) = 0 & t \in [0,\, \mathrm{T}],\, \omega \in \Omega \\[2mm]
u(x, 0;\, \omega) = u_0(x, \omega) & x \in [0,\, 10],\, \omega \in \Omega
\end{cases}
$$
$$(4.28)$$

where $f(u) = Au(u - 1)(\alpha - u)$ with A, α deterministic parameters and the initial condition is defined as:

$$
u_0(x, \omega) = 0.5 + z(\omega)\cos\left(\frac{\pi x}{5}\right) \qquad x \in [0,\, 10],\, \omega \in \Omega
$$

and $z \in \mathrm{L}_P^2(\Omega)$ uniform zero mean stochastic variable, with variance $\sigma^2 = 1/12$. The initial condition is bounded between 0 and 1 and, based on the value of α, the solution tends asymptotically either to the lower or the higher steady equilibrium of the bistable equation. In this example we consider $\alpha = 0.1$ and $A = 100$. Figure 4.9(left) illustrates the time evolution of the total variance of the solution. We observe that, because of the reaction term, the total variance increases during the first part of the process and then goes to zero when the solution approaches the steady level. Consequently we expect an analogous trend for the rank and the eigenvalues of the covariance matrix, associated to the DO approximate solution.

The DO approach leads to a system of equations as in (4.10). The initial datum is expanded according to (4.10) and in particular the deterministic basis functions are

initialized as:

$$u_i(x,0) \,=\, \sqrt{\frac{1}{5}} \cos\left(\frac{(i-1)\pi x}{5}\right) \qquad\qquad i=1,...,N$$

that implies:

$$u_0(x,t) \,=\, \bar{u}(x,0) + \sum_{i=1}^{N} y_i(0,\omega) u_i(x,0) \qquad\qquad x\in[0,10],\ \omega\in\Omega$$

where $\bar{u}(x,0)=0.5$, $y_2(0,\omega)=\sqrt{5}z(\omega)$ and $y_i(0,\omega)=0$ for all $i=1$ and $i=3,...,N$.
It follows that the rank of the covariance matrix is initially equal to one. Figure 4.10
(left) confirms the expected evolution of the rank of the covariance matrix. Contrary to
what discussed in the Chapter 3, even if the initial condition is a 1-rank function, the
solution evolves in a multidimensional manifold. This is due to the presence of the non
linear reaction term and it means that more terms in the DO expansion are needed to
well describe the solution. On the other hand figure 4.10 (right) shows that, even if many
stochastic coefficients are "activated" during the process, only few of them reach relevant
levels of variance. This means that good level of approximation can be still achieved
by using few modes. More precisely we consider the error in norm $L^2(D)\otimes L^2_P(\Omega)$
at time t fixed. In the Figure 4.9 (right) we compare the error of the DO approximate
solution with that of the best N-rank approximation with respect to N. The best N rank
approximation, that corresponds to the truncated KL expansion is computed numerically
by using the solution computed through the Stochastic Collocation method with $N_y=41$
collocation points. The figure shows that by increasing N, the error of the DO method
decreases more or less at the same rate as the best approximation error. Moreover good
level of accuracy can be achieved with few modes.

4.5.1 Comparison with the Stochastic Collocation method

The Stochastic Collocation method and the DO approach are based on two different
concepts of approximation. Given a stochastic field $u\in L^\infty([0,\,T],\,L^2(D)\otimes L^2_P(\Omega))$ that
is a solution of a problem as in (1.28), the Stochastic Collocation method provides, at any
time step, a global polynomial approximation of u in the stochastic space, interpolatory in
the case of tensor grids or nested collocation points, that is built upon specific evaluations
of the time dependent process in the collocation points. On the contrary the DO method
develops an approximate solution that is a linear combination of few basis functions
which depend on the solution and which aim to globally approximate it. However, the
DO method described in this thesis is closely related to the Stochastic Collocation method
since the latter is used to solve the ODEs for the stochastic coefficients in (2.6). It follows
that the error of the DO solution, in mean square sense, is related to the error of the
Stochastic Collocation method. Specifically, by using the same number of collocation
points, the error of the Stochastic Collocation method represents a lower bound for the
DO method. Indeed, according to the numerical methods used to solve the DO system,
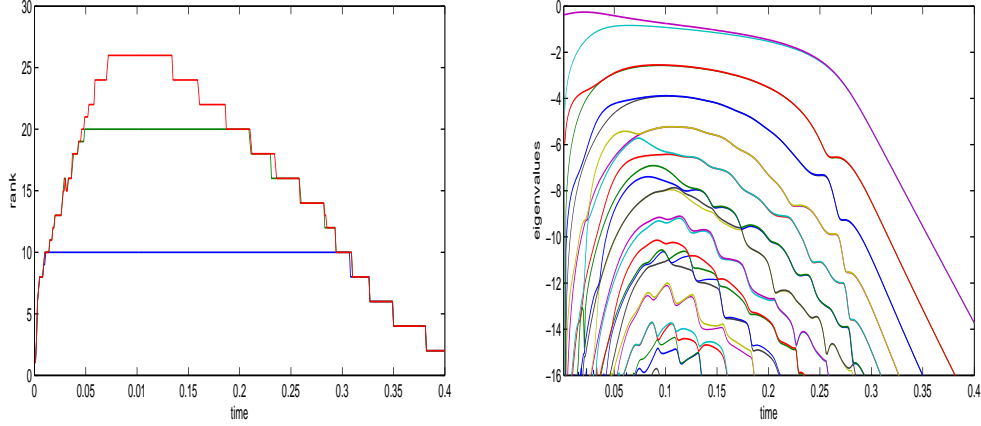
Figure 4.10: On the left: The rank evolution with $N = 10, 20, 30$ and corresponding number of collocation points $N_y = N + 1$. Excitation rate $A = 100$. On the right: Time evolution of the eigenvalues, in logarithmic scale with $N = 30$. Excitation rate $A = 100$.

the approximate solution can be expanded as:

$$
\begin{aligned}
u_N(\mathbf{x}, t; \omega) &= \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N} y_i(t; \omega) u_i(\mathbf{x}, t) \\
&= \bar{u}(\mathbf{x}, t) + \sum_{j=1}^{N_y} \left[\sum_{i=1}^{N} y_i(t; \xi_j(\omega)) u_i(\mathbf{x}, t) \right] \mathcal{L}_j(\xi(\omega))
\end{aligned}
\tag{4.29}
$$

that coincides to the approximate solution of the Stochastic Collocation method if $N = N_y - 1$. It follows that the error of the DO method is bigger than the error of the Stochastic Collocation method when we use the same number of collocation points and $N < N_y - 1$. On the other hand it is interesting to verify how much the error increases by decreasing N. In figure 4.11 (left) we compare the DO solution computed with N_y collocation points to the solution obtained through the Stochastic Collocation method with the same N_y, by varying the number of modes N. Specifically the plot concerns the numerical test discussed in the section 4.28 and the error computed is defined as:

$$
\epsilon(N) = \frac{1}{T} \int_0^T \| u_N(\cdot, t, \cdot) - u_{sc}(\cdot, t, \cdot) \|_{\mathrm{L}^2(\mathrm{D}) \otimes \mathrm{L}_P^2(\Omega)} dt
$$

where u_{sc} denotes the solution of Stochastic Collocation method with $N_y = 21$. In the figure 4.11 (right) we instead compare two solutions obtained by the DO method with different number of collocation points. We computed the error of the two approximate solutions with different values of N. We considered the error in mean square sense, with respect to a reference solution computed through the Stochastic Collocation method with many more collocation points. The plot shows that in the case analyzed, for small values of N, the trend of the error is independent to the the number of collocation points. Moreover it confirms that is not reasonable to use $N > N_y$.
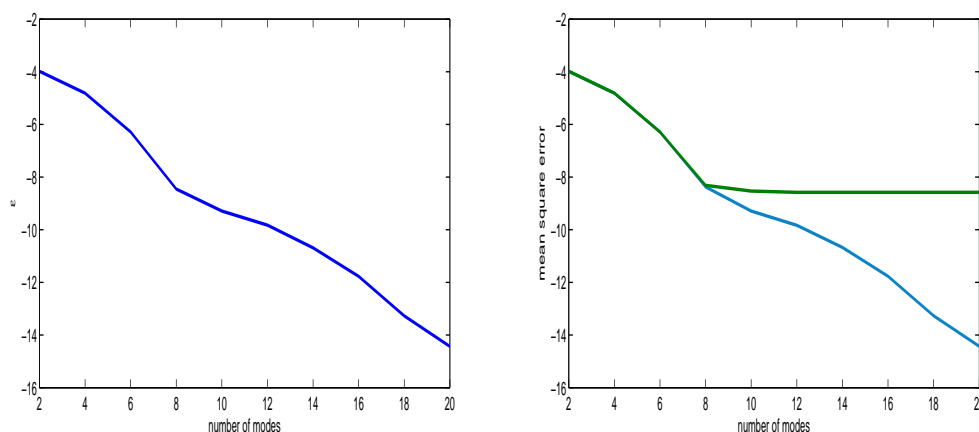
Figure 4.11: On the left: the error of the DO method compared to the Stochastic Collocation method, with the same number of collocation points $N_y = 21$, with respect to N (log scale). On the right: The error of the DO solution with $N_y = 11$ (green) and $N_y = 21$(blu) compared to a reference solution, with respect to N

4.6   Adaptive Dimensionality

In this section we describe an adaptive method for the dimensionality of the manifold where the solution is approximated, by following the criteria introduced in [17] [16]. According to the DO approach described in the Chapter 2, given N, the approximate solution is represented in terms of N deterministic orthonormal basis functions associated to N stochastic coefficients. Adaptive methods basically consist in supposing N a function of time. A number of modes that is fixed in time and chosen "a priori" leads indeed to two important questions: how many basis functions are needed to well describe the solution during the whole time interval and how is it possible to minimize this number? The DO approach gives a first answer to the problem by looking directly for a low rank approximate solution with a spectral representation as in (2.1). On the other hand there are many situation in which the low rank approach is not a suitable choice. The bistable equation with stochastic threshold potential value described in the section (4.4) provides an example. In that case indeed the effective rank of the solution, that is initially equal to zero for deterministic initial conditions, grows fast up to high levels and then decreases again to zero. Adaptive dimensionality criteria aim to use a time dependent number of modes $N(t)$ that follows the trend of the effective rank of the solution in order to obtain at any time instant an approximate representation which uses only the minimum number of terms to achieve the accuracy required. The focal points of these approaches concerns the choice of the basis functions to add or drop out.

4.6.1   Decreasing the dimensionality

The criterion to reduce the dimensionality is based on the rank of the covariance matrix. If the covariance matrix is singular, the basis functions associated to the zero variance stochastic coefficients, are dropped. In oder to do this we use the observation in (2.21). First of all we underline that, according to adaptive criteria, the dimension of the covariance matrix changes in time, i.e. $C(t) \in \mathbb{R}^{N(t) \times N(t)}$. Being $\lambda_1(t), ..., \lambda_{N(t)}(t)$ and $v_1(t), ... v_{N(t)}(t)$ the sequences of the eigenvalues and eigenvector of the covariance matrix at time t, the approximate solution $u_N \in \mathcal{M}_N$ can be expressed in terms of orthogonal components in both the physical and stochastic space:

$$u_N(\mathbf{x}, t; \omega) = \bar{u}(\mathbf{x}, t) + \sum_{i=1}^{N(t)} z_i(t; \omega) w_i(\mathbf{x}, t) \qquad (4.30)$$

where

- $w_j(\mathbf{x}, t) = \sum_{i=1}^{N(t)} u_i(\mathbf{x}, t) v_{ij}(t)$

- $z_j(t; \omega) = \sum_{i=1}^{N(t)} y_i(t; \omega) v_{ji}(t)$

Moreover one can verify that the basis functions $w_1, ..., w_{N(t)}$ correspond to the principal components of the approximate solution. Let $\mathbf{w}$ and $\mathbf{z}$ be the vector of functions such that $\mathbf{w}(\mathbf{x}, t) = \big(w_1(\mathbf{x}, t), ..., w_{N(t)}(\mathbf{x}, t)\big)$ and $\mathbf{z}(\omega, t) = \big(z_1(\omega, t), ..., z_{N(t)}(\omega, t)\big)$ and $\mathbb{D}$ the diagonal matrix of the eigenvalues, it holds:

$$C_{u(t)u(t)}(\mathbf{x}, \mathbf{x}') = \mathbb{E}[\mathbf{w}(\mathbf{x}, t)\mathbf{z}^\top(t, \cdot)\mathbf{z}(t, \cdot)\mathbf{w}^\top(\mathbf{x}', t)] = \mathbf{w}(\mathbf{x}, t)\mathbb{D}(t)\mathbf{w}^\top(\mathbf{x}', t) \qquad (4.31)$$

Reminding that the basis functions are orthonormal in $L^2(D)$, it is easy to check that $\lambda_1(t), ..., \lambda_{N(t)}(t)$ and $w_1, ..., w_{N(t)}$ are the solutions of the eigenvalue problem associated to $C_{u(t)u(t)}$. In light of that, if the covariance matrix singular with one zero eigenvalue, we drop the basis function associated to the zero eigenvalue and the dimensionality is reduced to $N(t^+) = N(t) - 1$. In practice, from a computational point of view, we fix a threshold under which the stochastic coefficients are considered having zero variance stochastic variables and at any time step we check if any random coefficient is under the threshold, in which case it is dropped.

4.6.2   Increasing the dimensionality

Given a stochastic problem as in (1.28), the DO method develops an approximate solution in the manifolds $\mathcal{M}_N$ that is mapped by the N orthonormal basis functions $u_1, ..., u_N$ at any time instant. Following the adaptive dimensionality approach, we denote with $\mathcal{W}_{N(t)}$ the $N(t)$ dimensional subspace spanned by $u_1, ..., u_{N(t)}$ and, at the fixed time instant $t^* \in [0, T]$, we look for the "direction" in the subspace orthogonal to $\mathcal{W}_{N(t^*)}$, that is associated the largest potential variance. Let us first explain the idea by applying the it to the truncated KL expansion, to which the DO approach is inspired. Fixed the time instant t^* and the number of basis functions $N^* = N(t^*)$, the method aims to add

the $(N^* + 1)^{th}$ principal component of u if the associated eigenvalue is bigger than the threshold. By transferring this idea in the DO framework, we underline that the basis function to add is "a priori" unknown. We followed the approach proposed in [16], [16] according to which we study the stability of the reduced system to perturbation normal to $\mathcal{W}_{N(t)}$ by computing the Normal Infinitesimal Lyapunov Exponents introduced in [35] to study the normal stability proprieties of invariant manifolds. In view of that we define the Fréchet derivative that is a basic element for optimization problems involving functional derivatives. Let X and Y be two Banach spaces and $F : A \subset X \to Y$ with A open in X. F is Fréchet differentiable in $x \in U$ if there exists a linear operator $dF(x) : X \to Y$ such that for any $x + h \in U$ it holds:

$$\lim_{h \to 0} \frac{\|F(x + h) - F(x) - dF(x)h\|_Y}{\|h\|_X} = 0 \tag{4.32}$$

Let $u_{N^*} \in \mathcal{M}_{N^*}$ the approximate solution at $t = t^*$, we seek a new basis function $u^* \in \mathcal{W}_{N^*}^\top$ orthonormal in $\mathrm{L}^2(\mathrm{D})$ to $\{u_1, ..., u_{N^*}\}$. Let u_{N^*+1} be the perturbed approximate solution defined as:

$$u_{N^*+1}(\mathbf{x}, t^*, \omega) = u_{N^*}(\mathbf{x}, t^*, \omega) + hy^*(t^*, \omega)u^*(\mathbf{x}, t^*) \qquad \mathbf{x} \in \mathrm{D}, \omega \in \Omega \tag{4.33}$$

where $0 < h << 1$. We assume $y^*(t^*, \cdot) \in \mathrm{L}_P^2(\Omega)$ is a random variable with zero mean and independent to $y_1(t^*, \omega), ..., y_{N^*}(t^*, \omega)$. By deriving the DO equations as in (2.6) we obtain:

$$h\frac{\partial y^*(t, \omega)}{\partial t} = < \mathcal{L}(u_{N^*+1}(\cdot, t, \omega); \omega) - \mathbb{E}[\mathcal{L}(u_{N^*+1}(\cdot, t, \omega); \omega)], u^*(\cdot, t^*) > \tag{4.34}$$

Supposed $\mathcal{L}$ Fréchet differentiable in $\mathrm{L}^2(\mathrm{D})$, it holds:

$$\mathcal{L}(u_{N^*+1}(\mathbf{x}, t, \omega), \omega) = \mathcal{L}(u_{N^*}(\mathbf{x}, t, \omega), \omega) + hy^*(t, \omega)d\mathcal{L}(u_{N^*}(\mathbf{x}, t, \omega), \omega)u^*(\mathbf{x}, t) + o(h^2) \tag{4.35}$$

Being y^* a zero mean stochastic process, the expected value of (4.35) at $t \to t^*$ leads to:

$$\lim_{t \to t^*} \mathbb{E}[\mathcal{L}(u_{N^*+1}(\mathbf{x}, t, \cdot))] = lim_{t \to t^*}\mathbb{E}[\mathcal{L}(u_N(\mathbf{x}, t, \cdot))] + o(h^2) \tag{4.36}$$

By replacing (4.36) and (4.35) in (4.34) for $t \to t^*$ we get:

$$\begin{aligned} lim_{t \to t^*} h\frac{\partial y^*(t, \omega)}{\partial t} &= < \mathcal{L}(u_N(\cdot, t^*, \omega); \omega) - \mathbb{E}[\mathcal{L}(u_N(\cdot, t^*, \omega); \omega)], u^*(\cdot, t^*) > + \\ &\quad hy^*(t^*, \omega) < d\mathcal{L}(u_N(\cdot, t^*, \omega), \omega)u^*(\mathbf{x}, t), u^*(\mathbf{x}, t^*) > + o(h^2) \end{aligned} \tag{4.37}$$

Then we multiply by y^* and integrate in Ω. By using again that y^* is a zero mean stochastic process and that it is independent of $y_1, ..., y_{N^*}$ when h that tends to zero it yields:

$$\frac{d\mathbb{E}[(y^*(t^*, \cdot))^2]}{dt} = 2\mathbb{E}[y^*(t^*, \cdot)^2] < \mathbb{E}[d\mathcal{L}(u_N(\cdot, t^*, \omega), \omega)u^*(\cdot, t^*)], u^*(\cdot, t^*) > \tag{4.38}$$

Finally the basis function that we are looking for is given by the $u^* \in \mathcal{W}_{N*}^{\top}$ orthonormal in $L^2(D)$ that maximizes:

$$Q(v) = <\mathbb{E}[d\mathcal{L}(u_N(\cdot, t^*, \omega), \omega)v^*(\cdot, t^*)], v(\cdot, t^*)> \tag{4.39}$$

under the assumption that all the stochastic variables associated to the basis functions not included in $\mathcal{W}_{N*}$ have the same variance.

4.6.3   An heuristic approach

In this section we give an heuristic criterion to increment the dimensionality. It is based on verifying if there is any direction, along which the solutions evolves, that can potentially develop stochasticity. The direction we look for "lives " in the complementary of the stochastic subspace generated by the random variable already included in the approximation. In light of that we can assume that the subspace spanned by the new basis function is included in $\mathbb{E}[\mathcal{L}(u(x, t, \cdot), \cdot)]$ and it is governed by the equation for the mean field in the DO system (2.6). According to the DO approach, we have:

$$\frac{\partial baru(\mathbf{x}, t)}{\partial t} = \mathbb{E}[\mathcal{L}(u(x, t, \cdot), \cdot)]$$

Once discretized the time derivative of the mean function by a finite difference, we project it onto the orthogonal to $\mathcal{W}_N$:

$$u^*(\mathbf{x}, t^n) = \Pi_{\mathcal{W}_N^{\top}}\left(\bar{u}(\mathbf{x}, t^{n+1}) - \bar{u}(\mathbf{x}, t^n)\right)/\Delta t$$

We assume that y^* is the stochastic coefficient associated to u^*. At $t = t^n$, y^* is identically zero since the u^* is not included in the stochastic space. In order to verify if y^* is going to increase its variance, according to the DO approach, we estimate:

$$\frac{\partial y^*(t; \omega)}{\partial t} = <\mathcal{L}(u(\cdot, t; \omega); \omega) - \mathbb{E}[\mathcal{L}(u(\cdot, t; \omega); \omega)], u^*>$$

At the discretized level, since y^* is identically zero at t^n we have:

$$y^*(t^{n+1}; \omega) = <\mathcal{L}(u(\cdot, t^{n+1}; \omega); \omega) - \mathbb{E}[\mathcal{L}(u(\cdot, t^{n+1}; \omega); \omega)], u^*> \Delta t$$

Then by computing $[\mathbb{E}[y^*(t^{n+1}, \cdot)^2]$ we have an estimate of the variance along the direction u^*. If that variance is bigger than a threshold we orthonormalize u^* and we include it in the stochastic subspace.

4.6.4   Numerical approach

We give here a brief idea of a possible numerical approach for problem (4.39) We have seen in Section 4.6.1 that the problem of adding the new mode can be re-interpreted in the optimization problem in (4.39). From the computational point of view we adopt the strategy proposed in [16], [17] which consists in sampling the space orthogonal to
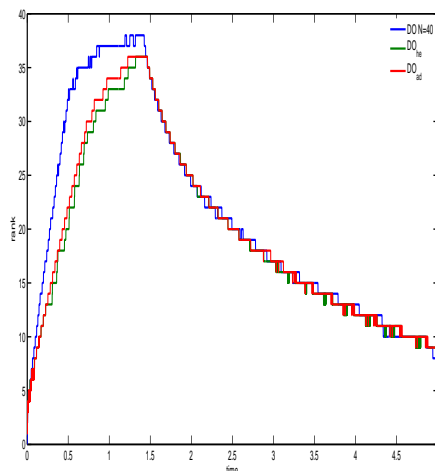
Figure 4.12: The evolution of the rank of the DO approximate solution (blu) with $N = 40$, of the adaptive DO solution (red) with approach in 4.6.4, adaptive DO solution with the heuristic approach (green) in 4.6.3

$\mathcal{W}_N$ (that is the subspace spanned by the basis functions already in the expansion 2.1 of the DO approximate solution). With this aim we apply the Gram-Schmidt method to a finite set of N_2 Fourier basis functions. Alternative we select a finite set of Fourier basis functions and them we project them into the orthogonal to $\mathbf{W}_N$. Say $\phi_1, ..., \phi_{N_2}$ the sampling basis functions, then mode which we are looking for is written as:

$$u^*(\mathbf{x}, \mathbf{t^n}) = \sum_{i=1}^{N_2} a_i^* \phi_i(\mathbf{x}) \tag{4.40}$$

and 4.39 is reduced to:

$$Q(v)^n = a_i a_j < \mathbb{E}[d\mathcal{L}(u_N(\cdot, t^n, \omega); \omega)\phi_i], \, \phi_j >$$

with $v = \sum_{i=1}^{N_2} a_i \phi_i(\mathbf{x})$ Defined

$$Q_{ij} = < \mathbb{E}[d\mathcal{L}(u_N(\cdot, t^n, \omega); \omega)\phi_i], \, \phi_j >$$

the problem 4.39 is reduced to the optimization of the quadratic functional $\tilde{Q} = \dfrac{1}{2}(Q_{ij} + Q_{ji})$ and in conclusion the new basis function is choice to correspond to the eigenvector associated to the maximum eigenvalues of $\tilde{Q}$.

4.6.5   Illustrative example

We apply the method proposed in [16] as well we tested the heuristic approach in 4.6.3 to problem (4.24). This represents a challenging example since the rank of the covariance

matrix fast increases up to large values. Figure 4.12 shows the evolution of the rank of
the DO approximate solution with $N = 40$ and the rank of the adaptive approximate
solutions. Observe that for the adaptive solution the rank corresponds to the number of
modes. Figure 4.12 shows that the dimension of the adaptive solutions well follows the
trend of the rank of the DO approximate solution, which arrives up to the saturation
level. We remark that this section concerns starting results about the adaptive approach
for the DO method, but however they are encouraging for further analysis.

Chapter 5

Conclusion

In this thesis we have investigated a low rank approximation method concerning the Dynamically Orthogonal approach for time dependent PDEs with stochastic parameters or initial data. This consists in developing an approximate solution expanded in terms of mean field, stochastic coefficients and deterministic basis functions, all of them time dependent that adapt to the solution as it evolves. Without imposing any polynomial structure to the term of the expansion we directly look for an approximate solution of the form in DO. This is achieved by projecting at any time instant the residual of the governing SPDE in (2.5) onto the tangent space to $\mathcal{M}_N$, $\mathcal{M}_N$ the manifold where all the rank N stochastic fields. Then we recover a coupled system of evolution equations for all the terms of the expansion (2.1), which consists in N+1 deterministic PDEs plus N stochastic ODEs. This allows to evolve a low rank solution that adapts at each time instant both the basis functions and the deterministic coefficients to what best describes the global structure of the solution. This idea suggests some relationships between the DO approximate solution and the N-truncated KL expansion.

On the other hand we showed that the DO approach and DDO decomposition provide the same numerical solution if a Galerkin formulation is adopted. This is a remarkable and encouraging starting point since convergence and error estimates are present in the literature for the DDO decomposition in finite dimensional setting. In particular it is shown that for evolution matrix equations the error of the DDO approximate solution is bounded in terms of optimal approximation error, under specific conditions. In light of that we investigated the relationships between the DO approach and the N truncated KL expansion, that is a representation of the best N rank approximation in mean square sense. We first focused on liniar parabolic diffusion equations with initial stochastic condition. In this framework theoretical considerations, confirmed by numerical tests, show that the DO approximate solution coincides with the optimal one only under very strong assumptions and that generally the convergence rate of the error is determined by the smallest eigenvalue of the Laplace operator. However we remark that the KL expansion does not represents an alternative method to the DO approach but a lower bound for the approximation error. Encouraging numerical results are provided by the analysis of the more challenging problem, governed by a parabolic diffusion equations with

non linear reaction term with initial stochastic condition, where we see that the error of *DO* approximate solution results is proportional to the optimal error and decreases with the same rate. In conclusion, even if the question remains already open, the achieved results make the DO approach suitable to a further analysis. In view of that, the probably more interesting feature of the DO approach concerns the adaptability of the dimension. As we have seen in the analysis of parabolic equations with non linear reaction term, during the evolution of the process the effective rank of the solution might significantly change. If decreasing the dimensionality is an easy task, the questions concerning when add and how to select new directions is already open. The starting results show that this is suitable and effective approach and furthermore several strategies can be investigated. We tested the idea of dimension adaptability by following the approach proposed in [17], [16] which consists in sampling the space orthogonal to the modes already included in the approximation, but more effective method can be investigated. One of the more promising is maybe a method based on power-type or Arnoldi iteration, in the same spirit as what proposed in [37].

Bibliography

[1] I. T. Jolli e, *Principal component analysis*, second ed., Springer Series in Statistics (SpringerVerlag, 2002).

[2] O.P. Le Maitre, O.M. Knio, *Spectral methods for uncertainty quantifcation*, Springer, 2010.

[3] F. Nobile and R. Tempone. Analysis and implementation issues for the numerical approximation of parabolic equations with random coefficients. *Int. J. Num. Methods Engrg.*, 80(6-7): 979-1006, 2009. Special Issue: Uncertainty Quanti cation in Computational and Prediction Science.

[4] I. Babuska, R. Tempone, and G. E. Zouraris, Galerkin finite element approximations of stochastic elliptic partial differential equations, SIAM J. Numer. Anal. 42 (2004) 800-825.

[5] S. Salsa, *Partial Differential Equations in Action: From Modelling to Theory*, Springer-Verlag, 2008

[6] R.J. Alder, J.E. Taylor, *Random Fields and Geometry*, Springer, 2007

[7] F. Nobile, R. Tempone, C. G. Webster, A sparse grid stochastic collocation method for partial differential equations with random input data. SIAM Journal, Vol. 46, No.5, pp. 2309-2345

[8] X. Wan and G.E. Karniadakis. Long-term behavior of polynomial chaos in stochastic flow simulations. *Comput. Methods Appl. Mech. Engrg.*, 195(41-43): 5582-5596, 2006. Art 5 da citare

[9] H. G. Matthies and A. Keese. Galerkin methods for linear and nonlinear elliptic stochastic partial differential equations. *Comput. Methods Appl. Mech. Engrg.*, 194(12-16):1295 1331, 2005.

[10] C. Lubich, T. Rohwedder, R. Schneider, and B. Vandereycken. Dynamical approximation of hierarchical tucker and tensor-train tensors. MATHICSE Technical Report 28.2012, École Polytechnique Fédérale de Lausanne, 2012.

[11] O. Koch and C. Lubich. Dynamical tensor approximation. SIAM J. *Matrix Anal. Appl.*, 31(5):2360 2375, 2010.

[12] O. Koch and C. Lubich. Dynamical low-rank approximation. SIAM J. *Matrix Anal. Appl.*, 29(2):434 454, 2007.

[13] V. Heuveline and M. Schick. A local time dependent generalized polynomial chaos method for stochastic dynamical systems. EMCL Preprint Series 04, EMCL, Karlsruhe Institute of Technology, 2011.

[14] M. Gerritsma, J-B. van der Steen, P. Vos, and G. Karniadakis. Time-dependent generalized polynomial chaos. *J. Comput. Phys.*, 229(22):8333-8363, 2010.

[15] M.S. Eldred. Recent advances in non-intrusive polynomial chaos and stochastic collocation methods for uncertainty analysis and design. In AIAA, 2009.

[16] Themistoklis P. Sapsis, and Pierre F.J. Lermusiaux, Dynamical criteria for the evolution of the stochastic dimensionality in flows with uncertainty, Physica D, 241(2-12) 60-76.

[17] Themistoklis P. Sapsis and Pierre F.J. Lermusiaux, Dynamically orthogonal field equations for continuous stochastic dynamical systems, Physica D, 238 (2009) 2347-2360.

[18] F. Nobile, R. Tempone and C. Webster, An anisotropic sparse grid stochastic collocation method for partial differential equations with random input data, SIAM J. Numer. Anal., 2008, vol. 46/5, pp. 2411-2442.

[19] M. P. Ueckermanna, P. F. J. Lermusiauxa, and T. P. Sapsis, Numerical Schemes for Dynamically Orthogonal Equations of Stochastic Fluid and Ocean Flows, J. Comput. Phys., submitted

[20] A. Quarteroni A. Valli Numerical Approximation of Partial Differential Equations. Springer-Verlag, Berlin Heidelberg, 1994

[21] J. Beck, F. Nobile, L. Tamellini, R. Tempone, *Optimal polynomial approximation of stochastic PDEs by Galerkin and Collocation methods* MOX report, 23/2011.

[22] I. Babuŝka, F. Nobile, R. Tempone, *A stochastic collocation method for elliptic partial differential equations with random input data*, SIAM REVIEW Vol. 52, No. 2, pp. 317-355.

[23] R. G. Ghanem and P. D. Spanos, *Stochastic finite elements: a spectral approach* (Springer Verlag, 1991).

[24] B. Ganapathysubramanian and N. Zabaras, Sparse grid collocation schemes for stochastic natural convection problems, *Journal of Computational Physics* 225 (2007) 652-685.

[25] N. Wiener, The homogeneous chaos, American Journal of Mathematics 60 (4) (1938) 897-936.

[26] D. Xiu, G. Karniadakis, The Wiener-Askey polynomial chaos for stochastic differential equations, SIAM Journal on Scientific Computing 24 (2) (2002) 619-644.

[27] J. Stoer, R. Bulirsch, Introduction to Numerical Analysis, Springer-Verlag, New York, 1979.

[28] A.J. Pullan, M.L. Buist, L.K. Cheng *Mathematically Modelling the Electrical Activity of the Heart* World Scientific Co. Pte. Ltd.

[29] J. Keener, J. Sneyd *Mathematical Physiology* Springer

[30] R.H. Cameron, W.T. Martin, The orthogonal development of non-linear functionals in series of Fourier-Hermite functionals, Annals of Mathematics 48(2) (1947) 385-392.

[31] R. A. Todor and C. Schwab. Convergence rates for sparse chaos approximations of elliptic problems with stochastic coe cients. IMA J Numer Anal, 27(2):232-261, 2007.

[32] A. Cohen, R. Devore, and C. Schwab. Analytic regularity and polynomial approximation of parametric and stochastic elliptic PDE's. Anal. Appl. (Singap.), 9(1):11-47, 2011.

[33] D. Xiu and J.S. Hesthaven. High-order collocation methods for differential equations with random inputs. SIAM J. Sci. Comput., 27(3):1118-1139,2005

[34] T. Zhou, F. Nobile *On Dynamically Orthogonal Fields Approach for Time Depen dent Stochastic PDE*: in preparation

[35] G. Haller and T.P. Sapsis. *Localized instability and attraction along invariant manifolds*. SIAM J. of Appl. Dynamical Systems, 9:611-633, 2010

[36] G.wanner, E.Hairer, C. Lubich *Geometric Numerical Integrtion: Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer

[37] L. Tamellini, O. Le Maitre, and A. Nouy. Model reduction based on proper generalized decomposition for the stochastic steady incompressible navier-stokes equations. MOX-Report 26/2012, Department of Mathematics, Politecnico di Milano, Italy, 2012. submitted