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Sparse high order FEM for elliptic sPDEs

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Abstract

We describe the analysis and the implementation of two Finite Element (FE) algorithms for the deterministic numerical solution of elliptic boundary value problems with stochastic coefficients.

They are based on separation of deterministic and stochastic parts of the input data by a Karhunen-Loève expansion, truncated after M terms. With a change of measure we convert the problem to a sequence of M-dimensional, parametric deterministic problems. Two sparse, high order polynomial approximations of the random solution's joint pdf's, parametrized in the input data's Karhunen-Loève expansion coordinates, are analyzed: a *sparse stochastic Galerkin FEM* (sparse sGFEM) and a *sparse stochastic Collocation FEM* (sparse sCFEM).

A-priori and a-posteriori error analysis is used to tailor the sparse polynomial approximations of the random solution's joint pdf's to the stochastic regularity of the input data. sCFEM and sGFEM yield deterministic approximations of the random solutions joint pdf's that converge spectrally in the number of deterministic problems to be solved.

Numerical examples with random inputs of small correlation length in diffusion problems are presented. High order gPC approximations of solutions with stochastic parameter spaces of dimension up to $M = 80$ are computed on workstations.

1 Introduction

Many engineering models of physical phenomena are subject to significant uncertainties. We mention subsurface flow, soil mechanics, earthquake engineering, to name but a few. Uncertainty can be crudely categorized as *aleatoric* (inherent parameter uncertainty) and *epistemic* (model uncertainty). Aleatorically uncertain quantities are very often modeled as random fields, see e.g. [1, 37]. Neglecting epistemic uncertainty, PDE models with aleatoric uncertainty can be formulated as stochastic partial differential equations (sPDEs).

Numerical analysis and implementational aspects for the solution of such equations by stochastic Galerkin Finite Element Method (sGFEM) and stochastic collocation FEM (sCFEM) will be the focus of this paper.

As in [2, 3, 8, 16, 39, 40, 44], our model problem is an elliptic diffusion problem with stochastic diffusion coefficient $a(\omega, \mathbf{x})$ (most, if not all techniques introduced here could be applied equally well to general elliptic problems with stochastic coefficients). We assume that the physical domain $D \subset \mathbb{R}^d$ is a known, bounded open set with Lipschitz boundary ∂D where, in the present work, d is either 1 or 2. We also consider a "zero-dimensional" model problem which admits a closed form solution in order to steer a feedback algorithm for adaptive discretization in probability space (see Section 2.6 and Algorithm 3.8 below).

By X we denote a Banach space of admissible input data for the PDE under consideration. Specifically, for isotropic diffusion problems with stochastic coefficients, we will have $X = L^\infty(D)$ or a separable subspace of it.

For *mathematical modelling of uncertainty in input data*, we specify "events" which correspond here to (sets of) possible realizations of random diffusion coefficients; the set of all possible realizations of coefficients is a sigma algebra Σ which we assume to be a sub-sigma algebra of the Borel sets of the data space X and a probability measure P on (Σ, X). The choice of Σ and P on the data space X is used to describe the information known to us on the data – roughly speaking, the larger Σ, the more information we assume can in principle be known. We adopt a particular construction of measures P based on the covariance operator of the input data detailed in Remark 2.11. To this end, we make the following assumption on the random diffusion coefficient $a(\omega, \mathbf{x})$.

Assumption 1.1. Let $a \in L^\infty(\Omega \times D)$ be strictly positive, with lower and upper bound $\alpha > 0$ and $\beta < \infty$ respectively, i.e.

$$P\left\{a(\omega,\cdot) \in X | \alpha \leq \operatorname*{ess\,inf}_{\mathbf{x}\in D} a(\omega,\mathbf{x}) \ \wedge \ \operatorname*{ess\,sup}_{\mathbf{x}\in D} a(\omega,\mathbf{x}) \leq \beta\right\} = 1 \tag{1.1}$$

where the essential infimum and supremum are understood with respect to the Lebesgue Measure in $D \subset \mathbb{R}^d$.

Some form of boundedness away from zero for $a(\omega, \mathbf{x})$ holding P-a.s. is essential to guarantee existence and uniqueness of a solution to the diffusion problem with stochastic coefficient introduced next, see e.g. [3].

Under Assumption 1.1, our model problem can be formally written as

$$\begin{cases} -\mathrm{div}(a(\omega,\mathbf{x})\nabla u(\omega,\mathbf{x})) = f(\mathbf{x}) \quad D, \\ u(\omega,\mathbf{x})|_{\mathbf{x}\in\partial D} = 0, \end{cases} \quad P\text{−a.e. } \omega \in \Omega \tag{1.2}$$

where the diffusion coefficient $a(\omega, \mathbf{x})$ and the solution $u(\omega, \mathbf{x})$ are random fields in the spatial domain D.

We emphasize that neither homogeneity nor ergodicity of the input random field $a(\omega, \mathbf{x})$ are usually available in practice. Accordingly, they are not assumed in the

following. Based on the stochastic input data $a(\omega, \mathbf{x})$, solutions $u(\omega, \mathbf{x})$ of (1.2) are themselves random fields.

Our goal is to compute statistical quantities of the random solution $u(\omega, \mathbf{x})$.

The simplest approach for deriving the statistics of $u(\omega, \mathbf{x})$ is Monte Carlo (MC) simulation, see e.g. [9]. This means that given the prescribed statistics of $a(\omega, \mathbf{x})$, a set of N_Ω many, i.i.d coefficient samples $a_j(\mathbf{x})$ is generated and, for each sample, a (deterministic) PDE is solved. Then, the desired solution statistics are obtained from the set (or "ensemble") of computed solutions of the deterministic PDEs obtained from inserting the (numerically generated) data samples. A first comparison of accuracy vs. complexity between this Monte Carlo Approach and the stochastic Galerkin (sG) strategy is given in [3]. Even though the sG error analysis in [3] was based on full tensor product error estimates, it substantiated mathematically the potential superiority of the sG approach over MC type methods, at least in certain cases (e.g. dominant long-range spatial correlations in input data with smooth two-point correlation matrix) which had earlier also been reported in numerical experiments (e.g. [13] and the references therein). The MC method allows a convergence rate of $O(N_\Omega^{-1/2})$ for approximating the random solution's mean field, see e.g. [3]. The rate for computing higher order moments by a MC approach might be even lower.

Sparse approximations of higher order moments together with a perturbation approach for problem (1.2) leads to a class of deterministic algorithms for the approximation of $\mathcal{M}^k u$, see [30, 31, 36, 38]. These FEM are of log-linear complexity in N_D, the number of degrees of freedom in the physical domain D. Like all perturbation methods, they require even for computing the mean field $\mathbb{E}[u]$ knowledge of the distribution function of the random input $a(\cdot, \mathbf{x})$ at any $\mathbf{x} \in D$, which is not a realistic assumption.

The sGFEM and sCFEM discussed here are based on the following assumption on $a(\omega, \mathbf{x})$:

Assumption 1.2. For the diffusion coefficient $a(\omega, \mathbf{x})$, the mean field

$$\mathbb{E}_a(\mathbf{x}) = \int_\Omega a(\omega, \mathbf{x})\, dP(\omega) \tag{1.3}$$

and covariance

$$V_a(\mathbf{x}, \mathbf{x}') = \int_\Omega (a(\omega, \mathbf{x}) - \mathbb{E}_a(\mathbf{x}))(a(\omega, \mathbf{x}') - \mathbb{E}_a(\mathbf{x}'))\, dP(\omega). \tag{1.4}$$

are known.

An equivalent assumption would be that the mean field $\mathbb{E}_a$ and the 2-point-correlation C_a are known, since

$$V_a(\mathbf{x}, \mathbf{x}') = C_a(\mathbf{x}, \mathbf{x}') - \mathbb{E}_a(\mathbf{x})\mathbb{E}_a(\mathbf{x}'). \tag{1.5}$$

Note that for V_a and C_a to exist, $a(\omega, \mathbf{x})$ must have finite second moments ($a \in L^2(\Omega \times D)$) which follows immediately from Assumption 1.1. The source term $f(\mathbf{x})$ is assumed to be a known deterministic function of $L^2(D)$. Both methods consist not only of discretizing the spatial variable $\mathbf{x}$ but also the stochastic variable ω which is usually based on a *Wiener* polynomial chaos or *generalized polynomial chaos* (PC/gPC) expansion, see [41, 43]. This approach leads to a parametric family of deterministic problems with a countable number of parameters. For the deterministic approximation, the number of parameters is restricted to a finite number M.

Note that *the truncation dimension M of the PC parameter space can be arbitrarily large in this approach* - it is, in fact, a discretization parameter. The sGFEM

is the mean-square projection of the unknown random solution onto a *sparse polynomial chaos* (SPC) expansion in the first M Karhunen-Loève parameters of the input data.

Similar ideas lead to a sparse collocation method, the sCFEM, where we present a sparse tensor family of collocation points which lead to an sCFEM algorithm. We prove that it has essentially the same complexity as the sGFEM, but without the need for the solution of a large number of coupled, deterministic problems. However, the sCFEM *requires pointwise control of the error incurred in the truncation of the Karhunen-Loève expansion* whereas for any choice of the SPC space, *the sGFEM is, due to Galerkin orthogonality and unlike the sCFEM, exact on the full KL-expansion of the input data*, as observed by Matthies et al. [21] (cf. also Remark 3.2 ahead).

The outline of the paper is as follows: in Section 2 our formulation of PDEs with stochastic input data is presented, starting with some basic results on Karhunen-Loève expansions of the input data, deriving the variational formulation and introducing a "zero-dimensional" model problem.

Section 3 then discusses the stochastic Galerkin FEM. A particular family of sparse polynomial chaos approximation spaces first introduced in [35] will be presented. We prove that based on these spaces and under the assumption of piecewise analytic two-point correlation of the diffusion coefficient, the sGFEM achieves *exponential convergence rates in terms of the degree of the gPC approximations*. More importantly, we estimate the dimension of the gPC space and prove *spectral convergence rates in terms of the number N_Ω of deterministic PDEs to be solved*.

Section 4 briefly describes the stochastic collocation method by using the ideas and constructions of the previous section and states the second main results providing essentially the same convergence rates as for the sGFEM. Section 5 deals with details regarding the implementation of the proposed algorithms and in Section 6, numerical examples will be given. Finally, the technical Appendices A and B provide the proofs of the convergence rates of the SPC approach and the collocation method, respectively. We point out that (1.2) is just a model problem. The numerical analysis and implementation can be generalized straightforward to any stochastic elliptic operator. The FE-space in the deterministic variable and the assumptions on the stochastic coefficients will then in general change.

2 Uncertainty parametrization

In the deterministic numerical solution of problem (1.2), the random field $a(\omega, \mathbf{x})$ is based on its parametrization in both the spatial and the stochastic variables. This is achieved by expanding the stochastic diffusion coefficients into a so-called *Karhunen-Loève* (KL) expansion described in Subsection 2.1, which is a Fourier-type representation of random fields in probability space. Based on this parametrization the problem (1.2) will be solved by either a stochastic Galerkin finite element method (sGFEM), Section 3 (corresponding to a maximum likelihood estimate of the random solution's joint pdf's) or a stochastic collocation method (sCFEM), Section 4 (corresponding to MC-like sampling of the solution's joint pdf's, albeit in sampling points adapted to the input data's regularity).

2.1 Karhunen-Loève (KL) expansion

The KL-expansion can be understood as a Fourier representation of a random field in which the spatial and stochastic parts are naturally separated into an infinite number of random variables $\alpha_i(\omega)$ and functions $N_i : D \subset \mathbb{R}^d \longrightarrow \mathbb{R}$ (for example

finite element shape functions) in the sense of

$$a(\omega, \mathbf{x}) = \sum_{m \geqslant 0} N_m(\mathbf{x}) \alpha_m(\omega).$$

There exist infinitely many such representations, see e.g. [17]. We use the Karhunen-Loève expansion [19].

2.1.1 Definition of the KL-expansion

First we define what we will later refer to as an *admissible covariance function*

Definition 2.1. A covariance function $V_a(\mathbf{x}, \mathbf{x}') \in L^2(D \times D)$ given by (1.4) is said to be admissible if it is symmetric and positive definite in the sense that

$$0 \leqslant \sum_{k=1}^{n} \sum_{j=1}^{n} a_k V_a(x_k, x_j) \bar{a}_j \qquad \forall x_k, x_j \in D,\ a_k, a_j \in \mathbb{C} \tag{2.1}$$

We refer to [28] for basic results on positive definite functions and examples.

The covariance operator of a random permeability $a(\omega, \mathbf{x}) \in L^2(\Omega \times D)$ is

$$\mathcal{V}_a : L^2(D) \longrightarrow L^2(D), \quad (\mathcal{V}_a u)(\mathbf{x}) := \int_D V_a(\mathbf{x}, \mathbf{x}') u(\mathbf{x}')\, d\mathbf{x}'. \tag{2.2}$$

Given an admissible covariance function $V_a(\mathbf{x}, \mathbf{x}')$ in the sense of Definition 2.1, the associated covariance operator $\mathcal{V}_a$ is a symmetric, non-negative and compact integral operator.

Therefore it has a countable sequence of eigenpairs $(\lambda_m, \varphi_m)_{m \geqslant 1}$

$$\mathcal{V}_a \varphi_m = \lambda_m \varphi_m \qquad m = 1, 2, ... \tag{2.3}$$

where the sequence (real and positive) KL-eigenvalues λ_m is enumerated with decreasing magnitude and is either finite or tends to zero as $m \to \infty$, i.e. $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant 0$ (with multiplicity counted). The KL-eigenfunctions $\varphi_m(\mathbf{x})$ are assumed to be $L^2(D)$-orthonormal, i.e.

$$\int_D \varphi_m(\mathbf{x}) \varphi_n(\mathbf{x}) d\mathbf{x} = \delta_{mn}, \qquad m, n = 1, 2, ... \tag{2.4}$$

Definition 2.2 (Karhunen-Loève expansion)**.** The Karhunen-Loève (KL) expansion of a random field $a(x, \omega)$ with finite mean (1.3) and covariance (1.4) which is admissible in the sense of Definition 2.1 is given by

$$a(\omega, \mathbf{x}) = \mathbb{E}_a(\mathbf{x}) + r(\omega, \mathbf{x}) = \mathbb{E}_a(\mathbf{x}) + \sum_{m \geqslant 1} \sqrt{\lambda_m} \varphi_m(\mathbf{x}) Y_m(\omega). \tag{2.5}$$

Here, $\{\varphi_m(x)\}_{m=1}^{\infty}$ denote the $L^2(D)$-orthonormalized KL-eigenfunctions. The family of random variables $(Y_m)_{m \geqslant 1}$ is given by

$$Y_m(\omega) = \frac{1}{\sqrt{\lambda_m}} \int_D (a(\omega, \mathbf{x}) - \mathbb{E}_a(\mathbf{x})) \varphi_m(\mathbf{x})\, d\mathbf{x} : \Omega \to \mathbb{R}. \tag{2.6}$$

The KL-eigenfunctions $\varphi_m(\mathbf{x})$ in (2.3) - (2.6) can be efficiently computed in general domains D from a given, analytic covariance $V_a(\mathbf{x}, \mathbf{x}')$ of the data by means of a (generalized) Fast Multipole Method (gFMM), see [32]. Once the $\varphi_m(\mathbf{x})$ are available, probability densities $\rho_m(x_m)$ of the Y_m in (2.6) may be estimated from

sample input fields $a(\omega, \mathbf{x})$ — the KL-eigenfunctions are, in effect, a tool to process such sampling data via (2.6).
One immediately verifies that

$$\mathbb{E}[Y_m] = 0, \quad \mathbb{E}[Y_m \cdot Y_n] = \delta_{mn}, \quad \forall\, m, n \geqslant 1, \tag{2.7}$$

i.e. the $Y_m(\omega)$ are centered with unit variance and pairwise uncorrelated.

In order to be able to numerically treat the KL-expansion, the series is truncated after M terms, and we define

$$a_M(\omega, \mathbf{x}) := \mathbb{E}_a(\mathbf{x}) + \sum_{m=1}^{M} \sqrt{\lambda_m}\varphi_m(\mathbf{x})Y_m(\omega). \tag{2.8}$$

2.1.2 Properties of the KL-expansion

The (truncated) KL-series (2.8) converges in $L^2(\Omega \times D)$ to $a(\omega, \mathbf{x})$ as shown in [19] and is an optimal approximation of $a(\omega, \mathbf{x})$ in the mean square sense, that is for any other linear combination $\tilde{a}_M(\omega, \mathbf{x})$ of M functions, the error $||a(\omega, \mathbf{x}) - \tilde{a}_M(\omega, \mathbf{x})||_{L^2(\Omega\times D)}$ is not smaller than for the KL-expansion, see e.g. [13]. Since the truncation order M determines the dimension of the stochastic parameter space in which we have to find an approximation to the random solution, the Karhunen-Loève expansion is therefore our preferred choice. Estimates on the KL-eigenvalue decay determine the error of truncating the KL-expansion after M terms due to

$$\mathbb{E}\left[\int_D \left(a(\omega, \mathbf{x}) - a_M(\omega, \mathbf{x})\right)^2 d\mathbf{x}\right] = \sum_{m>M} \lambda_m \tag{2.9}$$

The KL-eigenvalue decay in turn is highly dependent on the regularity of the correlation kernel (1.4). First results on the eigenvalue decay of integral operators with positive definite kernels have been proved by J.B. Reade [25, 26, 18]. The results presented in the following are an extension of those results to the case $d > 1$.

Proposition 2.3 (KL-eigenvalue decay([32], Proposition 2.18))**.**
Let $V_a \in L^2(D \times D)$ be a symmetric covariance satisfying (2.1). If V_a is piecewise analytic on $D \times D$, i.e. there exists a finite family $(D_i)_{1\leqslant i\leqslant I} \subset \mathbb{R}^d$ of mutually disjoint, open subdomains of D such that $\overline{D} \subseteq \bigcup_{i=1}^{I} \overline{D_i}$ and $V|_{D_i\times D_j}$ has an analytic continuation in a neighborhood of $\overline{D_i} \times \overline{D_j}$ for any pair (i, j), then there exist constants $c_1, c_2 > 0$ such that

$$0 \leqslant \lambda_m \leqslant c_1 e^{-c_2 m^{\kappa}}, \quad \forall\, m \geqslant 1 \tag{2.10}$$

where $\kappa := 1/d$. If $V_a \in L^2(D \times D)$ has piecewise $C^s(D \times D)$ regularity,

$$\forall\, m \geqslant 1: \qquad 0 \leqslant \lambda_m \leqslant c_1 m^{-\kappa s}. \tag{2.11}$$

Remark 2.4. The case of a Gaussian covariance kernel of the form

$$V_a(\mathbf{x}, \mathbf{x}') = \sigma^2 e^{-\frac{|\mathbf{x}-\mathbf{x}'|^2}{\gamma^2 \mathrm{diam}(D)^2}}, \qquad (\mathbf{x}, \mathbf{x}') \in D \times D, \tag{2.12}$$

is particularly interesting since it appears in many applications. The fact that this function can be extended to an entire function in $\mathbb{C}^d$ leads to a faster than exponential KL-eigenvalue decay, namely

$$0 < \lambda_m \lesssim \frac{\sigma^2}{\gamma^2} \frac{(1/\gamma)^{m^{1/d}}}{\Gamma(0.5m^{1/d})}, \quad \forall\, m \geqslant 1. \tag{2.13}$$

A proof of this assertion is given in Appendix C. The parameters $\sigma, \gamma > 0$ in (2.12) and (2.13) refer to the standard deviation and the correlation length, respectively.

Regularity of the correlation kernel implies pointwise estimates on the eigenfunctions $\varphi_m(\mathbf{x})$ of the associated covariance operator ([32], Proposition 2.24):

Proposition 2.5 (Pointwise eigenfunction estimate)**.** *Let $V_a(\mathbf{x}, \mathbf{x}')$ be symmetric and piecewise C^s, $s \geq 1$ in the sense of Proposition 2.3. For any fixed multiindex $\alpha \in \mathbb{N}_0^d$ and any $t > 0$ there exists $C(t, |\alpha|) > 0$ such that*

$$\forall 1 \leqslant i \leqslant I, \forall m \geqslant 1 : \qquad ||\partial^\alpha \varphi_m||_{L^\infty(D_i)} \leqslant C\lambda_m^{-t}. \tag{2.14}$$

Remark 2.6. From Proposition 2.3 and (2.14) it follows that for covariances which are piecewise analytic in the sense of Proposition 2.3 there exist constants $c_1(|\alpha|) > 0$ and $c_2 > 0$ independent of m, such that for all $\alpha \in \mathbb{N}_0^d$ we have *pointwise exponential decay* of the KL-terms in the following sense:

$$\forall m \in \mathbb{N}, \alpha \in \mathbb{N}^d : \qquad \sqrt{\lambda_m}||\partial^\alpha \varphi_m||_{L^\infty(D_i)} \leqslant c_1 e^{-c_2 m^\kappa}. \tag{2.15}$$

Similarly, for covariances which are piecewise C^s in the sense of Proposition 2.3 there exist constants $c_1(|\alpha|) > 0$ and $c_2 > 0$ independent of m, such that for all $\alpha \in \mathbb{N}_0^d$ we have *pointwise algebraic decay* of the KL-terms in the following sense:

$$\forall m \in \mathbb{N}, \alpha \in \mathbb{N}^d : \qquad \sqrt{\lambda_m}||\partial^\alpha \varphi_m||_{L^\infty(D_i)} \leqslant c_1 m^{-\kappa s}. \tag{2.16}$$

Recall that in (2.15), (2.16) we have $\kappa = 1/d$. The pointwise KL-eigenfunction bounds (2.15), (2.16) in terms of the KL-eigenvalues are crucial in the (uniform in M) stability of the sCFEM.

2.1.3 Structure of the probability measure P

In the following we assume that the diffusion coefficient $a(\omega, \mathbf{x})$ satisfies (1.1) and admits a Karhunen-Loève expansion (2.5). Furthermore we require

Assumption 2.7. The covariance (1.4) is admissible and piecewise analytic in the sense of Proposition 2.3.

We also make the following assumptions on the random variables Y_m in the KL-representation (2.5) of the input data.

Assumption 2.8. i) The family $(Y_m)_{m\geqslant 1} : \Omega \to \mathbb{R}$ is *independent*,

ii) the KL-expansion (2.5) of the input data is finite, i.e. there exists $\bar{M} < \infty$ such that $Y_m = 0$ for all $m > \bar{M}$,

iii) with each $Y_m(\omega)$ in (2.5), (2.6) is associated a probability space $(\Omega_m, \Sigma_m, P_m)$, $m \in \mathbb{N}$ with the following properties:

   a) the range of Y_m, $I_m := \mathrm{Ran}(Y_m) = \mathrm{supp}(\rho_m) \subseteq \mathbb{R}$, is assumed to be compact,

   b) the probability measure P_m admits a probability density function $\rho_m : I_m \longrightarrow [0, \infty)$ such that $dP_m(\omega) = \rho_m(y_m)dy_m$, $m \in \mathbb{N}$, $y_m \in I_m$ and

   c) the sigma algebras Σ_m are subsets of the Borel sets of the interval I_m, i.e. $\Sigma_m \subseteq \mathcal{B}(I_m)$.

Assumption 2.8, ii) is made to be able to represent the measure P on the space of input data as an $\bar{M}$-fold product measure and to avoid technical issues related to countable product measures on the space X of input data. We have

$$\Sigma = \bigotimes_{m\geqslant 1} \Sigma_m, \quad dP = \bigotimes_{m\geqslant 1} dP_m, \quad I = \bigotimes_{m\geqslant 1} I_m$$

Assumption 2.8, iiia) is used in our analysis ahead in an essential fashion. It precludes the case of Gaussian densities for the Y_m. Upon rescaling the Y_m, by Assumption 2.8, iiib) it can be assumed without loss of generality that

$$I_m = \mathrm{Ran}(Y_m) \subset [-1, 1], \quad \forall\, m \geqslant 1.$$

Remark 2.9. In general, (2.7) does not imply independence of the random variables. The case of dependent random variables has been treated in [33] where an orthonormal system of polynomials are constructed to serve as a basis for the chaos representation. An alternative way of overcoming the problem of dependent RV's has been proposed in [2] by introducing auxiliary probability density functions $\tilde{\rho}_m$ with $\|\rho_m/\tilde{\rho}_m\|_{L^\infty}$ such that the random variables Y_m are independent with respect to $\tilde{\rho} = \prod_{m\geqslant 1} \tilde{\rho}_m$.

2.2 Variational formulation of the sBVP

Multiplying (2.25) with a test function and integrating yields the variational formulation: Find $u \in L^2_P(\Omega) \otimes H^1_0(D)$ such that $\forall\, v \in L^2_P(\Omega) \otimes H^1_0(D)$

$$b(u, v) := \mathbb{E}\left[\int_D a(\omega, \mathbf{x}) \nabla u(\omega, \mathbf{x}) \cdot \nabla v(\omega, \mathbf{x})\, d\mathbf{x}\right] = \mathbb{E}\left[\int_D f(\mathbf{x}) v(\omega, \mathbf{x})\, d\mathbf{x}\right]. \quad (2.17)$$

By (1.1), the bilinear form $b(\cdot, \cdot)$ is continuous and coercive on the Hilbert space $L^2_P(\Omega) \otimes H^1_0(D)$.

2.3 Parametric deterministic formulation of the sBVP

As a consequence of the independence in Assumption 2.8, the multivariate probability density on $I = I_1 \times I_2 \times \ldots$ is given by

$$\rho(\mathbf{y}) = \rho(y_1, \ldots, y_m, \ldots) := \Pi_{m\geqslant 1} \rho_m(y_m). \quad (2.18)$$

We substitute $Y_m(\omega)$ by y_m and equip the range I of the vector $(Y_1, Y_2 ...)$ with the product measure $dP(\omega) = \bigotimes_{m\geqslant 1} \rho_m(y_m) dy_m$. Changing measure from $dP(\omega)$ to $\Pi_{m\geqslant 1}\rho_m(y_m)dy_m$, problem (2.17) *is equivalent to the parametric, deterministic problem*

$$-\mathrm{div}(a(\mathbf{y}, \mathbf{x}) \nabla u(\mathbf{y}, \mathbf{x})) = f(\mathbf{x}) \quad \mathbf{y} \in I,\, \mathbf{x} \in D \quad (2.19)$$

where $\mathbf{y} = (y_1, y_2 \ldots)$. Its variational form reads:
Find $u \in L^2_\rho(I) \otimes H^1_0(D)$ such that $\forall\, v \in L^2_\rho(I) \otimes H^1_0(D)$

$$b(u, v) = l(v). \quad (2.20)$$

with

$$\begin{aligned} b(u, v) &= \mathbb{E}\left[\int_D a(\cdot, \mathbf{x}) \nabla u(\cdot, \mathbf{x}) \cdot \nabla v(\cdot, \mathbf{x})\, d\mathbf{x}\right] \quad (2.21) \\ &= \int_I \int_D a(\mathbf{y}, \mathbf{x}) \nabla u(\mathbf{y}, \mathbf{x}) \cdot \nabla v(\mathbf{y}, \mathbf{x}) \rho(\mathbf{y})\, d\mathbf{x} d\mathbf{y} \end{aligned}$$

and

$$l(v) = \mathbb{E}\left[\int_D f(\mathbf{x}) v(\cdot, \mathbf{x})\, d\mathbf{x}\right] = \int_I \int_D f(\mathbf{x}) v(\mathbf{y}, \mathbf{x}) \rho(\mathbf{y})\, d\mathbf{x} d\mathbf{y}. \quad (2.22)$$

2.4 Stochastic Regularity

By stochastic regularity we mean the *smoothness of the parametrized random solution* $u(\mathbf{y}, \mathbf{x})$ with respect to the parameters $\mathbf{y}$. It can be shown that the solution to (2.19) is analytic with respect to $\mathbf{y}$. We have ([2], Lemma 5)

Lemma 2.10. *The solution $u(\mathbf{y})$ as a function of y_m admits an analytic extension to the region of the complex plane*

$$\Sigma(I_m, \tau_m) = \{z \in \mathbb{C} : \mathrm{dist}(z, I_m) \leqslant \tau_m\}, \tag{2.23}$$

with $0 < \tau_m < 1/\eta_m$, where

$$\eta_m = \frac{\sqrt{\lambda_m}||\varphi_m(x)||_{L^\infty(D)}}{2a_{\min}} \tag{2.24}$$

and $a_{\min} = \alpha$ as in (1.1).

In particular there exists a so-called "Bernstein-ellipse" in $\mathbb{C}$ with foci at $\Re z = \pm 1$ and for which the sum of semiaxes is bigger than 1, s.t. $u(\mathbf{y}, \mathbf{x})$, as a function of y_m for $m \leq \bar{M}$, is analytic in the closure of the Bernstein-ellipse, *uniformly with respect to y_i for all $i \neq m$.*

2.5 Dimension Reduction

The parametric deterministic problem (2.19) is, in principle, amenable to numerical treatment by standard discretization schemes. However, in general $\bar{M}$ in Assumption 2.8 could be prohibitively large and a reduction of the (possibly infinite) stochastic dimension to a finite, possibly large, value M, is necessary. To this end, the "truncated problem"

$$\begin{cases} -\mathrm{div}(a_M(\omega, \mathbf{x})\nabla u_M(\omega, \mathbf{x})) = f(\mathbf{x}) & D, \\ u_M(\omega, \mathbf{x})|_{\mathbf{x}\in\partial D} = 0, \end{cases} \quad P-\text{a.e. } \omega \in \Omega \tag{2.25}$$

is considered, where the truncated KL-expansion $a_M(\omega, \mathbf{x})$ of the input data is as in (2.8). It has been shown in [3] that due to Assumption 1.1 there exists a unique solution to problem (2.25) in the space $\mathcal{H}^1_0(D) = L^2_P(\Omega, H^1_0(D))$ which is isomorphic to $L^2_P(\Omega) \otimes H^1_0(D)$, where $L^2_P(\Omega) := \left\{\xi(\omega) | \int_\Omega \xi^2(\omega)\, dP(\omega) < \infty\right\}$.

Remark 2.11. (On the structure of the probability measure P and its truncated approximations $P_{\leqslant M}$) By Assumption 2.8, P is the (essentially unique, cf. e.g. [4]) product measure

$$P(\omega) = \bigotimes_{m\geqslant 1} P_m(\omega) \tag{2.26}$$

with $dP_m(\omega) = \rho_m(y_m)dy_m$, $m \in \mathbb{N}$ on the product sigma algebra $\Sigma = \bigotimes_{m\geq 1} \Sigma_m$ in the set of events $\Omega = \prod_{m\geqslant 1} \Omega_m$ (i.e. the essentially unique, smallest sigma algebra in Ω for which each of the projections $\pi_m : \Omega \to \Omega_m$ is $\Omega - \Omega_m$ measurable).

For every $M \in \mathbb{N}$ and for $m > M$ we define the sigma algebra $\tilde{\Sigma}_m = \{\emptyset, \Omega_m\} \subset \Sigma_m$ and denote by $\Sigma_{\leqslant M}$ the corresponding product sub-sigma algebra of Σ, i.e.

$$\Sigma_{\leqslant M} := \left(\prod_{m=1}^{M} \Sigma_m\right) \times \left(\prod_{m>M} \tilde{\Sigma}_m\right) \subset \Sigma$$

Since, for $m > M$, each P_m is a probability measure on $\tilde{\Sigma}_m$, it holds $P_m(\emptyset) = 0$ and $P_m(\Omega_m) := 1$. The *M-truncated probability measure for the family $(Y_m)_{m\geqslant 1}$* is

the restriction of P to $\Sigma_{\leqslant M}$. It satisfies for every elementary event $\omega \in \Sigma_{\leqslant M}$ of the form $\omega = (\omega_1, \omega_2, ..., \omega_M, \Omega_{M+1}, \Omega_{M+2}, ...)$

$$P_{\leqslant M}(\omega) = \bigotimes_{m=1}^{M} P_m(\omega_m) \tag{2.27}$$

The truncated problem (2.25) can be obtained from (2.17) by taking the conditional expectation over $\Sigma_{\leqslant M}$.

2.6 "zero-dimensional" model problem

In the sGFEM and sCFEM, each "stochastic degree of freedom" corresponds to a solution of one boundary value problem for a deterministic, elliptic PDE. It is therefore of utmost importance to discretize (2.19) with as few DoFs in $\mathbf{y}$ as possible, without compromising accuracy.

Our methodology to achieve this consists, as mentioned above, in identification of the most important "active" gPC modes by *a-priori error analysis*. We also present a heuristic algorithm for *a-posteriori* and adaptive choice of such "active" DoFs by relating the original problem (1.2) to a "zero-dimensional" model problem whose solutions take values in $\mathbb{R}$ rather than in $H_0^1(D)$.

This zero-dimensional problem had been first introduced in [8], to motivate the sGFEM. Here, we propose to use this stochastic model problem *as a tool for on-the-fly prediction and optimization* of relevant gPC solution modes in both, adaptive sGFEM and adaptive sCFEM.

It consists of the algebraic problem

$$a^0(\omega)u^0(\omega) = 1, \qquad P-\text{a.e. } \omega \in \Omega. \tag{2.28}$$

Clearly, the exact solution of this problem is $u^0(\omega) = \frac{1}{a^0(\omega)}$. It is assumed that $a^0(\omega)$ has a formal KL expansion of the form

$$a^0(\omega) = \gamma_0 + \gamma_1\sqrt{\lambda_1}Y_1 + \cdots + \gamma_m\sqrt{\lambda_m}Y_m + \cdots, \tag{2.29}$$

where the eigenvalues λ_m stem from the underlying original problem in (2.8) and Y_m are i.i.d. random variables as described above. The γ_i's represent the values that can be taken by the functions $E_a(x)$ (in the case $i = 0$) and $\varphi_i(x)$, respectively. The truncated zero-dimensional problem which corresponds to (2.25) then reads

$$a_M^0(\mathbf{y})u_M^0(\mathbf{y}) = 1 \tag{2.30}$$

where $a_M^0(\mathbf{y}) = \gamma_0 + \gamma_1\sqrt{\lambda_1}y_1 + \cdots + \gamma_M\sqrt{\lambda_M}y_M$. For any $M < \bar{M}$, $u_M^0 = \frac{1}{a_M^0}$ and we have

$$||\partial^\alpha u_M^0||_{L^\infty(I)} = \alpha! \prod_{m=1}^{M} \gamma_m^{\alpha_m} \cdot (||u_M^0||_{L^\infty(I)})^{|\alpha|}. \tag{2.31}$$

The regularity (2.31) of the model problem (2.28) is determined by the coefficients γ_m, $m = 0, ..., M$. *We propose to use the explicit solution $u_M^0 = 1/a_M^0$ of (2.30) with coefficients γ_i related to the KL-data of the full problem to predict significant coefficients of sGFEM approximations of the full problem (1.2) resp. of its approximation (2.25)*, see Subsection 3.2.3 ahead for more details.

To relate the truncated problem (2.25) to the zero dimensional problem (2.30), we proceed as follows: based on the first M KL-eigenfunctions $\varphi_m(x)$, $m = 1, .., M$, a conservative choice of the parameters γ_i to assess the approximability of $u_M(\mathbf{x}, \omega)$ in (2.25) is

$$\gamma_0 := \inf_D E_a(\mathbf{x}), \quad \gamma_m := ||\varphi_m(\mathbf{x})||_{L^\infty(D)}, \qquad m = 1, 2, 3, ... \tag{2.32}$$

To avoid singularities we assume that the expansion (2.29) satisfies

$$0 < \alpha^* \leqslant a_M^0(\mathbf{y}) \leqslant \beta^* \tag{2.33}$$

which is not restrictive due to (2.10), (2.11) and (2.14).

Multiplying equation (2.30) with a test function $v(\mathbf{y}) \in L^2_\rho(I)$ and integrating yields to the variational form corresponding to (2.20): Find $u_M^0(\mathbf{y}) \in L^2_\rho(I)$ s.t.

$$b^0(u_M^0, v) = l^0(v) \quad \forall v \in L^2_\rho(I) \tag{2.34}$$

with the bilinear form

$$b^0(u, v) := \mathbb{E}\left[a_M^0(\mathbf{y})u(\mathbf{y})v(\mathbf{y})\right], \tag{2.35}$$

and the linear functional

$$l^0(v) := \mathbb{E}\left[v(\mathbf{y})\right]. \tag{2.36}$$

Furthermore, problem (2.30) is equipped with the stochastic energy norm

$$||v||_E^2 := b^0(v, v) = \mathbb{E}\left[a_M^0(\mathbf{y})v(\mathbf{y})^2\right]. \tag{2.37}$$

3 Stochastic Galerkin FEM

We will discuss the Galerkin discretization of the variational problem (2.20). For a general discussion of the sGFEM we refer to [13, 3, 8, 17] and references therein. Here, due to the high dimensionality of $L^2_\rho(I)$, we will primarily focus on sparse techniques to reduce the complexity of the stochastic approximation.

We discretize the variational formulation (2.20) by Galerkin projection onto a sequence of finite dimensional subspaces of

$$L^2_\rho(I, H^1_0(D)) \simeq L^2_\rho(I) \otimes H^1_0(D). \tag{3.1}$$

Specifically, we choose a gPC discretization in I based on two-parametric families of finite dimensional subspaces $Y^M_{\mu,\nu} \subset L^2_\rho(I)$. Here, μ and ν refer to the polynomial degree and the maximal number of "active gPC dimensions", respectively (see Remark 3.6 ahead). Denoting the FE-space in the physical domain $V_h^D \subset H^1_0(D)$, the sGFEM is based on the tensor product space

$$Y^M_{\mu,\nu} \otimes V_h^D \subset L^2_\rho(I) \otimes H^1_0(D). \tag{3.2}$$

Then the sGFEM approximation of (2.20) reads:

$$\text{Find} \quad u_M \in Y^M_{\mu,\nu} \otimes V_h^D : \quad b_M(u_M, v) = l(v) \quad \forall v \in Y^M_{\mu,\nu} \otimes V_h^D \tag{3.3}$$

where

$$b_M(u_M, v) = \mathbb{E}\left[\int_D a_M(\mathbf{y}, \mathbf{x})\nabla u_M(\mathbf{y}, \mathbf{x}) \cdot \nabla v(\mathbf{y}, \mathbf{x})\, d\mathbf{x}\right]. \tag{3.4}$$

Remark 3.1. Note that the 'factor'-subspaces in the tensor product (3.2) can be chosen independently of each other. In fact, the spatial and stochastic variables of the random solution only interact with each other when building up the combined stiffness matrix, as we will show in Section 5.3 ahead.

Remark 3.2. The dimensional reduction from $b(\cdot, \cdot)$ in (2.21) to $b_M(\cdot, \cdot)$ in (3.3) was done by truncating the Karhunen-Loève expansion (2.5) of $a(\mathbf{x}, \omega)$ to $a_M(\mathbf{x}, \omega)$ in (2.8), resulting in (2.25). By Remark 2.11, a "probabilistic interpretation" of this transition is to take in (2.17) instead of $\mathbb{E}[\cdot]$ expectations $\mathbb{E}[\cdot|\Sigma_{\leq M}]$ conditional on $\Sigma_{\leq M} \subset \Sigma$ as in Remark 2.11. Therefore, the solution u_M of (3.3) is a maximum likelihood estimate of u subject to the (reduced) information $\Sigma_{\leq M}$ on coefficient $a(\mathbf{x}, \omega)$.

Remark 3.3. In order for (2.25) or, equivalently, for (3.3) to be well-posed, coercivity of $b_M(\cdot,\cdot)$ is necessary. In the sCFEM, $a_M(\omega,\mathbf{x})$ in (2.8) must satisfy (1.1) at least for M sufficiently large, possibly with worse constants $0<\alpha\leq\beta<\infty$ but uniformly in M to ensure the V-coercivity of

$$\int_D a_M(\cdot,\mathbf{x})\nabla u_M(\cdot,\mathbf{x})\cdot\nabla v(\cdot,\mathbf{x})\,d\mathbf{x} : V\times V\to\mathbb{R}$$

uniformly in $\mathbf{y}\in I$ which is necessary for the stability of the scFEM. In the sGFEM this assumption is redundant, as pointed out in [21]: Due to the fact that the random variables y_m are centered, see (2.7), an easy computation shows that

$$b_M(u_M,v)=b(u_M,v)\qquad\forall u_M,v\in Y_{\mu,\nu}^M\otimes V_h^D,$$

with $b(u_M,v)$ and $b_M(u_M,v)$ as in (2.21) and (3.4), respectively, so that $b_M(\cdot,\cdot)$ satisfies (1.1) for any M.

3.1 Multilevel hierarchic spatial discretization

For the sake of simplicity, we assume that the spatial domain D is a bounded Lipschitz polyhedron with straight faces in $\mathbb{R}^d$. In order to find a hierarchic sequence of discrete spaces $V_h^D\subset H_0^1(D)$ we introduce piecewise polynomial wavelet discretizations. For a discussion of spline wavelets we refer to [6, 5] and references therein.

$$V_0^D\subset V_1^D\subset\ldots\subset V_l^D\subset V_{l+1}^D\subset\ldots\subset H_0^1(D)$$

be a dense sequence of finite dimensional subspaces, given by e.g. $V_l^D:=S_0^p(D,\mathcal{T}_l)$ where $p\geq 1$ is a (fixed) polynomial degree and $\{\mathcal{T}_l\}$ is a nested sequence of regular simplicial triangulations of D and define

$$S_0^p(D,\mathcal{T}_l)=\left\{u\in H_0^1(D):u|_T\in\mathcal{P}_p(T)\text{ for }T\in\mathcal{T}_l\right\},\qquad l=0,1,\ldots$$

i.e. the space of continuous piecewise polynomials of total degree at most p on the triangulation $\mathcal{T}_l$. We denote by P_l^D the $H_0^1(D)$ projection onto V_l^D, i.e.

$$\big(\nabla(u-P_l^Du),v\big)=0\quad\forall v\in V_l^D,$$

where $(\cdot,\cdot)$ denotes the $L^2(D)$ inner product, and define the *detail spaces* W_l^D such that

$$W_0^D:=V_0^D\quad\text{and}\quad V_l^D=V_{l-1}^D\oplus W_l^D\text{ for }1\leqslant l\leqslant L.$$

The FE-space V_L^D admits a multilevel decomposition $V_L^D:=\bigoplus_{l=0}^L W_l^D$. Furthermore, let $\psi_l=\{\psi_{lk}:k\in\nabla_l\}$, where ∇_l is an index set, be a basis of the "increment space" W_l^D. The ensemble of basisfunctions $\Psi=\{\psi_{lk}:l\geqslant 1,k\in\nabla_l\}$ are then called *wavelets*, whereas ψ_{0k} are the *scaling functions*.

Every function $u\in H_0^1(D)$ can be decomposed in terms of the scaling functions at the coarsest level $l=0$ and wavelets on levels $l\geqslant 1$ as

$$u=\sum_{l\geqslant 0}\sum_{k\in\nabla_l}d_{lk}\psi_{lk}=\sum_{l\geqslant 0}\mathbf{d}_l^\top\Psi_l=\mathbf{d}^\top\Psi,\tag{3.5}$$

and the following norm equivalences hold (see e.g. [5]):

$$\begin{array}{rcl}\|u\|_{L^2(D)}&\sim&\|\mathbf{d}\|_{\ell^2}\\ \|\nabla u\|_{L^2(D)}^2&\sim&\sum_{l\geqslant 0}2^{2l}\|\mathbf{d}_l\|_{\ell^2}^2.\end{array}\tag{3.6}$$

Remark 3.4. We emphasize that for the computation of the FE stiffness matrices, any h-version FE-code in conjunction with a wavelet transformation can be used, since the matrices correspond to diffusion FE stiffness matrices with the KL-eigenfunctions $\varphi_m(x)$ as coefficients, see Section 5.3 for details.

3.2 Discretization in the stochastic variable

In the sGFEM (3.3), judicious choice of $Y^M_{\mu,\nu} \subset L^2_\rho(I)$ is crucial, since the complexity of the sGFEM (3.3) is at least that of solving $N_\Omega = \dim Y^M_{\mu,\nu}$ deterministic problems D. Since the solution of (2.19) is analytic with respect to $\mathbf{y}$, a *Polynomial Chaos* (PC) approximation by Hermite Polynomials of Gaussian random variables due to N. Wiener [41] seems appropriate. As the measure P in (1.1) is not necessarily Gaussian, generalized Polynomial Chaos (gPC) has been proposed, see e.g. [44, 43]. This leads to exponential convergence rates in numerical experiments, even if non-Gaussian probability density functions are present, see [44, 16] and references therein. Multi-element gPC (ME-gPC) have then been considered in [40, 39] and can be viewed as an *hp*-version of the gPC approach, where the probability domain I is partitioned and a gPC approximation is performed in each subdomain. However, gPC and ME-gPC suffer from the curse of dimension when M gets large which is the case for 'rough' covariances as well as for problems in space dimensions $d = 2$ and $d = 3$, since due to (2.10), (2.11) the corresponding slow decay of the KL-eigenvalues forces a large value of M.

Sparse polynomial tensor product [35] expansions allow to treat high truncation orders M with only algebraic growth of the number N_Ω of deterministic problems to be solved uniformly, as $M \to \infty$.

3.2.1 Sparse polynomial chaos

For every coordinate y_m, $m \in \{1, 2, \dots M\}$ let a family of one-dimensional polynomials $(\pi^m_i(y_m))_{i\in\mathbb{N}_0}$ be given, where $\pi^m_i(y_m)$ is a polynomial of degree i on I_m, and denote by

$$\zeta_{M,\alpha}(y_1, \dots, y_M) := \pi^1_{\alpha_1}(y_1)\pi^2_{\alpha_2}(y_2)\cdots\pi^M_{\alpha_M}(y_M), \quad \alpha \in \mathbb{N}_0^M. \tag{3.7}$$

their tensor product. Assume that the polynomials $(\pi^m_i(y_m))_{i\in\mathbb{N}_0}$ form a basis for $L^2_{\rho_m}(I_m)$. Then it follows that the tensorized polynomials (3.7) form a basis in $L^2_\rho(I)$. The gPC representation for the solution of (2.19) is

$$u_M(\mathbf{y}, \mathbf{x}) = \sum_{\alpha\in\mathbb{N}_0^M} u_\alpha(\mathbf{x})\zeta_{M,\alpha}(\mathbf{y}), \tag{3.8}$$

where only a finite number of coefficients $u_\alpha(\mathbf{x})$ are nonzero. Our aim is to choose an appropriate subset $\Lambda \subset \mathbb{N}_0^M$ such that an as small as possible number N_Ω of functions $\zeta_{M,\alpha}(\mathbf{y})$ are considered in the approximation of u_M while still retaining spectral convergence rates of the sGFEM discretization in $\mathbf{y}$. That this is in principle possible has been proved for exponential KL-eigenvalue decay (2.10) in [35]. Here, we will present a more sophisticated selection of $\Lambda \subset \mathbb{N}_0^M$ with a still moderate cardinality $N_\Omega := |\Lambda|$ such that, up to a given accuracy, u_M can be approximated as

$$u_{M,\Lambda}(\mathbf{y}, \mathbf{x}) = \sum_{\alpha\in\Lambda} u_\alpha(\mathbf{x})\zeta_{M,\alpha}(\mathbf{y}). \tag{3.9}$$

Moreover, we show *spectral convergence* in terms of the number N_Ω of gPC "modes" (where each mode corresponds to a deterministic problem).

Following [35], we introduce the gPC approximation space as follows:

Definition 3.5. For $M, \mu, \nu \in \mathbb{N}$ with $\nu \leqslant M$ let the index set $\Lambda_{M,\mu,\nu} \subset \mathbb{N}_0^M$ be given by

$$\Lambda_{M,\mu,\nu} := \{\alpha \in \mathbb{N}_0^M : \|\alpha\|_1 \leqslant \mu, \|\alpha\|_0 := |\mathrm{supp}(\alpha)| \leqslant \nu\}, \tag{3.10}$$

where $|\mathrm{supp}(\alpha)|$ denotes the number of nonzero components of the multiindex α. The corresponding approximation space is then defined as

$$\mathcal{P}_{M,\mu,\nu} := \mathrm{span}\{\zeta_{M,\alpha} : \alpha \in \Lambda_{M,\mu,\nu}\}. \tag{3.11}$$

Remark 3.6. The approximation space $Y^M_{\mu,\nu} = \mathcal{P}_{M,\mu,\nu}$ in (3.10), (3.11) used in the gPC sGFEM discretization is inspired by Hoeffding's ANOVA decomposition of random fields [14]: there, a function $f(\mathbf{y}) = f(y_1, y_2, ...)$ of countably many variables y_i is represented by

$$\sum_{i^{(1)}\in\mathbb{N}_0^1} f^{(1)}_{i^{(1)}}(y_{i^{(1)}}) + \sum_{i^{(2)}\in\mathbb{N}_0^2} f^{(2)}_{i^{(2)}}(y_{i^{(2)}_1}, y_{i^{(2)}_2}) + ... + \sum_{i^{(k)}\in\mathbb{N}_0^k} f^{(k)}_{i^{(k)}}(y_{i^{(k)}_1}, ..., y_{i^{(k)}_k}) + ... \quad (3.12)$$

Our approximation space $Y^M_{\mu,\nu} = \mathcal{P}_{M,\mu,\nu}$ consists in a) truncation of the ANOVA representation (3.12) at levels $k = \nu$, b) in term $k \leq \nu$, truncating the ranges of the multiindices $i^{(k)}$ from $\mathbb{N}_0^k$ to $\{0, 1, ..., M\}^k$ and c) replacing for $k \leq \nu$ each function $f^{(k)}_{i^{(k)}}(\cdot)$ in (3.12) by a polynomial of degree at most μ in at most $k \leq \nu$ of the variables y_j, $j \leq M$.

3.2.2 Sparse orthogonal chaos

As a special choice of polynomials $(\pi^m_i(y_m))_{i\in\mathbb{N}_0}$, a family of univariate orthogonal polynomials in y_m with respect to the probability density ρ_m can be considered. Choosing orthogonal polynomials in each variable $y_1, \ldots, y_M$, spanning the same space as (3.11), will naturally sparsify the matrix of the stochastic discretization and, in addition, reduce its condition number. In case the multivariate probability density function $\rho(\mathbf{y})$ in (2.18) is uniform, the tensorized Legendre polynomials

$$\mathcal{L}_{M,\alpha}(\mathbf{y}) := L_{\alpha_1}(y_1)L_{\alpha_2}(y_2)\cdots L_{\alpha_M}(y_M) \quad (3.13)$$

form such an orthogonal family. Here $L_{\alpha_m}(y_m)$ is the Legendre polynomial of degree α_m on $I_m = [-1, 1]$ normalized such that $L_{\alpha_m}(1) = 1$, i.e. it satisfies

$$\int_{I_m} L_{\alpha_m}(y_m)L_{\alpha'_m}(y_m)\rho(y_m)\, dy_m = \delta_{\alpha_m\alpha'_m}\frac{1}{2\alpha_m + 1}. \quad (3.14)$$

The Legendre expansion with respect to $\mathbf{y}$ can then be written as

$$u_M(\mathbf{y}, \mathbf{x}) = \sum_{\alpha\in\mathbb{N}_0^M} u_\alpha(\mathbf{x})\mathcal{L}_{M,\alpha}(\mathbf{y}). \quad (3.15)$$

We denote by

$$u_{\Lambda_{M,\mu,\nu}}(\mathbf{y}, \mathbf{x}) = \sum_{\alpha\in\Lambda_{M,\mu,\nu}} u_\alpha(\mathbf{x})\mathcal{L}_{M,\alpha}(\mathbf{y}) \quad (3.16)$$

the Legendre chaos expansion restricted to the index set $\Lambda_{M,\mu,\nu}$ in (3.10).

For non-uniform probability density functions, other types of orthogonal functions can be considered. See e.g. [43] for a list of various probability density functions and their corresponding orthogonal polynomials.

3.2.3 Adaptive selection of active gPC modes

Although the family $\Lambda_{M,\mu,\nu}$ of index sets in Definition 3.5 represents a judicious, sparse choice of active gPC coefficients, its cardinality increases rapidly as M, μ and ν are increased.

Proposition 3.7. *For the sGFEM based on the gPC approximation with coefficients in the set $\Lambda_{M,\mu,\nu}$ specified in (3.10), it holds*

$$N_\Omega = |\Lambda_{M,\mu,\nu}| \leqslant 2M^\nu(\mu + 1)^{\nu+1}. \quad (3.17)$$

We refer to Appendix A.2 for the proof.

As every stochastic 'degree of freedom' entails the numerical solution of one deterministic boundary value problem in D, hence yielding a total number of $N_{\text{tot}} = N_\Omega N_D$ degrees of freedom, it is important to represent the unknown solution $u_M(\mathbf{y}, \mathbf{x})$ in (3.15) by as few gPC modes as possible. Hence, for a prescribed error bound ϵ and a given gPC dimension $M < \bar{M}$, we aim at finding an index set $\Lambda(\epsilon) \subset \mathbb{N}_0^M$ which satisfies

$$\Lambda(\epsilon) := \operatorname{argmin} \left\{ |\tilde{\Lambda}| : \tilde{\Lambda} \subset \mathbb{N}_0^M, \|u_M - u_{M,\tilde{\Lambda}}\|_{L^\infty(I)} < \epsilon \right\} \tag{3.18}$$

In the following we present a heuristic algorithm of selecting such an index set Λ adaptively in each step, based only on Karhunen-Loève data of $a(\omega, \mathbf{x})$. Motivated by Subsection 2.6, every stochastic elliptic diffusion problem corresponds to a purely stochastic problem of the form (2.30) with the formal solution

$$u_M^0(\mathbf{y}) = \frac{1}{\gamma_0 + \sum_{m=1}^\infty \gamma_m \sqrt{\lambda_m} y_m}. \tag{3.19}$$

It is easy to see that $u_M^0(\mathbf{y})$ can be expanded in a geometric series like

$$\Psi_M(\mathbf{y}) = \frac{1}{\gamma_0} + \sum_{n=1}^\infty (-1)^n \left(\frac{1}{\gamma_0} \sum_{m=1}^M \gamma_m \sqrt{\lambda_m} y_m \right)^n = \frac{1}{\gamma_0} + \sum_{\alpha \in \mathbb{N}_0^M} c_\alpha \tilde{\gamma}^\alpha \mathbf{y}^\alpha,$$

with $\tilde{\gamma} = \frac{1}{\gamma_0}(\gamma_1 \sqrt{\lambda_1}, \gamma_2 \sqrt{\lambda_2}, \ldots)$ and some constants c_α. By using a (finitely supported) index set $\Lambda \subset \ell_c^\infty(\mathbb{N})$, the sequence space of all bounded sequences with compact support, the series is truncated as

$$\mathcal{G}_M(\mathbf{y}) = \frac{1}{\gamma_0} + \sum_{\alpha \in \Lambda} c_\alpha \tilde{\gamma}^\alpha \mathbf{y}^\alpha. \tag{3.20}$$

The order of magnitude of the coefficients of $\mathbf{y}^\alpha$ are asymptotically determined by

$$\tilde{\gamma}^\alpha = \prod_{m \geqslant 1} \tilde{\gamma}_m^{\alpha_m}. \tag{3.21}$$

Hence, in the spirit of a best N-term approximation we propose the following Algorithm 3.8 for selecting an index set Λ containing the largest coefficients $\tilde{\gamma}^\alpha$. We emphasize here, that the presented algorithm is also *dimension-adaptive*, i.e. the maximum dimension of 'active' coefficients, previously called M, may vary when computing the modified index set $\tilde{\Lambda}$ from Λ.

Algorithm 3.8. (KL-adapted selection of indices)

Input:

- KL-data (γ_m, λ_m)
- Steering parameter $\theta > 0$
- Index set Λ

Output: Modified index set $\tilde{\Lambda}$ computed by

1. **Compute** $\forall \alpha \in \Lambda$ the numbers $\tilde{\gamma}^\alpha$ and denote by $\tilde{\gamma}_{\min} = \min_{\alpha \in \Lambda} \tilde{\gamma}^\alpha$ their minimum.

2. **Determine**

$$\tilde{\Lambda} = \{\alpha \in \ell_c^\infty(\mathbb{N}) : \tilde{\gamma}^\alpha > \theta\tilde{\gamma}_{\min}\}.$$

Choosing $0 < \theta < 1$ corresponds to an extension of the index set Λ whereas for $\theta > 1$ Λ will be contracted, i.e.

$$\begin{cases} 0 < \theta < 1: & \tilde{\Lambda} \supseteq \Lambda \\ \theta = 1: & \tilde{\Lambda} = \Lambda \\ 1 < \theta: & \tilde{\Lambda} \subseteq \Lambda \end{cases} \tag{3.22}$$

Starting e.g. with $\Lambda^{(0)} = \{\mathbf{0}\}$ and applying Algorithm 3.8 with $0 < \theta < 1$ repeatedly provides a hierarchic sequence of index sets

$$\Lambda^{(0)} \subseteq \Lambda^{(1)} \subseteq \cdots \subseteq \Lambda^{(l)} \subseteq \cdots \subseteq \ell_c^\infty(\mathbb{N}) \tag{3.23}$$

to be used in conjunction with the deterministic FE-spaces V_l^D. Numerical examples in Section 6 will show that the adaptive refinement of stochastic modes by Algorithm 3.8 results in accurate representations of the random solution involving considerably less degrees of freedom than by using $\Lambda_{M,\mu,\nu}$ instead.

Remark 3.9. The values of $\gamma_0, \gamma_1, \ldots$ have been set to the minima and maxima of $\mathbb{E}_a(\mathbf{x})$ and $\varphi_m(\mathbf{x})$, respectively, over the domain D, see (2.32). Consider now a decomposition of D into open, nonempty, disjoint subsets $\{D_i\}_{0 \leqslant i \leqslant I}$, s.t. $\overline{D} = \cup_{i=0}^I \overline{D_i}$ and set

$$\gamma_0^{(i)} := \inf_{D_i} \mathbb{E}_a(\mathbf{x}), \quad \gamma_m^{(i)} := \|\varphi_m(\mathbf{x})\|_{L^\infty(D_i)}, \quad m = 1, 2, 3, \ldots$$

Consequently, by Algorithm (3.8), we get sequences $\Lambda_{D_i}^{(0)} \subseteq \Lambda_{D_i}^{(1)} \subseteq \cdots \subseteq \ell_c^\infty(\mathbb{N})$ taking into account that $a(\omega, \mathbf{x})$ might behave differently on each D_i. Solving now (2.20) on separate subdomains D_i, together with the appropriate index sets $\Lambda_{D_i}^{(j)}$, might lead to a better approximation of the random solution's joint pdf's.

3.3 Error analysis

By choosing the discrete spatial space $V_h^D = V_L^D$ and the discrete stochastic space $Y_{\mu,\nu}^M = \mathcal{P}_{M,\mu,\nu}(I)$ as discussed in the previous subsections we obtain the full discretization

$$\mathcal{P}_{M,\mu,\nu}(I) \otimes V_L^D \subset L_\rho^2(I) \otimes H_0^1(D) \simeq L_\rho^2(I, H_0^1(D)). \tag{3.24}$$

The approximate solution $u_{\Lambda_{M,\mu,\nu}}^L(\mathbf{y}, \mathbf{x}) \in \mathcal{P}_{M,\mu,\nu}(I) \otimes V_L^D$ to the stochastic elliptic problem (2.17) is then represented as a series of the form

$$u_{\Lambda_{M,\mu,\nu}}^L(\mathbf{y}, \mathbf{x}) = \sum_{\alpha \in \Lambda_{M,\mu,\nu}} u_\alpha(\mathbf{x}) \mathcal{L}_{M,\alpha}(\mathbf{y}) \tag{3.25}$$

where, according to (3.5), $u_\alpha \in V_L^D$ can be written as

$$u_\alpha(\mathbf{x}) = \sum_{l=0}^{L} \sum_{k \in \nabla_l} u_{lk}^\alpha \psi_{lk}(\mathbf{x}). \tag{3.26}$$

Let us denote by $P_L^D : H_0^1(D) \to V_L^D$ the Galerkin finite element projection operator in the physical domain D. It satisfies quasi optimality in $H_0^1(D)$, i.e.

$$||v - P_L^D v||_{H_0^1(D)} \leqslant C \min_{v^L \in V_L} ||v - v^L||_{H_0^1(D)}, \quad \forall v \in H_0^1(D) \tag{3.27}$$

were C depends only on α and β in (1.1).

Similarly we can define an interpolation operator $P^I_{\Lambda_{M,\mu,\nu}} : L^2_\rho(I) \to \mathcal{P}_{M,\mu,\nu}$ which projects functions from $L^2_\rho(I)$ onto their truncated sparse Legendre chaos expansion (3.16) defined by

$$P^I_{\Lambda_{M,\mu,\nu}} u_M(\mathbf{y},\mathbf{x}) = \sum_{\alpha\in\Lambda_{M,\mu,\nu}} u_\alpha(\mathbf{x})\mathcal{L}_{M,\alpha}(\mathbf{y}), \quad u_\alpha(\mathbf{x}) = \prod_{m=1}^{M}(2\alpha_m+1)\int_I u_M(\mathbf{y},\mathbf{x})\mathcal{L}_{M,\alpha}(\mathbf{y})\,d\mathbf{y}.$$

Let us recall that we use the notation u for the solution of (1.2), u_M for the solution of the dimensionally truncated problem (2.25) and $u^L_{\Lambda_{M,\mu,\nu}}$ for the sGFEM approximation (3.25). To estimate the overall sGFEM error

$$\epsilon^L_{\Lambda_{M,\mu,\nu}} := ||u - u^L_{\Lambda_{M,\mu,\nu}}||_{\mathcal{H}^1_0(D)}. \tag{3.28}$$

we split it into three parts, namely

$$\epsilon^L_{\Lambda_{M,\mu,\nu}} \leqslant \underbrace{||u-u_M||_{\mathcal{H}^1_0}}_{\epsilon_M} + \underbrace{||u_M - P^D_L u_M||_{\mathcal{H}^1_0}}_{\epsilon_{V^D_L}} + \underbrace{||P^D_L(u_M - P^I_{\Lambda_{M,\mu,\nu}} u_M)||_{\mathcal{H}^1_0}}_{\epsilon_{\mu,\nu}} \tag{3.29}$$

Here, ϵ_M denotes the Karhunen-Loève truncation error due to replacing $a(\mathbf{y},\mathbf{x})$ by $a_M(\mathbf{y},\mathbf{x})$, $\epsilon_{V^D_L}$ is the FE discretization error and $\epsilon_{\mu,\nu}$ stems from the gPC discretization in the stochastic variables $\mathbf{y}$. We choose M, L, μ, ν in relation to each other such that the corresponding error contributions are equilibrated while the total number of degrees of freedom is minimal. We use numerical analysis of the error to identify sets $\Lambda_{M,\mu,\nu}$ of 'active' gPC modes of small cardinality $N_\Omega = |\Lambda_{M,\mu,\nu}|$, the number of deterministic FE solutions needed to approximate the random field.

We start with the spatial finite element discretization error $\epsilon_{V^D_L}$. A-priori FE-estimates on quasiuniform meshes of width h in the physical domain D are well known, see, e.g. [29]: as the meshwidth $h \to 0$ and $p \geq 1$ is fixed, we have

$$\epsilon_{V^D_L} \sim h^p \qquad \text{as} \quad h \to 0.$$

In the case of an arbitrary but fixed polynomial degree $p \geq 1$, we therefore choose L as

$$L \sim |\ln \epsilon_{V^D_L}|/p. \tag{3.30}$$

Next, we aim at choosing M, such that $\epsilon_M \sim \epsilon_{V^D_L}$. To obtain an estimate for ϵ_M, recall the definition of the (truncated) bilinear and linear forms $b(u_M, v)$, $b_M(u_M, v)$ and $l(v)$ from (2.21),(3.4) and (2.22), respectively. The variational formulation of the model problem (1.2) and its truncated version (2.17) are:

$$\text{Find } u \in L^2_P(\Omega, H^1_0(D)) \text{ s.t. } \forall v \in L^2_P(\Omega, H^1_0(D)) \text{ holds } b(u,v) = l(v)$$

and

$$\text{Find } u_M \in L^2_P(\Omega, H^1_0(D)) \text{ s.t. } \forall v \in L^2_P(\Omega, H^1_0(D)) \text{ holds } b_M(u_M,v) = l(v),$$

respectively.

Using a Strang-type perturbation argument, the error ϵ_M due to the truncation of the KL-expansion can be estimated as follows: we use

$$||u_M||^2_{\mathcal{H}^1_0} \overset{(1.1)}{\leqslant} \frac{2}{\alpha} b_M(u_M,u_M) = l_M(u_M) \leqslant \frac{2}{\alpha} C_P ||f||_{L^2(D)} ||u_M||_{\mathcal{H}^1_0},$$

where C_P is the Poincaré constant, and obtain

$$||\epsilon_M||_{\mathcal{H}^1_0} \leqslant C_P \frac{2}{\alpha^2} ||a_M - a||_{L^\infty(I,H^1_0(D))} ||f||_{L^2(D)}.$$

A stochastic source term $f(x,\tilde{\omega})$ would lead here to an additional term of the form $||f - f_{M'}||_{L^\infty}$, where $f_{M'}$ denotes the truncated Karhunen-Loève expansion of f.

From (2.9) and Proposition 2.3 it follows that

$$\epsilon_M \sim \exp(-cM^\kappa),$$

where $\kappa = 1/d$. Hence, together with (3.30)

$$M \sim |\ln \epsilon_M|^d \sim L^d p^d \tag{3.31}$$

It remains to choose μ, ν, such that $\epsilon_{\mu,\nu}$ is of the same order as $\epsilon_{V_L^D}$ and ϵ_M. Due to (3.27) the third term in (3.29) reduces to

$$||P_L^D(u_M - P^I_{\Lambda_{M,\mu,\nu}} u_M)||_{\mathcal{H}_0^1} \leqslant C||u_M - P^I_{\Lambda_{M,\mu,\nu}} u_M||_{\mathcal{H}_0^1} \tag{3.32}$$

The following Lemma provides a pointwise estimate for the stochastic approximation error $\epsilon_{\mu,\nu}$ in (3.29):

Lemma 3.10. *If u_M solves (2.19) then there exist constants $c_1, c_2, c_3, c_4 > 0$, depending only on the data a, r, f but are independent of M, μ, ν such that the expansion of u_M into tensorized Legendre polynomials of $\mathcal{P}_{M,\mu,\nu}(I)$ satisfies*

$$||u_M - u_{\Lambda_{M,\mu,\nu}}||_{L^\infty(I,H_0^1(D))} \leqslant c_1 \left(e^{-c_2 \nu^{1+\kappa}} + e^{c_3 \nu (\ln M + \ln \mu) - c_4 \mu} \right) \tag{3.33}$$

for any $M, \mu, \nu \in \mathbb{N}$ with $\nu \leqslant M$.

For the proof we refer again to Appendix A.2. Choosing $\mu \sim M^\kappa$ and $\nu \sim M^{\kappa/(\kappa+1)}$ yields asymptotically, as $\mu, \nu, L, M \to \infty$, that $\epsilon_{\mu,\nu} \sim \epsilon_M \sim \epsilon_{V_L^D}$. With the complexity estimate (3.17), we have proved

Proposition 3.11. *There exist positive constants c_L, c_M, c_μ, c_ν, independent of L, M, μ, ν, s.t. for any $\varepsilon > 0$, by choosing*

$$\begin{aligned} L(\varepsilon) &:= \left\lceil c_L \tfrac{|\ln \varepsilon|}{p} \right\rceil, \qquad & M(\varepsilon) &= \lceil c_M L(\varepsilon)^d p^d \rceil, \\ \mu(\varepsilon) &= \lceil c_\mu M(\varepsilon)^\kappa \rceil, & \nu(\varepsilon) &= \lceil c_\nu M(\varepsilon)^{\kappa/(\kappa+1)} \rceil \end{aligned} \tag{3.34}$$

for $m = 1, 2, ..., M(\varepsilon)$, we have

$$\|u - u^L_{\Lambda_{M,\mu,\nu}}\|_{\mathcal{H}_0^1(D)} \leqslant \varepsilon \tag{3.35}$$

and the number N_Ω of deterministic problems to be solved is asymptotically, as $\varepsilon \to 0$ for any fixed $s > 0$ bounded by

$$N_\Omega = |\Lambda_{M,\mu,\nu}| \lesssim \varepsilon^{-1/s}, \quad \varepsilon \to 0 \tag{3.36}$$

with a constant independent of the parameters in (3.34)

Note that (3.36) inserted in (3.35) implies for all $s > 0$ as the number N_Ω of stochastic DOFs tends to ∞ the convergence rates

$$\|u - u^L_{\Lambda_{M,\mu,\nu}}\|_{\mathcal{H}_0^1(D)} \leqslant C_s N_\Omega^{-s} \tag{3.37}$$

while, by (3.29)-(3.30), the total number N of degrees of freedom necessary for computing the sGFEM approximation $u^L_{\Lambda_{M,\mu,\nu}}$ of u which is accurate of order ε in $L^2_\rho(I, H_0^1(D))$ is bounded by

$$N = N_\Omega N_D \sim \varepsilon^{-1/s - d/p} \quad \text{as} \quad \varepsilon \to 0 \tag{3.38}$$

4 Stochastic Collocation FEM

A stochastic collocation method for sPDEs has first been proposed in [42, 2] by using numerical quadrature for the approximate evaluation of the stochastic integrals. Whereas [42] already proposed the usage of Smolyak grids to reduce the number of collocation points, this was further analyzed and developed in [22] and [23]. We propose here a stochastic collocation method based on our sGFEM approach. Judicious selection of a two-parameter sequence of collocation points is shown to overcome the problem of high dimensionality for random coefficients $a(\omega, \mathbf{x})$ with Karhunen-Loève eigenvalue decay (2.10) for any $\kappa > 0$. Our sCFEM uses the sGFEM subspaces $Y^M_{\mu,\nu}$ in Definition 3.5. For the resulting sCFEM we prove, under (2.10) for any $\kappa > 0$, similar convergence rates as the sGFEM approach, see Lemma 4.1 below, while having complexity equal to that of the MC method with N_Ω "samples", i.e. N_Ω many solutions of deterministic problems in D.

4.1 Formulation of the collocation algorithm

The functions a_M, u_M, v, f are viewed as functions taking values in $V = H^1_0(D)$, parametrized by $\mathbf{y} \in I$. We consider again the parametric deterministic formulation introduced in (2.19). By projecting it in the spatial variable $\mathbf{x}$ onto a subspace $V^D_L \subset H^1_0(D)$ we obtain a parametric semidiscrete problem which can be written in variational form as: Find $u^L_M : I \longrightarrow V^D_L$ s.t. $\forall v^L \in V^D_L$, $\forall \mathbf{y} \in I$:

$$\int_D a_M(\mathbf{y}, \mathbf{x}) \nabla u^L_M(\mathbf{y}, \mathbf{x}) \cdot \nabla v^L(\mathbf{y}, \mathbf{x})\, d\mathbf{x} = \int_D f(\mathbf{x}) v^L(\mathbf{y}, \mathbf{x})\, d\mathbf{x}. \tag{4.1}$$

Equation (4.1) is collocated w.r. to $\mathbf{y}$ at the roots of polynomials which are orthogonal w.r. to $\bigotimes_{m \geqslant 1} L^2(I_m, \rho_m(y_m)dy_m)$. Approximate joint pdf's of the unknown random solution are recovered by interpolation and statistical moments are computed by ANOVA-composite, tensorized Gaussian Quadratures associated with the collocation points (postprocessing, see Subsection 5.5) .

Specifically, for each parameter $m \in \{1, \dots M\}$ we denote by y_{m,k_m}, $1 \leqslant k_m \leqslant \mu_m + 1$ the $\mu_m + 1$ roots of the orthogonal polynomial $\pi^m_{\mu_m+1}(y_m)$ with respect to the probability measure ρ_m. We will restrict the discussion to the case of Jacobi polynomials $J^{\alpha,\beta}_{\mu_m+1}(y_m)$, i.e. $\rho_m(y_m) = \frac{1}{2}(1-y_m)^\alpha(1+y_m)^\beta$, which covers the case of Legendre and Chebyshev polynomials. For any multiindex $\mathbf{k} = (k_1, \dots, k_M)$ we write $\mathbf{y_k} = (y_{1,k_1}, \dots, y_{M,k_M})$. For a vector $\underline{\mu} = (\mu_1, \dots, \mu_M)$ of polynomial degrees, the (anisotropic) Lagrange interpolation operator is defined by

$$\mathcal{I}_{\underline{\mu}} u^L(\mathbf{y}) = \sum_{\mathbf{1} \leqslant \mathbf{k} \leqslant \underline{\mu}+\mathbf{1}} u^L(\mathbf{y_k}) l_{\mathbf{k}}(\mathbf{y}), \tag{4.2}$$

where $u^L(\mathbf{y_k})$ is the solution of (4.1) for $\mathbf{y} = \mathbf{y_k}$ and where $l_{\mathbf{k}}(\mathbf{y}) = \prod_{m=1}^M l_{m,k_m}(y_m)$ where $l_{m,k_m}(y_m)$ is the Lagrange interpolation polynomial of degree μ_m at the point y_{m,k_m}, defined by

$$l_{m,k_m}(y_m) \in \mathcal{P}_{\mu_m}(I_m), \qquad l_{m,k_m}(y_{m,j_m}) = \delta_{k_m j_m}, \quad 1 \leqslant k_m, j_m \leqslant \mu_m + 1. \tag{4.3}$$

Now, let $S \subset \{1, \dots, M\}$ be the index set of 'active' coordinate axes and denote by u^L_S the restriction of u^L to $y_m = 0$ for all $m \notin S$. Define the interpolation operator

$$\mathcal{I}_{M,\underline{\mu},\nu} : L^\infty(I, H^1_0(D)) \longrightarrow H^1_0(D) \otimes \mathcal{P}_{\underline{\mu}}(I) \tag{4.4}$$

$$\begin{aligned} \mathcal{I}_{M,\underline{\mu},\nu} u^L_M(\mathbf{y}) &= \sum_{\substack{S \subset \{1,\dots,M\} \\ |S| \leqslant \nu}} \gamma_{M,|S|,\nu} \sum_{\substack{\mathbf{k} \in \mathbb{N}^M_0 \\ \mathbf{k} \leqslant \underline{\mu}+\mathbf{1}, \mathrm{supp}(\mathbf{k}) = S}} u^L_M(\mathbf{y_k}) l_{\mathbf{k}}(\mathbf{y}) \\ &= \sum_{\substack{S \subset \{1,\dots,M\} \\ |S| \leqslant \nu}} \gamma_{M,|S|,\nu} \mathcal{I}_{\underline{\mu}} u^L_{M,S}(\mathbf{y}), \end{aligned} \tag{4.5}$$

where

$$\gamma_{M,s,\nu} := \sum_{r=s}^{\nu} (-1)^{r-s} \binom{M-s}{r-s} \tag{4.6}$$

and $y_{m,0} = 0$. In the isotropic case we will write $\mathcal{I}_{M,\mu,\nu} := \mathcal{I}_{M,\underline{\mu},\nu}$ with $\underline{\mu} = (\mu, \dots, \mu)$.

4.2 Analysis of the sCFEM

The interpolation error then satisfies the following bound:

Lemma 4.1. *If u_M^L solves (4.1) then there exist constants $c, \tilde{c}, c_1, \dots, c_M > 0$, depending only on the data a, r, f but not on $M, \underline{\mu}, \nu$ such that the sCFEM solution satisfies*

$$\|u_M^L - \mathcal{I}_{M,\underline{\mu},\nu} u_M^L\|_{L^\infty(I, H_0^1(D))} \leqslant c \left(e^{-\tilde{c}\nu^{1+\kappa}} + (M+1)^{2\nu} e^{c_0 \nu} \left(\sum_{m=1}^{M} e^{-c_m \mu_m} \right) \right) \tag{4.7}$$

for any $M, \underline{\mu}, \nu \in \mathbb{N}$ with $\nu \leqslant M$.

The proof will be given in Appendix B. By similar arguments as in Proposition 3.7, we can provide an estimate on the number of collocation points.

Proposition 4.2. *For input data $a(\omega, \mathbf{x})$ with piecewise analytic covariance $V_a(\mathbf{x}, \mathbf{x}')$ in the sense of Proposition 2.3, the number N_Ω of collocation points in the sCFEM satisfies the bound*

$$N_\Omega = \#(Col.points) \leqslant M^\nu \max_{m \in \{1,\dots,M\}} (\mu_m)^\nu \tag{4.8}$$

Similar as in the sGFEM, the a-priori error analysis of the collocation algorithm is based on splitting the total error $\epsilon^L_{I_{M,\underline{\mu},\nu}}$ into three parts. Adopting the notations of Subsection 3.3 we obtain

$$\epsilon^L_{I_{M,\underline{\mu},\nu}} \leqslant \underbrace{||u - u_M||_{\mathcal{H}_0^1}}_{\epsilon_M} + \underbrace{||u_M - P_L^D u_M||_{\mathcal{H}_0^1}}_{\epsilon_{V_L^D}} + \underbrace{||P_L^D(u_M - \mathcal{I}_{M,\underline{\mu},\nu} u_M)||_{\mathcal{H}_0^1}}_{\epsilon_{\underline{\mu},\nu}}. \tag{4.9}$$

Following the analysis presented in Subsection 3.3, replacing Lemma 3.10 by Lemma 4.1, we obtain the following proposition for choosing the parameters $L, M, \nu, \mu_1, \dots, \mu_M$ in order to equilibrate the error contributions in (4.9).

Proposition 4.3. *There exist positive constants $c_L, c_M, c_\nu, c_{\mu_1}, \dots, c_{\mu_M}$ s.t. by choosing for any $\varepsilon > 0$*

$$\begin{aligned} L(\varepsilon) &= \left\lceil c_L \tfrac{|\ln \varepsilon|}{p} \right\rceil, & M(\varepsilon) &= \lceil c_M L(\varepsilon)^d p^d \rceil, \\ \mu_m(\varepsilon) &= \lceil c_{\mu_m} M(\varepsilon)^\kappa \rceil, & \nu(\varepsilon) &= \lceil c_\nu M(\varepsilon)^{\kappa/(\kappa+1)} \rceil, \end{aligned} \tag{4.10}$$

for $m = 1, 2, ..., M(\varepsilon)$, we have

$$\|u - u^L_{\Lambda_{M,\underline{\mu},\nu}}\|_{\mathcal{H}_0^1(D)} \leqslant \varepsilon \tag{4.11}$$

and the number N_Ω of deterministic problems to be solved is asymptotically, as $\varepsilon \to 0$ for any fixed $s > 0$ bounded by

$$N_\Omega = \#(Col.points) \lesssim \varepsilon^{-1/s}, \quad \varepsilon \to 0. \tag{4.12}$$

Hence, inserting (4.11) in (4.12) yields for all $s > 0$ the asymptotic convergence rates

$$\|u - u^L_{\Lambda_{M,\underline{\mu},\nu}}\|_{\mathcal{H}^1_0(D)} \leqslant C_s N_\Omega^{-s} \tag{4.13}$$

as the number of collocation points N_Ω tends to ∞. The total number of DoFs satisfies, like in (3.38)

$$N_{\text{tot}} = N_\Omega N_D \sim \varepsilon^{-1/s-d/p} \quad \text{as} \quad \varepsilon \to 0 \tag{4.14}$$

for any fixed $s > 0$.

4.3 Discussion: sGFEM versus sCFEM

So far, two sparse methods for solving (1.2) have been presented: sGFEM and sCFEM. Starting point for both methods is its parametric reformulation (2.19). While the sGFEM projects the solution onto a finite dimensional subspace $\mathcal{P}_{M,\mu,\nu}(I) \subset L^\infty(I)$, the sCFEM samples the solution on a set of predetermined points $\mathbf{y_k}$ and interpolates its probability densities on these points. Both methods make reduce the problem of approximating a function in $L^\infty(I)$ to a sum of approximation problems in $L^\infty(\hat{I})$, $\hat{I} = I_{i_1} \times \cdots \times I_{i_\nu}$, $i_j \in \{1, \ldots, M\}$ with lower "active" dimension $\nu \ll M$, while still providing arbitrary high algebraic convergence rates for both, sGFEM and sCFEM.

One major difficulty of the sGFEM lies in the fact that it leads to a fully coupled system of N_Ω linear deterministic equations whereas in the sCFEM they are naturally decoupled. Parallelization is therefore straightforward in the latter case. Comparing Lemma 3.10 with Lemma 4.1 already indicates that the sGFEM approach may converge faster than the sCFEM in terms of N_Ω, the number of deterministic problems to be solved, as μ and ν are increased. This will also be illustrated in the numerical examples, see Section 6. Furthermore, due to the restriction $\|\alpha\|_1 \leqslant \mu$ in (3.10), the sGFEM algorithm uses considerably less degrees of freedom than the collocation approach. The main advantage of the sGFEM algorithm, however, lies in the fact that it provides much more flexibility regarding adaptively increasing or decreasing the index set $\Lambda_{M,\mu,\nu}$. An example of this flexibility has already been given by Algorithm 3.8, where a sequence of 'optimal', in the sense of (3.18), sets $\Lambda^{(j)}$ of "active" indices have been constructed to approximate $u_M(\mathbf{y})$.

In summary, the sGFEM may be preferable over the sCFEM for the following reasons:

- The system of linear equations is smaller in the sGFEM, which, despite the fact that they are coupled, dramatically affects the run-time of the algorithm,
- in the absence of spatial discretization, sGFEM yields a maximum likelihood estimate of the unkown random field u, conditional on the information $\Sigma_{\leq M}$ about the random coefficient,
- sGFEM provides faster convergence rates w.r.t. the total number of degrees of freedom $N_{\text{tot}} = N_D N_\Omega$,
- sGFEM is stable on any subspace $Y^M_{\mu,\nu} \subseteq L^2_\rho(I)$ (cf. Remark 3.3) providing maximum flexibility in the adaptive selection active gPC modes, to be discussed below.

5 Implementation

5.1 Algorithms

A crucial point in the implementation of the sGFEM and the collocation algorithm is to equilibrate their different sources of error as pointed out in Subsection 3.3. The main error sources are

- truncating the KL-expansion
- spatial discretization
- stochastic discretization and stochastic interpolation error, respectively

Proposition 3.11 and Theorem 4.3 provide guidelines on how to choose the parameters of the algorithms in order to equilibrate the error contributions.

Given a tolerance ϵ on the solution u and input data $V_a(\mathbf{x}, \mathbf{x}')$, $E_a(\mathbf{x})$, we propose the following algorithms

Algorithm 5.1. (sGFEM algorithm) .

1. Given $\epsilon > 0$, **determine** a KL-truncation order M such that
$$||u(\omega, \mathbf{x}) - u_M(\omega, \mathbf{x})||_{\mathcal{H}_0^1(D)} \leqslant \epsilon.$$
2. **Compute** eigenpairs (λ_m, φ_m), $m = 1, ..., M$ of the covariance operator (2.2) by [32].
3. **Choose** a spatial discretization level L, such that the associated error $\epsilon_{V_L^D}$ in (3.29) is less than ϵ.
   Compute the stiffness matrices (5.7) and the spatial load vector (5.9).
4. **Determine** μ and ν such that the stochastic error $||u_M - P^I_{\Lambda_{M,\mu,\nu}} u_M||_{\mathcal{H}_0^1} \leqslant \epsilon$.
   Compute the stiffness matrices (5.6) and the stochastic load vector in (5.8).
5. **Solve** the resulting system.
6. **Calculate** the required statistical data from the solution.

Algorithm 5.2. (sCFEM algorithm).

1. Given $\epsilon > 0$, **determine** a truncation order M such that
$$||u(\omega, \mathbf{x}) - u_M(\omega, \mathbf{x})||_{\mathcal{H}_0^1(D)} \leqslant \epsilon.$$
2. **Compute** the eigenpairs (λ_m, φ_m) of the covariance operator (2.2) by [32].
3. **Choose** a spatial FE discretization level L, such that the associated spatial error is less than ϵ.
4. **Determine** the parameters $\underline{\mu}, \nu$ such that the interpolation error (4.9) is less than ϵ and **compute** the corresponding collocation points.
5. **Solve** (4.1) for each collocation point $\mathbf{y_k}$ by finite element projection.
6. **Calculate** the required statistical data from the set of solutions.

As it can be seen above, both algorithms consist of several key tasks, namely for the sGFEM

- Eigenvalue and eigenfunction computation of the covariance operator $(V_a u)(\mathbf{x})$ defined in (2.2).
- Assembly of the stochastic and spatial stiffness matrices.
- Solving the global system.
- Postprocessing the deterministic solution to obtain statistics.

and in the sCFEM

- Eigenvalue and eigenfunction computation of the covariance operator $(V_a u)(\mathbf{x})$ defined in (2.2).
- Computing the collocation points.
- Deriving the response statistics from the interpolated solution (postprocessing).

The following subsections briefly address those computational tasks.

5.2 KL - Eigenpair Computation

The eigenproblem to be solved can be formulated as: Find $(\lambda, \varphi) \in \mathbb{R}^+ \times L^2(D)$ s.t.

$$(V_a u)(\mathbf{x}) = \int_D V_a(\mathbf{x}, \mathbf{x}')\varphi(\mathbf{x}')\, d\mathbf{x}' = \lambda\varphi(\mathbf{x}), \tag{5.1}$$

where $V_a(\mathbf{x}, \mathbf{x}')$ is an admissible covariance function in the sense of Definition 2.1. This is a Fredholm integral equation of the second kind. For some special correlation functions like exponential ones and simple domains D, analytical solutions to (5.1) can be obtained by separation of variables, [13]. For more general correlation functions and arbitrary domains D, however, the KL-eigenpairs have to be computed numerically [32]. In variational form, the KL-Eigenvalue problem (5.1) becomes:
Find $\lambda \in \mathbb{R}$ and $0 \neq \varphi \in L^2(D)$ s.t. $\forall v \in L^2(D)$

$$\int_D \int_D V_a(\mathbf{x}, \mathbf{x}')\varphi(\mathbf{x}')v(\mathbf{x})\, d\mathbf{x}' d\mathbf{x} = \lambda \int_D \varphi(\mathbf{x})v(\mathbf{x})\, d\mathbf{x}. \tag{5.2}$$

For the numerical examples in Section 6 the discretization was done by piecewise linear finite element shape functions. The obtained generalized matrix eigenvalue problem was then solved by using JDBSYM, a Jacobi Davidson method optimized for large symmetric eigenproblems, see [11, 12] for details.

5.3 Assembly of sGFEM stiffness matrix

Once discrete spaces $\mathcal{P}_{M,\mu,\nu}$ and V_L^D have been selected in Algorithm 5.1, any choice of basis functions $(\zeta_i(\mathbf{y}))_{i=1}^{N_\Omega} \in \mathcal{P}_{M,\mu,\nu}$ and $(\psi_i(\mathbf{x}))_{i=1}^{N_D} \in V_L^D$ will lead to a linear system

$$A\mathbf{u} = \mathbf{l}, \tag{5.3}$$

where

$$A = G_0 \otimes A_0 + \sum_{m=1}^{M} G_m \otimes A_m, \tag{5.4}$$

$$\mathbf{l} = \mathbf{g}_0 \otimes \mathbf{f}_0, \tag{5.5}$$

with the stochastic mass matrices

$$\begin{aligned}[G_0]_{ij} &= \int_I \zeta_i(\mathbf{y})\zeta_j(\mathbf{y})\rho(\mathbf{y})\,d\mathbf{y},\\ [G_m]_{ij} &= \int_I \sqrt{\lambda_m} y_m \zeta_i(\mathbf{y})\zeta_j(\mathbf{y})\rho(\mathbf{y})\,d\mathbf{y},\end{aligned} \tag{5.6}$$

the deterministic finite element stiffness matrices

$$\begin{aligned}[A_0]_{ij} &= \int_D E_a(\mathbf{x})\nabla\psi_i(\mathbf{x})\nabla\psi_j(\mathbf{x})\,d\mathbf{x},\\ [A_m]_{ij} &= \int_D \varphi_m(\mathbf{x})\nabla\psi_i(\mathbf{x})\nabla\psi_j(\mathbf{x})\,d\mathbf{x}\end{aligned} \tag{5.7}$$

and the load vectors

$$[g_0]_i = \int_I \zeta_i(\mathbf{y})\rho(\mathbf{y})\,d\mathbf{y}, \tag{5.8}$$

$$[f_0]_i = \int_D f(\mathbf{x})\psi_i(\mathbf{x})\,d\mathbf{x}. \tag{5.9}$$

Hence, the resulting linear system has a block structure with a total number of $N_{\text{tot}} = N_\Omega \cdot N_D$ degrees of freedom. Even though the number of variables in the system grows polynomially with M, the memory consumption consists of saving the (M+1) spatial matrices (5.7), the stochastic mass matrices (5.6) and the vectors $\mathbf{g}_0$ and $\mathbf{f}_0$ given in (5.5). As it can be seen in (5.6) and (5.7) all of them are sparse and can therefore be efficiently stored using an appropriate storage scheme.

The assembly procedures for the spatial and stochastic stiffness matrices can be run independently from each other. Since the spatial matrices (5.7) are generic finite element stiffness matrices, their assembly is standard and will not be discussed here.

For the computation of the stochastic stiffness matrices we use tensor products of polynomials which are orthogonal w.r. to the marginal probability densities $\rho_m(y_m)$ in Assumption 2.8, iiib). Such polynomial systems can be generated for each marginal coordinate y_m independently and in parallel once the densities $\rho_m(\cdot)$ are known using standard algorithms (see e.g. [10] and the references therein). In certain cases they are known explicitly as e.g. in the case when $I_m = [-1, 1]$ and $\rho_m = \frac{1}{2}$ for all m where they are tensorized Legendre polynomials. Denoted again by $\mathcal{L}_{M,\alpha}$. According to (5.6), the integrals

$$\int_I \mathcal{L}_{M,\alpha}(\mathbf{y})\mathcal{L}_{M,\alpha'}(\mathbf{y})\,d\mathbf{y} \quad \text{and} \quad \int_I y_m \mathcal{L}_{M,\alpha}(\mathbf{y})\mathcal{L}_{M,\alpha'}(\mathbf{y})\,d\mathbf{y} \tag{5.10}$$

have to be computed. The evaluation of the integrals can be done analytically, since formulae for Legendre polynomials are known explicitly. Due to L^2-orthogonality the first integral is nonzero if and only if $\alpha = \alpha'$. Specifically,

$$\int_{I_m} L_{\alpha_m}(y_m)L_{\alpha'_m}(y_m)\,dy_m = \frac{2}{2\alpha_m + 1}\delta_{\alpha_m\alpha'_m}. \tag{5.11}$$

The second integral can be computed by the formula

$$\int_{I_m} y_m L_{\alpha_m}(y_m)L_{\alpha'_m}(y_m)\,dy_m = \begin{cases} \frac{2\alpha_m+1}{(2\alpha_m+1)(2\alpha_m+3)} & \alpha'_m = \alpha_m + 1\\ \frac{2\alpha_m}{(2\alpha_m-1)(2\alpha_m+1)} & \alpha'_m = \alpha_m - 1\\ 0 & \text{else.}\end{cases} \tag{5.12}$$

Hence, the second integral in (5.10) is nonzero if and only if α and α' differ exactly by one in the m'th entry.

We define the sum of the stochastic mass matrices as

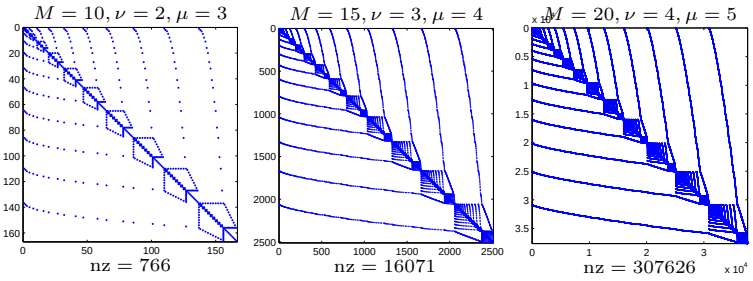

Figure 5.1: Sparsity patterns of the cumulated mass matrix G. Different Parameter choices of M, μ, ν are considered as indicated.

Definition 5.3 (cumulated stochastic mass matrix)**.**

$$G := G_0 + G_1 + \ldots + G_M. \tag{5.13}$$

The sparsity pattern of the cumulated stochastic mass matrix is illustrated in Figure 5.1. The index set $\Lambda_{M,\mu,\nu}$ in conjunction with a Legendre basis has been used to assemble the matrices (5.6). The eigenvalues and eigenvectors stem from an underlying spatial problem, using a covariance function $V_a(x, x') = e^{-10|x-x'|^2}$ on $D = [-1, 1]$.

From the integral formulae (5.11) and (5.12) it follows immediately that G has at most $2M+1$ nonzero entries per row and column. Note that the structure of the combined stiffness matrix A in (5.3) remains the same as of G where every entry of G is multiplied with a spatial FE-matrix, hence becoming a tensor of order four.

Remark 5.4. In case of an additional stochastic right hand side in problem (1.2) the source $f(\mathbf{x}, \tilde{\omega})$, like the diffusion coefficient, could be represented as a truncated Karhunen-Loève series. Then, the vector $\mathbf{l}$ in (5.5) would have a similar representation as A in (5.4), namely as the sum of tensor products between deterministic and stochastic load vectors with eigenfunctions and associated random variables as weighting functions cf. [21].

5.4 Iterative solution of the combined system

For the solution of the symmetric and positive definite combined system $A\mathbf{u} = \mathbf{l}$ (5.3) a conjugate gradient algorithm is used. The matrix vector multiplication is done blockwise whereas the outer iteration runs over the stochastic degrees of freedom. It is well-known, see e.g. [27], how the number of CG-steps to achieve a given accuracy can be estimated in terms of the condition number of the matrix A.

Proposition 5.5 (CG-steps)**.** *Let $A\mathbf{u} = \mathbf{l}$ be a symmetric positive definite linear system. Denote by $\mathbf{e}^{(k)} := \mathbf{u}^{(k)} - \mathbf{u}$ the residual in the k-th CG-step. The number of required CG-steps to achieve a given accuracy*

$$\|\mathbf{e}^{(k)}\|_A / \|\mathbf{e}^{(0)}\|_A \leqslant \epsilon \tag{5.14}$$

can be estimated as

$$k \leqslant \frac{1}{2}\sqrt{\kappa(A)} \ln\left(\frac{2}{\epsilon}\right) + 1, \tag{5.15}$$

where $\kappa(A)$ denotes the condition number of A measured in the 2-norm.

For an efficient iterative solver, we must reduce the condition number of A by means of preconditioning. As the matrix A in (5.4) is a (sum of) Kronecker

products of the stochastic moment matrices and the finite element stiffness matrices, preconditioners must be built as Kronecker products of preconditioners of each factor.

For the finite element stiffness matrix, we propose the usage of biorthogonal FE wavelets on $L^2(D)$ to build the stiffness matrices (5.7) and the load vector (5.9), see also Subsection 3.1. Given a FE-wavelet discretization, the following proposition then ensures the existence of a diagonal matrix Π, such that the preconditioned linear system

$$\Pi^{-1} A\mathbf{u} = \Pi^{-1}\mathbf{l} \tag{5.16}$$

has a bounded condition number, independent of the deterministic and stochastic discretization parameters.

Proposition 5.6. *There exists a robust preconditioner* Π *for the sGFEM, such that*

$$\kappa(\Pi A) \leqslant C, \tag{5.17}$$

where the constant C *is independent of* M, μ, ν, L.

Proof Let us denote by $\Psi = \{\psi_\lambda, \lambda \in \nabla\}$, where ∇ denotes an index set, the ensemble of biorthogonal wavelets on $L^2(D)$. Hence, every function $\tilde{v} \in L^2(D)$ can be represented in terms of wavelets as

$$\tilde{v} = \sum_{\lambda\in\nabla} d_\lambda \psi_\lambda = \mathbf{d}^\top \Psi \tag{5.18}$$

From (3.6) we recall the fact that biorthogonal wavelets in $L^2(D)$ satisfy (by construction) the *norm equivalence* $\|\mathbf{d}\|_{l^2(\nabla)} \sim \|\mathbf{d}^\top\Psi\|_{L^2(D)}$. Since every function $v \in H_0^1(D)$ can be represented equivalently as in (3.5), there exists a diagonal matrix Π_1, such that the following norm equivalence holds:

$$\|\Pi_1^{-1}\mathbf{d}\|_{l^2(\nabla)} \sim \|\mathbf{d}^\top\Psi\|_{H_0^1(D)}, \tag{5.19}$$

i.e. the scaled wavelets form a Riesz basis for the FE energy space $H_0^1(D)$. Therefore, *diagonal preconditioning* of the FE stiffness matrix leads to bounded condition numbers of A, independent of the meshwidth in the physical domain D.

Let us address the preconditioning of the stochastic moment matrix G. To this end, let $w \in L^2(I)$ and denote by $\mathcal{L}_{M,\alpha}$ the tensorized Legendre polynomials defined earlier in (3.13). Then

$$w = \sum_{\alpha\in\mathbb{N}^M} w_\alpha \mathcal{L}_\alpha = \mathbf{w}\mathcal{L}_M, \quad w_\alpha = (w, \mathcal{L}_\alpha)_{L^2(D)} \tag{5.20}$$

Define the diagonal matrix $\Pi_2 = \{\prod_{m=1}^M \frac{2}{2\alpha_m+1}\delta_{\alpha\alpha'}\}_{\alpha\alpha'}$. It follows (Parseval)

$$\|\Pi_2^{-1}\mathbf{w}\|_{l^2(\mathbb{N}^M)} = \|\mathbf{w}^\top\mathcal{L}\|_{L^2(I)}. \tag{5.21}$$

We then set $\Pi := \Pi_2 \otimes \Pi_1$. Any function $u \in L^2_\rho(I, H_0^1(D))$ can be written as

$$u = \sum_{\alpha\in\mathbb{N}^M}\sum_{\lambda\in\nabla} u_{\lambda,\alpha}\psi_\lambda \otimes \mathcal{L}_{M,\alpha}$$

Denote $\mathbf{u} = \{u_{\lambda,\alpha}\}_{\lambda,\alpha}$. Therefore, by (5.19), (5.21) and Assumption 1.1,

$$(\Pi A\mathbf{u}, \mathbf{u})_{L^2(I)\otimes H_0^1(D)} \sim \|\mathbf{u}\|_{l^2(\mathbb{N}^M)\otimes l^2(\nabla)} \tag{5.22}$$

which ensures (5.17) □

Remark 5.7. From the previous proof it follows immediately that the sequence of linear systems obtained by the collocation algorithm can be preconditioned by means of Π_1, since the diffusion parameter $a_M(\mathbf{y_k}, \mathbf{x})$ is bounded for any choice of collocation point $\mathbf{y_k}$.

5.5 Postprocessing

5.5.1 sGFEM postprocessing

In order to extract the statistical information from the sGFEM solution

$$u^L_{\Lambda_{M,\mu,\nu}}(\mathbf{y},\mathbf{x}) = \sum_{\alpha\in\Lambda_{M,\mu,\nu}} u_\alpha(\mathbf{x})\mathcal{L}_{M,\alpha}(\mathbf{y})$$

some sort of postprocessing is necessary. For the mean value we obtain, due to the orthogonality relation (5.11), the simple formula

$$\mathbb{E}[u^L_{\Lambda_{M,\mu,\nu}}] = u_{\mathbf{0}}(\mathbf{x}), \tag{5.23}$$

where $\mathbf{0} = \underbrace{(0,0,\ldots,0)}_{M \text{ times}}$.
Since the variance can be expressed as $\mathrm{Var}[u^L_{\Lambda_{M,\mu,\nu}}] = \mathbb{E}[(u^L_{\Lambda_{M,\mu,\nu}})^2] - \mathbb{E}[u^L_{\Lambda_{M,\mu,\nu}}]^2$ we obtain the formula

$$\mathrm{Var}[u^L_{\Lambda_{M,\mu,\nu}}] = \sum_{\alpha\neq\mathbf{0}} u_\alpha(\mathbf{x})^2 \tag{5.24}$$

5.5.2 sCFEM postprocessing

To retrieve statistics from the set of collocation solutions $u^L_M(\mathbf{y_k},\mathbf{x})$ we use formula (4.5) and the fact that the collocation points $\mathbf{y_k}$ are nodes of a weighted tensor product Gaussian quadrature formula. Denote by $\omega_{\mathbf{k}}$ the weights associated with $\mathbf{y_k}$. For the mean we obtain

$$\mathbb{E}[u^L_{\mathcal{I}_{M,\underline{\mu},\nu}}] = \sum_{\substack{S\subset\{1,\ldots,M\}\\ |S|\leqslant\nu}} \gamma_{M,|S|,\nu} \sum_{\substack{\mathbf{k}\in\mathbb{N}_0^M\\ \mathbf{k}\leqslant\underline{\mu}+\mathbf{1},\mathrm{supp}(\mathbf{k})=S}} \omega_{\mathbf{k}} u^L_M(\mathbf{y_k}). \tag{5.25}$$

The computation of higher order moments can be done similarly, e.g. in the case of $\mathbb{E}[(u^L_{\mathcal{I}_{M,\underline{\mu},\nu}})^2]$ we have

$$\mathbb{E}[(u^L_{\mathcal{I}_{M,\underline{\mu},\nu}})^2] = \sum_{\substack{S\subset\{1,\ldots,M\}\\ |S|\leqslant\nu}} \gamma_{M,|S|,\nu} \sum_{\substack{\mathbf{k}\in\mathbb{N}_0^M\\ \mathbf{k}\leqslant\underline{\mu}+\mathbf{1},\mathrm{supp}(\mathbf{k})=S}} \omega_{\mathbf{k}} (u^L_M(\mathbf{y_k}))^2. \tag{5.26}$$

The quadratures in (5.25), (5.26) are summed and tensorized Gaussian quadrature rules which are exact for the ANOVA type spaces $\mathcal{P}_{M,\mu,\nu}$.

6 Numerical examples

This section provides numerical examples illustrating sparse polynomial chaos approximation, the sGFEM (Algorithm 5.1) and sparse collocation method (Algorithm 5.2). The sGFEM and collocation examples will be given in one and two space dimensions. A uniform pdf of the random variables y_m on $I = I_1 \times I_2 \times \ldots$ is assumed in all examples. Therefore, gPC spaces based on active modes given by $\Lambda_{M,\mu,\nu}$ in combination with Legendre polynomials are used for the stochastic discretization. For the spatial discretization, if considered, piecewise linear finite elements are used. All examples have been run on a single processor AMD64 machine.

6.1 Sparse polynomial chaos approximation

To illustrate the convergence of SPC approximations we will, on one hand, consider the variational "zero-dimensional" model problem (2.34) and, on the other hand, approximate the solution of the semidiscrete problem (4.1).

Motivated by the fact that

$$u_M^0 = \frac{1}{\gamma_0 + \gamma_1\sqrt{\lambda_1}y_1 + \ldots + \gamma_M\sqrt{\lambda_M}y_M} \tag{6.1}$$

is the exact solution to the "zero-dimensional" problem, we try to approximate (6.1) by a sparse polynomial chaos expansion. Discretizing (2.34) with $\mathcal{P}_{M,\mu,\nu} \subset L^2_\rho(I)$ as in Subsection 5.3 results in a linear system

$$G\mathbf{u}^0_{\Lambda_{M,\mu,\nu}} = \mathbf{g_0}, \tag{6.2}$$

for the discrete solution $u^0_{\Lambda_{M,\mu,\nu}}$ with G and $\mathbf{g_0}$ denoting the same matrix and vector as in the underlying spatial problem, see (5.13) and (5.8), respectively.

Hence the error $\epsilon_{\mu,\nu}$, see Section 3.3, of the y-approximation in (3.29) can be measured by looking at the algebraic problem (2.28) where the exact solution is known. In fact, the numerical examples will show that the y-approximation error of the "zero-dimensional" problem is mostly higher than the corresponding error of the semidiscrete problem. Since

$$||u_M^0 - u^0_{\Lambda_{M,\mu,\nu}}||^2_{L^2_\rho(I)} \leqslant \frac{1}{\alpha^*} b^0(u_M^0 - u^0_{\Lambda_{M,\mu,\nu}}, u_M^0 - u^0_{\Lambda_{M,\mu,\nu}}) \tag{6.3}$$

we compute the ("zero-dimensional") energy error as follows.

Proposition 6.1 ("zero-dimensional" energy error)**.**

$$b^0(u_M^0 - u^0_{\Lambda_{M,\mu,\nu}}, u_M^0 - u^0_{\Lambda_{M,\mu,\nu}}) = \int_I \frac{\rho(\mathbf{y})}{\gamma_0 + \sum_{m=1}^M \gamma_m\sqrt{\lambda_m}y_m}\, d\mathbf{y} - \mathbb{E}[u^0_{\Lambda_{M,\mu,\nu}}], \tag{6.4}$$

i.e. the difference between the mean values of u_M^0 and $u^0_{\Lambda_{M,\mu,\nu}}$.

Proof The variational formulations of (2.30) and its discretized version read

$$b^0(u_M^0, v) = l^0(v), \qquad \forall v \in L^2_\rho(I) \tag{6.5}$$

$$b^0(u_{N_y}^0, v) = l^0(v), \qquad \forall v \in \mathcal{P}_{M,\mu,\nu}. \tag{6.6}$$

The energy error

$$\mathbf{e} = b^0(u_M^0 - u^0_{\Lambda_{M,\mu,\nu}}, u_M^0 - u^0_{\Lambda_{M,\mu,\nu}})$$

is given by

$$\begin{aligned} \mathbf{e} &= b^0(u_M^0, u_M^0) - 2b^0(u_M^0, u^0_{\Lambda_{M,\mu,\nu}}) + b^0(u^0_{\Lambda_{M,\mu,\nu}}, u^0_{\Lambda_{M,\mu,\nu}}) \\ &\overset{(6.5),(6.6)}{=} l^0(u_M^0) - 2l^0(u^0_{\Lambda_{M,\mu,\nu}}) + l^0(u^0_{\Lambda_{M,\mu,\nu}}) = l^0(u_M^0) - l^0(u^0_{\Lambda_{M,\mu,\nu}}), \end{aligned}$$

which concludes the proof. □

The integral in formula (6.4) we found best evaluated with a Smolyak cubature based on the Clenshaw-Curtis rule, see [24].

Hence, in the following we will always consider a semidiscrete problem (4.1) and, at the same time, use it as an underlying problem for the "zero-dimensional" case using the same Karhunen-Loève data to compute γ_m. We will compare the stochastic sGFEM error $\|u_M^L - u^L_{\Lambda_{M,\mu,\nu}}\|$, measured in the $L^2(D)$-norm and the $H^1(D)$-seminorm, to the "zero-dimensional" energy error (6.4).

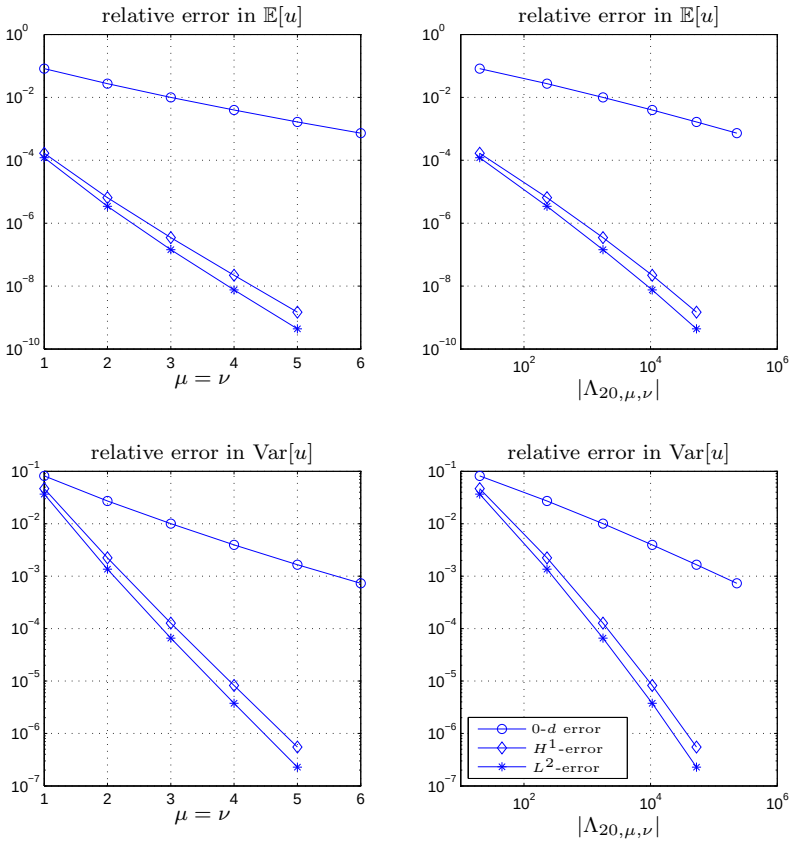

Figure 6.1: Numerical example to show the SPC approximation for $M = 20$ in terms of the "zero-dimensional" relative energy error (6.4) and the relative semidiscrete error $\|u_M^L - u_{\Lambda_{M,\mu,\nu}}^L\|$ as described in Subsection 6.1.1. The left graphs show the errors w.r.t. the parameter choices μ, ν and the right graphs w.r.t. the cardinality $|\Lambda_{20,\mu,\nu}|$

6.1.1 SPC approximation in $M = 20$ dimensions, Example 1

This example considers a one-dimensional problem on $[-1, 1]$ with $V_a(x, x') = e^{-4|x-x'|^2}$ and $\mathbb{E}_a(x) = 3 + x$. The Karhunen-Loève expansion is truncated after $M = 20$ terms. For the semidiscrete problem, 800 spatial elements have been used for discretization. The stochastic approximation has been computed using different values of μ, ν as indicated in Figure 6.1. There, the top graphs show the approximation of the mean field whereas the bottom graphs show the approximation error w.r.t. the variance.

6.1.2 SPC approximation in $M = 20$ dimensions, Example 2

Choosing the same correlation function as in the previous example but a different mean field $\mathbb{E}_a(x) = 5 - x$ should lead to a better convergence due to the fact that u_M^0 in (6.1) is now "more" bounded away from its singularity, i.e. α^* (2.33) is larger. This is indeed shown in Figure 6.2.

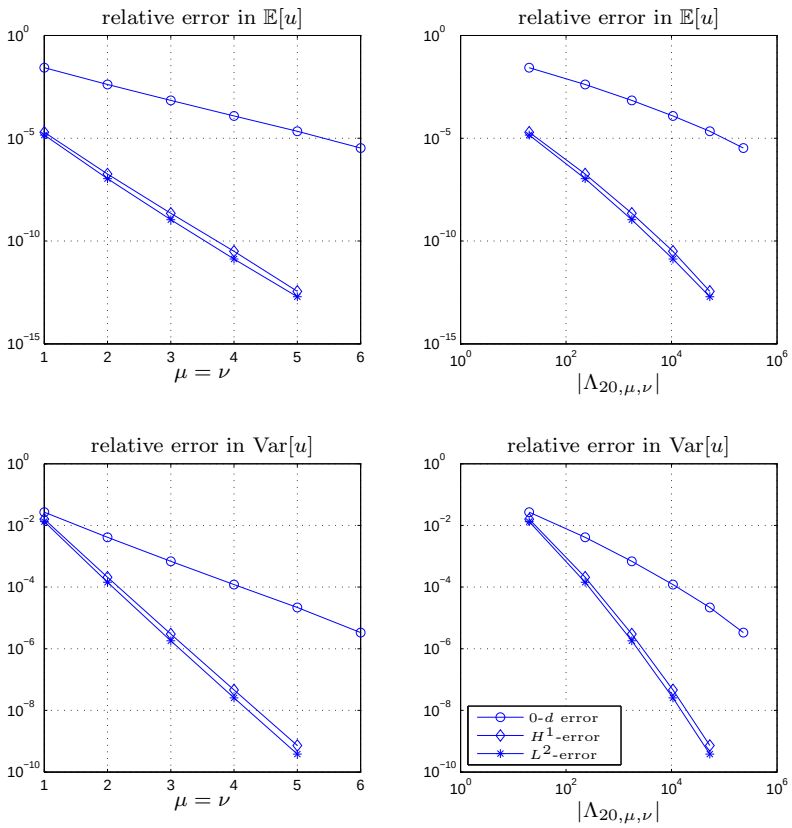

Figure 6.2: Numerical example to show the SPC approximation for $M = 20$ in terms of the "zero-dimensional" relative energy error (6.4) and the relative semidiscrete error $\|u_M^L - u_{\Lambda_{M,\mu,\nu}}^L\|$ as described in Subsection 6.1.2. The left graphs show the errors w.r.t. the parameter choices μ, ν and the right graphs w.r.t. the cardinality $|\Lambda_{20,\mu,\nu}|$

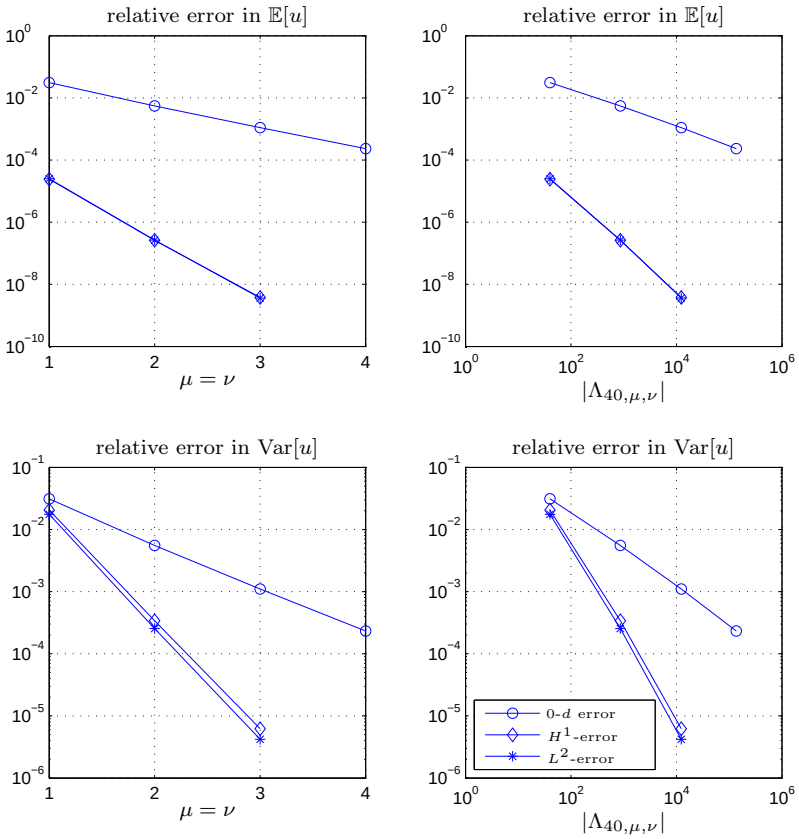

Figure 6.3: Numerical example to show the SPC approximation for $M = 40$ in terms of the "zero-dimensional" relative energy error (6.4) and the relative semidiscrete error $\|u_M^L - u_{\Lambda_{M,\mu,\nu}}^L\|$ as described in Subsection 6.1.3. The left graphs show the errors w.r.t. the parameter choices μ, ν and the right graphs w.r.t. the cardinality $|\Lambda_{40,\mu,\nu}|$

6.1.3 SPC approximation in $M = 40$ dimensions

This example considers a 1-d problem with $V_a(x, x') = e^{-25|x-x'|^2}$ and $\mathbb{E}_a(x) = 5-x$. The approximation is now carried out in $M = 40$ dimensions. Again the relative "zero-dimensional" energy error and the relative error measured in the $L^2(D)$-norm and the $H^1(D)$-seminorm are shown in Figure 6.3.

6.1.4 SPC approximation in $M = 80$ dimensions

This example considers again a Gaussian covariance on $[-1, 1] \times [-1, 1]$ but with short correlation length $\gamma = 0.0125$, hence $V_a(x, x') = e^{-400|x-x'|^2}$. By Remark 2.4, the KL-eigenvalue decay is at least exponential but with small constant in the exponent. To achieve reasonable accuracy with sGFEM, we are therefore forced to consider a tensor product gPC space in $M = 80$ independent variables in the stochastic approximation space $\mathcal{P}_{M,\mu,\nu}$. Figure 6.4 shows again the relative "zero-dimensional" energy error compared to the L^2 and H^1 error for both, mean field $\mathbb{E}[u]$ and variance $\mathrm{Var}[u]$.

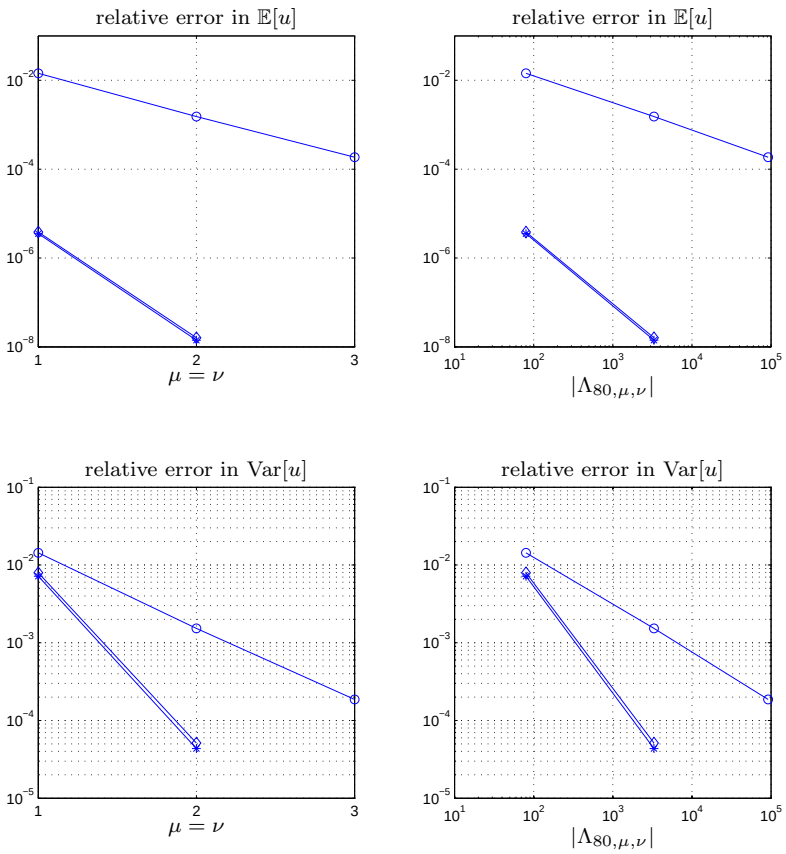

Figure 6.4: Numerical example to show the SPC approximation for $M = 80$ in terms of the "zero-dimensional" relative energy error (6.4) and the relative semidiscrete error $\|u_M^L - u_{\Lambda_{M,\mu,\nu}}^L\|$ as described in Subsection 6.1.4. The left graphs show the errors w.r.t. the parameter choices μ, ν and the right graphs w.r.t. the cardinality $|\Lambda_{80,\mu,\nu}|$

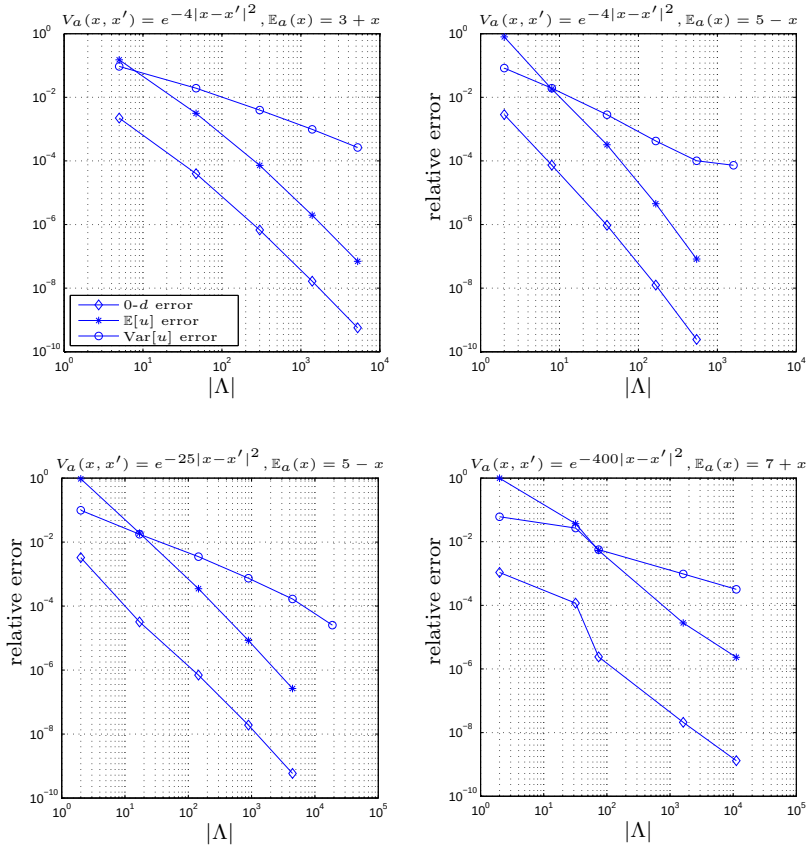

Figure 6.5: Numerical examples showing adapted SPC approximation using Algorithm 3.8. Various examples of two-point correlation functions $V_a(\mathbf{x}, \mathbf{x}')$ and mean fields $\mathbb{E}_a(\mathbf{x})$ are considered as indicated. The "zero-dimensional" error is compared against the $H^1(D)$ error of the mean and variance

6.1.5 Adapted SPC approximation

Here, we will again consider the numerical examples 6.1.1–6.1.4 but instead of using a sparse PC approximation based on $\Lambda_{\mu,\nu}$, we will use Algorithm 3.8 to obtain a hierarchic sequence of stochastic indices $\Lambda^{(0)} \subset \Lambda^{(1)} \subset \ldots$. The steering parameter θ is chosen equal to 0.1. Figure 6.5 shows the obtained results. Again, the "zero-dimensional" error is compared to the $H^1(D)$-error in mean and variance. By comparing the obtained results to the ones in Figure 6.1–6.4 it can clearly be seen, that the adapted approach takes considerably less stochastic DoFs into account than the $\Lambda_{M,\mu,\nu}$ approach considered earlier.

6.2 sGFEM and sCFEM

In the following we will consider 3 example problems of the form (1.2) in one and two space dimensions where the aim is to compute first- and second-order moments of the solution using Algorithm 5.1. The second example will again be an example where the correlation function has a short correlation length and therefore an

Step	M	N_{det}	$\Lambda_{M,\mu,\nu}$	N_{tot}	CG-steps	time [s]
1	7	10	$\Lambda_{7,1,1}$	84	9	0.01
2	10	40	$\Lambda_{10,2,2}$	2772	12	0.15
3	13	100	$\Lambda_{13,3,3}$	113120	14	3.49
4	15	400	$\Lambda_{15,4,4}$	1558152	15	114.02

Table 6.1: Sequence of discrete spaces used to approximate Example 1 by sGFEM

Step	M	N_{det}	ν/μ	N_{tot}	time [s]
1	7	10	1/1	88	0.01
2	10	40	2/2	8241	0.34
3	13	100	3/3	85484	31.6
4	15	400	4/4	152500701	5993

Table 6.2: Sequence of interpolants $\mathcal{I}_{M,\mu,\nu}$ for solving Example 1 by sparse collocation

a-priori reduction of the stochastic approximation space is necessary. We will, in particular, compare the performance of the sGFEM and the sCFEM for these problems with particular attention to the case of small correlation length, resp. large values of M.

6.2.1 Example 1, d=1

This one-dimensional example on $D = [-1, 1]$ compares the sGFEM to the sparse collocation algorithm. It considers a random coefficient $a(\omega, \mathbf{x})$ with $\mathbb{E}_a(x) = 3 + x$ and $V_a(x, x') = e^{-4|x-x'|^2}$. The deterministic right hand side is assumed to be periodic of the form $f(x) = 2\sin(x)$. Table 6.1 shows the sGFEM settings that have been used in each step as well as the number of iteration steps used to solve the global system and the total time used. Table 6.2 reports the corresponding settings for the sparse collocation algorithm. Figure 6.6 shows the numerical results obtained with these choices. To compare the obtained solutions, an "overkill" solution (i.e. a numerical solution on a substantially finer discretization) with $\Lambda_{20,5,5}$ and 800 spatial elements has been computed as a reference.

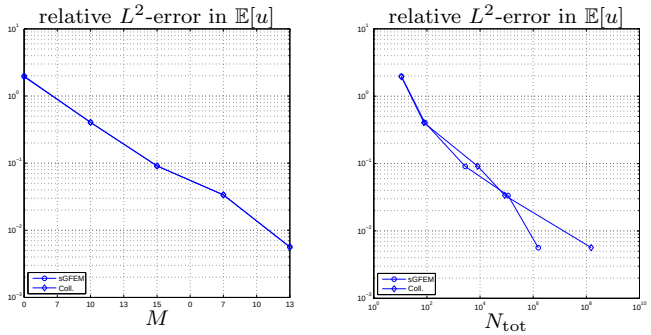

Figure 6.6: Numerical example to show convergence of sGFEM and sparse collocation as described in Subsection 6.2.1. Convergence of the mean field for discretization choices as shown in Tables 6.1 and 6.2 w.r.t. N_{tot} and M. is shown

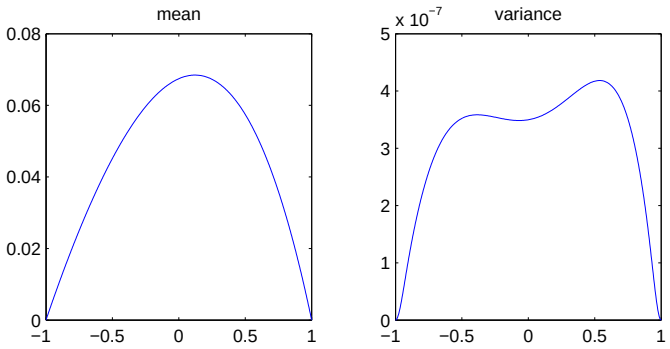

Figure 6.7: Numerical example with small correlation length: $V_a(x,x') = e^{-400|x-x'|^2}$. Mean and variance of the solution computed with 400 spatial elements and $\tilde{\Lambda}_{80,3,3}$ as stochastic discretization space.

6.2.2 Example 2, d=1

Here we consider the model problem (1.2) on $D = [-1,1]$ with small correlation length. The covariance kernel is given by $V_a(x,x') = e^{-400|x-x'|^2}$, hence the correlation length is $\gamma = 0.025$. The computation is done by using piecewise continuous linear elements for the spatial discretization in a uniform mesh $\mathcal{T}$ with 400 elements on $D = [-1,1]$ and the gPC space based on the index set $\Lambda_{80,3,3}$ for the discretization in the stochastic parameters. Note that the FE meshwidth $h = 2/400 = 0.005 < \gamma$, i.e. the FE mesh in D resolves the fluctuations of the random coefficient which occur on the length scale γ in this example.

We chose the mean field $\mathbb{E}_a(x) = 8 + x$ and a smooth right hand side $f(x) = e^x$. The above choices lead to a system with $N_{\text{tot}} \approx 30$ million. The total computation time was below 5 hours and the preconditioned block-CG algorithm converged in 9 steps. Figure 6.7 shows the computed mean value and variance of the solution.

6.2.3 Example 3, d=2

This last example considers the model problem in two dimensions, hence on $D = [-1,1]^2$. We consider a diffusion coefficient with a Gaussian correlation kernel $V_a(\mathbf{x},\mathbf{x}') = e^{-4|\mathbf{x}-\mathbf{x}'|^2}$ and mean field $\mathbb{E}_a(\mathbf{x}) = 5 + x_1$ and right hand side $f(\mathbf{x}) = 2e^{x_1+2x_2}$. The spatial discretization has been performed using piecewise linear finite elements on a triangular mesh with 7200 elements. The approximation space $\mathcal{P}_{20,2,2}$, hence $M = 20$, has been used for the stochastic discretization. Figure 6.8 shows the computed mean field and variance of the solution.

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A Technical Appendix on sGFEM

The appendix is devoted to the proof of Lemma 3.10. In the first subsection some auxiliary results will be stated, whereas in the second subsection the proof itself will be presented.

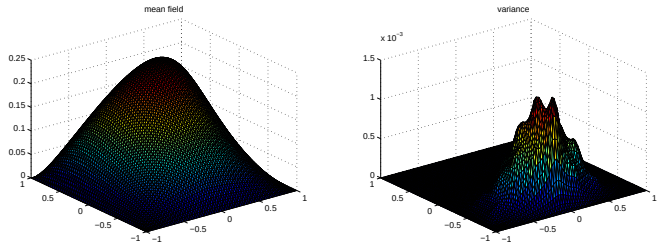

Figure 6.8: Numerical example in $[-1,1]^2$. $V_a(\mathbf{x},\mathbf{x}') = e^{-4|\mathbf{x}-\mathbf{x}'|^2}$, $\mathbb{E}_a(\mathbf{x}) = 5 + x_1$ and $f(\mathbf{x}) = 2e^{x_1+2x_2}$ are given. For the discretization piecewise linear finite elements and $\Lambda_{20,2,2}$ with Legendre polynomials have been used.

A.1 Auxiliary results

First we state two results which will be used in the proof of Lemma 3.10. As a first result, we prove

Lemma A.1. *For any fixed $t \in (0,1)$ and $N, L \in \mathbb{N}$ with $N \leqslant L$ it holds*

$$\sum_{n=N}^{\infty} \binom{L+n}{n} t^n = t^N (1-t)^{-(L+1)} e^{L(1+\ln N)} \tag{A.1}$$

$$\leqslant c_{1,t} e^{c_{2,t} L \ln N - c_{3,t} N} \tag{A.2}$$

with positive constants $c_{1,t}, c_{2,t}, c_{3,t}$.

Proof Define

$$S_L := \sum_{n=0}^{\infty} \binom{L+n}{L} t^n \tag{A.3}$$

Due to the binomial identity

$$\binom{L+n}{L} = \binom{L+n-1}{L} + \binom{L+n-1}{L-1} \tag{A.4}$$

we obtain the recursive formula $S_L = tS_L + S_{L-1}$, which leads to

$$S_L = (1-t)^{-L} S_0 = (1-t)^{-(L+1)} \tag{A.5}$$

It follows

$$\sum_{n=N}^{\infty} \binom{L+n}{n} t^n = t^N \sum_{n=0}^{\infty} \binom{L+N+n}{L} t^n. \tag{A.6}$$

By expanding the binomial coefficient into factorials we see that

$$\binom{L+N+n}{L} = \left(1 + \frac{L}{n+N}\right) \cdots \left(1 + \frac{L}{n+1}\right) \binom{L+n}{L} \tag{A.7}$$

Since for $x \geqslant 0$ it holds $1 + x \leqslant e^x$ and furthermore $\sum_{k=1}^{K} \frac{1}{k} \leqslant 1 + \int_1^K \frac{1}{x}\, dx$ the lemma follows □

The next result can be found in [35], Lemma A.2:

Lemma A.2. *If $\kappa > 0$ and $y > z > 0$, then there exists $c_{\kappa,y,z} > 0$ such that*

$$\sum_{1 \leqslant m_1 < \cdots < m_j < \infty} \prod_{i=1}^{j} e^{-y m_i^{\kappa}} \leqslant c_{\kappa,y,z} e^{-z \frac{1}{1+\kappa} j^{1+\kappa}} \tag{A.8}$$

for all $j \in \mathbb{N}_+$.

The following proposition is a generalization of a result in [7], Chapter 12.4 and provides a bound on the coefficients of the Legendre expansion (3.15)

Proposition A.3. *If u_M solves (2.19) and is expanded in a Legendre chaos series as in (3.15), then there exists a constant $c_{a,r,f}$, independent of M and α, such that the Legendre coefficients satisfy*

$$\|u_\alpha\|_{H_0^1(D)} \leqslant c_{a,r,f}\tilde{\mathbf{r}}^{-\alpha}, \tag{A.9}$$

where $\tilde{r}_m = \left(\frac{1}{2\eta_m m^{1+\delta}} + \sqrt{1+\frac{1}{(2\eta_m m^{1+\delta})^2}}\right)^{(1-\epsilon)}$ with any $0<\epsilon<1$, $0<\delta$ and η_m as defined in (2.24).

Proof The Legendre coefficients are given by the formula

$$u_\alpha = \left(\prod_{m=1}^{M} 2\alpha_m + 1\right) \int_I u_M(\mathbf{y})\mathcal{L}_\alpha(\mathbf{y})\rho(\mathbf{y})\, d\mathbf{y} \tag{A.10}$$

According to Lemma 2.10, u_M is separately analytic in each variable y_m, uniformly with respect to all other variables $y_j \in I_j$ with $j \neq m$, and the domain of analyticity is given by

$$\Sigma(I_m, \tau_m) = \{z \in \mathbb{C} : \operatorname{dist}(z, I_m) \leqslant \tau_m\}, \tag{A.11}$$

where $\tau_m = 1/2\eta_m$. It follows that u_M is also separately analytic in each variable y_m, assuming all other variables are given arbitrary but fixed values $y_j \in \Sigma(I_j, \frac{\tau_j}{j^{1+\delta}})$ with a $\delta > 0$. By Hartogs theorem (cf. [15], Theorem 2.2.8) such a separately analytic function is analytic. Hence, u_M is analytic in the product domain $\prod_{m=1}^{M}\Sigma(I_m, \frac{\tau_m}{m^{1+\delta}})$ and we can use the Cauchy formula to write

$$u_M(\mathbf{y}) = \frac{1}{(2\pi i)^M}\oint_\Gamma \frac{u_M(\mathbf{z})}{(\mathbf{z}-\mathbf{y})^{\mathbf{1}}}\, d\mathbf{z}, \tag{A.12}$$

where

$$\Gamma = \Gamma_1 \times \cdots \times \Gamma_M \tag{A.13}$$

and Γ_m is the largest possible ellipse in Σ_m with foci ± 1. It is easy to verify that the sum of its semiaxes is equal to

$$1 < r_m := \frac{\tau_m}{m^{1+\delta}} + \sqrt{1+\left(\frac{\tau_m}{m^{1+\delta}}\right)^2}. \tag{A.14}$$

Hence, we have

$$u_\alpha = \left(\prod_{m=1}^{M}\frac{2\alpha_m+1}{2\pi i}\right)\int_I \mathcal{L}_\alpha(\mathbf{y})\oint_\Gamma \frac{u_M(\mathbf{z})}{(\mathbf{z}-\mathbf{y})^{\mathbf{1}}}\, d\mathbf{z}\,\rho(\mathbf{y})d\mathbf{y} \tag{A.15}$$

$$= \left(\prod_{m=1}^{M}\frac{2\alpha_m+1}{2\pi i}\right)\oint_\Gamma u_M(\mathbf{z})\int_I \frac{\mathcal{L}_\alpha(\mathbf{y})}{(\mathbf{z}-\mathbf{y})^{\mathbf{1}}}\rho(\mathbf{y})\, d\mathbf{y}\, d\mathbf{z} \tag{A.16}$$

By [34] §4.9, the inner integral is a representation for the Legendre polynomials of the second kind,

$$\mathcal{Q}_\alpha(\mathbf{z}) = \int_I \frac{\mathcal{L}_\alpha(\mathbf{y})}{(\mathbf{z}-\mathbf{y})^{\mathbf{1}}}\rho(\mathbf{y})\, d\mathbf{y}. \tag{A.17}$$

Furthermore, if we substitute $z_m = \frac{1}{2}(w_m + w_m^{-1})$ (Joukowski transformation) with $|w_m| = r_m$, the Legendre polynomials of the second kind can be expanded like (cf. [7], Lemma 12.4.6)

$$Q_{\alpha_m}(\frac{1}{2}(w_m + w_m^{-1})) = \sum_{k=\alpha_m+1}^{\infty}\frac{q_{\alpha_m k}}{w_m^k}$$

with $|q_{\alpha_m k}| \leqslant \pi$. Hence,

$$|\mathcal{Q}_\alpha(\mathbf{z})| \leqslant \prod_{m=1}^{M} \sum_{k=\alpha_m+1}^{\infty} \frac{\pi}{r_m^k} = \frac{\pi^M \mathbf{r}^{-(\alpha+\mathbf{1})}}{\prod_{m=1}^{M}(1-r_m^{-1})}$$

Together with (A.16) we obtain

$$\begin{aligned}
|u_\alpha| &= \left| \left(\prod_{m=1}^{M} \frac{2\alpha_m+1}{2\pi i} \right) \oint_\Gamma u_M(\mathbf{z}) \mathcal{Q}_\alpha(\mathbf{z})\, dz \right| \\
&\leqslant \left(\prod_{m=1}^{M} \frac{2\alpha_m+1}{2\pi} \mathrm{Len}(\Gamma_m) \right) \max_{\Gamma} |u_M(\mathbf{z})| \max_{I} |\mathcal{Q}_\alpha| \qquad \text{(A.18)} \\
&\leqslant \left(\prod_{m=1}^{M} \frac{2\alpha_m+1}{2\pi} \mathrm{Len}(\Gamma_m) \right) \max_{\Gamma} |u_M(\mathbf{z})| \frac{\pi^M \mathbf{r}^{-(\alpha+1)}}{\prod_{m=1}^{M}(1-r_m^{-1})} \\
&\leqslant c_{a,r,f} \left(\prod_{m=1}^{M} 2(2\alpha_m+1) \right) \mathbf{r}^{-\alpha} \qquad \text{(A.19)}
\end{aligned}$$

where the last estimate holds due to the fact that $\mathrm{Len}(\Gamma_m) \leqslant 4r_m$. Since to every $\varepsilon > 0$ there exists a constant $C(\varepsilon) > 0$ s.t. $2\alpha_m + 1 \leqslant C(\varepsilon) r_m^{\varepsilon\alpha_m}$ for any $\varepsilon > 0$ the Proposition follows. □

Remark A.4. Note that due to the exponential decay of η_m, the same estimates for $\tilde{r}_m^{-1}$ hold as for η_m, i.e according to (2.15)

$$\tilde{r}_m^{-1} \leqslant c_r e^{-c_{1,r} m^{\kappa}} \qquad \text{(A.20)}$$

with constants depending on ε and δ if $\varepsilon \to 0$ and $\delta \to 0$.

A.2 Proof of Lemma 3.10 and of Proposition 3.7

Proof of Lemma 3.10 To get the error estimate (3.33) we estimate the part of the expansion

$$u_M = \sum_{\alpha \in \mathbb{N}^M} u_\alpha \mathcal{L}_{M,\alpha} \qquad \text{(A.21)}$$

that belongs to the complement of $\Lambda_{M,\mu,\nu}$. Since

$$\Lambda_{M,\mu,\nu} = \Lambda_{M,\mu} \cap \Lambda_{M,\nu},$$

where

$$\Lambda_{M,\mu} := \left\{ \alpha \in \mathbb{N}^M : |\alpha| \leqslant \mu \right\}, \quad \Lambda_{M,\nu} := \left\{ \alpha \in \mathbb{N}^M : \mathrm{supp}(\alpha) \leqslant \nu \right\},$$

we can split the complement into 2 parts, namely

$$\mathbb{N}^M \backslash \Lambda_{M,\mu,\nu} = \underbrace{(\Lambda_{M,\nu} \backslash \Lambda_{M,\mu})}_{\mathrm{I}} \cup \underbrace{\left(\mathbb{N}^M \backslash \Lambda_{M,\nu}\right)}_{\mathrm{II}}. \qquad \text{(A.22)}$$

We will then estimate parts I and II separately.

Part I: Denote $S_{\mathrm{I}} := || \sum_{\alpha \in \Lambda_{M,\nu} \backslash \Lambda_{M,\mu}} u_\alpha \mathcal{L}_\alpha(\mathbf{y}) ||_{L^\infty(I, H_0^1(D))}$. By using Proposition A.3 we get

$$\begin{aligned}
S_{\mathrm{I}} &\leqslant c_{a,r,f} \sum_{\substack{\alpha \in \Lambda_{M,\nu} \\ |\alpha| \geqslant \mu+1}} \tilde{\mathbf{r}}^{-\alpha} \leqslant c_{a,r,f} \sum_{\substack{\alpha \in \Lambda_{M,\nu} \\ |\alpha| \geqslant \mu+1}} \tilde{r}_1^{-|\alpha|} \\
&\leqslant c_{a,r,f} \sum_{n=\mu+1}^{\infty} \tilde{r}_1^{-n} \binom{\nu+n-1}{n} \binom{M}{\nu} \overset{(A.2)}{\leqslant} c_{a,r,f} e^{c_{1,a,r,f}\nu(\ln M + \ln \mu) - c_{2,a,r,f}\mu} \qquad \text{(A.23)}
\end{aligned}$$

where we used Lemma A.1 the last line.

Part II: Denote $S_{\mathrm{II}} := ||\sum_{\alpha\in\mathbb{N}^M\setminus\Lambda_{M,\nu}} u_\alpha \mathcal{L}_\alpha(\mathbf{y})||_{L^\infty(I,H_0^1(D))}$. Using again Proposition A.3 and by parametrizing the indices α through their support we get

$$\begin{aligned}
S_{\mathrm{II}} &\leqslant c_{a,r,f} \sum_{\substack{\alpha\in\mathbb{N}^M \\ \mathrm{supp}(\alpha)\geqslant\nu+1}} \tilde{\mathbf{r}}^{-\alpha} \\
&= c_{a,r,f} \sum_{j=\nu+1}^{M} \sum_{1\leqslant m_1<\cdots<m_j\leqslant M} \prod_{k=1}^{j} (\tilde{r}_{m_k}^{-1} + \tilde{r}_{m_k}^{-2} + \ldots) \\
&= c_{a,r,f} \sum_{j=\nu+1}^{M} \sum_{1\leqslant m_1<\cdots<m_j\leqslant M} \prod_{k=1}^{j} \left(\frac{\tilde{r}_{m_k}^{-1}}{1-\tilde{r}_{m_k}^{-1}}\right) \\
&\overset{(A.20)}{\leqslant} c_{a,r,f} \sum_{j=\nu+1}^{M} \sum_{1\leqslant m_1<\cdots<m_j\leqslant M} \prod_{k=1}^{j} c_1 e^{-c_{1,r} m_k^\kappa} \\
&\overset{(A.8)}{\leqslant} c_{a,r,f} \sum_{j=\nu+1}^{M} c_1^j e^{-c_{1,r} j^{1+\kappa}} \\
&\leqslant c_{a,r,f} e^{-c_{2,r}\nu^{1+\kappa}}. \qquad (A.24)
\end{aligned}$$

(A.23) together with (A.24) yields the desired result. □

Proof of Proposition 3.7 We adopt the notations of the previous proof of Theorem 3.10. Therefore $|\Lambda_{M,\mu,\nu}| = |\Lambda_{M,\mu} \cap \Lambda_{M,\nu}|$. Based on the fact that the equation $x_1 + x_2 + \ldots + x_q = l$ has exactly $\binom{l}{q}$ solutions $(x_1, x_2, \ldots, x_q) \in \mathbb{N}_+^q$, we obtain by a counting argument

$$\begin{aligned}
|\Lambda_{M,\mu} \cap \Lambda_{M,\nu}| &= \sum_{l=0}^{\mu}\sum_{q=0}^{\nu} \binom{M}{q}\binom{l}{q} = \sum_{q=0}^{\nu} \binom{M}{q}\binom{\mu+1}{q+1} \\
&\leqslant M^\nu \sum_{q=0}^{\nu} \binom{\mu+1}{q+1} \leqslant 2M^\nu(\mu+1)^{\nu+1}
\end{aligned}$$

□

B Technical Appendix on sCFEM

To prove Lemma 4.1 we establish bounds on the stability of the interpolation operator. Let $\mathcal{I}_p$ be the one-dimensional Lagrange interpolation operator as defined in (4.2) for $\underline{\mu} = p \in \mathbb{N}$.

Lemma B.1.

$$\|\mathcal{I}_p v\|_{L^\infty(I_m,H_0^1(D))} \leqslant \Lambda_{\alpha,\beta}(p+1)\|v\|_{L^\infty(I_m,H_0^1(D))} \qquad (B.1)$$

where $\Lambda_{\alpha,\beta}(p+1)$ denotes the Lebesgue constant which is in the case of Jacobi zeros given by

$$\Lambda_{\alpha,\beta}(p+1) = \begin{cases} \mathcal{O}(\log(p+1)) & -1 \leqslant \alpha,\beta \leqslant -1/2 \\ \mathcal{O}(p^{\gamma+1/2}),\ \gamma = \max(\alpha,\beta) & \text{else} \end{cases} \qquad (B.2)$$

(see e.g. [20]).

Proof

$$\begin{aligned}\|\mathcal{I}_p v\|_{L^\infty} &= \|\sum_{k=1}^{p+1} v(y_k) l_k(y)\|_{L^\infty} \leqslant \max_k v(y_k) \max_{y\in I_m} \sum_{k=1}^{p+1} |l_k(y)| \\ &\leqslant \Lambda_{\alpha,\beta}(p+1)\|v\|_{L^\infty}\end{aligned}$$

where $\Lambda_{\alpha,\beta}(p+1) := \max_{y\in I_m} \sum_{k=1}^{p+1} |l_k(y)|$ is the Lebesgue constant for Lagrange interpolation on the roots of Jacobi polynomials $J_{p+1}^{\alpha,\beta}(y)$. □

Hence, for fixed p, the interpolation operator satisfies a continuity estimate in L^∞. By writing $\mathcal{I}_{\underline{\mu}} = \mathcal{I}_{\mu_1} \otimes \cdots \otimes \mathcal{I}_{\mu_M}$ we immediately obtain a continuity estimate for the multivariate case.

Corollary B.2.

$$\|\mathcal{I}_{\underline{\mu}} v\|_{L^\infty(I,H_0^1(D))} \leqslant \prod_{m=1}^{M} \Lambda_{\alpha,\beta}(\mu_m+1)\|v\|_{L^\infty(I,H_0^1(D))} \tag{B.3}$$

Now let $u \in \mathcal{P}_{\underline{\mu}}(I)$ be a polynomial in $I = I_1 \times \cdots \times I_M$. It holds

$$\begin{aligned}\|v - \mathcal{I}_{\underline{\mu}} v\|_{L^\infty} &\leqslant \|v-u\|_{L^\infty(I)} + ||\mathcal{I}_{\underline{\mu}} u - \mathcal{I}_{\underline{\mu}} v||_{L^\infty(I)} &\text{(B.4)}\\ &\leqslant \left(1 + \prod_{m=1}^{M} \Lambda_{\alpha,\beta}(\mu_m+1)\right)\|v-u\|_{L^\infty(I)} &\text{(B.5)}\end{aligned}$$

Since this holds for any $u \in \mathcal{P}_{\underline{\mu}}$ we have proved

Lemma B.3.

$$\|v - \mathcal{I}_{\underline{\mu}} v\|_{L^\infty(I,H_0^1(D))} \leqslant \left(1 + \prod_{m=1}^{M} \Lambda_{\alpha,\beta}(\mu_m+1)\right) \min_{u\in\mathcal{P}_{\underline{\mu}}(I)} \|v-u\|_{L^\infty(I,H_0^1(D))} \tag{B.6}$$

Proof of Lemma 4.1 For notational convenience, we omit the subscript $L^\infty(I, H_0^1(D))$ of the norm in this paragraph. As it has been shown in [35] (Corollary 5.3), for every analytic function $g : I \to H_0^1(D)$ and $\nu \leqslant M$ the following equation holds:

$$g(\mathbf{y}) - \sum_{\substack{S\subset\{1,\dots,M\}\\ |S|\leqslant\nu}} \gamma_{M,|S|,\nu} g_S(\mathbf{y}) = \sum_{\substack{\alpha\in\mathbb{N}^M\\ |\mathrm{supp}(\alpha)|=\nu}} \frac{\partial^\alpha g(\mathbf{0})}{\alpha!}\mathbf{y}^\alpha. \tag{B.7}$$

where $\gamma_{M,s,\nu}$ is given as in (4.6). Therefore the interpolation error $\epsilon := \|u_M - \mathcal{I}_{M,\underline{\mu},\nu} u_M\|$ can be split into two parts, namely

$$\begin{aligned}\epsilon &\leqslant \|u_M^L - \sum_{\substack{S\subset\{1,\dots,M\}\\ |S|\leqslant\nu}} \gamma_{M,|S|,\nu} u_{M,S}^L\| &\text{(B.8)}\\ &\quad + \sum_{\substack{S\subset\{1,\dots,M\}\\ |S|\leqslant\nu}} |\gamma_{M,|S|,\nu}| \|u_{M,S}^L - \mathcal{I}_{\underline{\mu}} u_{M,S}^L\| &\text{(B.9)}\end{aligned}$$

As it has been shown in [35], Proposition 5.4 the first term is bounded by

$$\|u_M^L - \sum_{\substack{S\subset\{1,\dots,M\}\\ |S|\leqslant\nu}} \gamma_{M,|S|,\nu} u_{M,S}^L\| \leqslant c_{a,r,f} e^{-c_{1,a,r,f}\nu^{1+\kappa}}. \tag{B.10}$$

It remains to bound the second term. It has been shown in [35], Theorem 5.5 that the multivariate Chebyshev interpolant $\mathcal{I}_{\underline{\mu}}^{\mathrm{Cheb}}$ satisfies the following estimate for functions g analytic in a region as in (2.10):

$$\|g_S - \mathcal{I}_{\underline{\mu}}^{\mathrm{Cheb}} g_S\| \leqslant c e^{c_0 \nu} \left(\sum_{m \in S} e^{-c_m \mu_m} \right) \tag{B.11}$$

(B.11) together with Lemma B.3 then yields

$$\|u_{M,S}^L - \mathcal{I}_{\underline{\mu}} u_{M,S}^L\| \leqslant c_{a,r,f} e^{c_{0,a,r,f} \nu} \left(\sum_{m \in S} e^{-c_{m,a,r,f} \mu_m} \right) \tag{B.12}$$

Furthermore, [35] Lemma 5.3 assures that

$$\sum_{\substack{S \subset \{1,\dots,M\} \\ |S| \leqslant \nu}} |\gamma_{M,|S|,\nu}| \leqslant (\nu+1)(M+1)^{2\nu} \tag{B.13}$$

Combining (B.10),(B.12) and (B.13) we obtain the final result

$$\epsilon \leqslant c_{a,r,f} \left(e^{-\tilde{c}_{a,r,f} \nu^{1+\kappa}} + (M+1)^{2\nu} e^{c_{0,a,r,f} \nu} \left(\sum_{m=1}^{M} e^{-c_{m,a,r,f} \mu_m} \right) \right). \tag{B.14}$$

□

C Proof of Remark 2.4

Let H be a Hilbert space on D and denote by $\mathcal{B}(H)$ the set of bounded linear operators in H. In [32], Lemma 2.16 it has been proven that for a symmetric, nonnegative and compact operator $\mathcal{C} \in \mathcal{B}(H)$ with eigenpair sequence $(\lambda_m, \varphi_m)_{m \geqslant 1}$ it holds

$$\lambda_{m+1} \leqslant \|\mathcal{C} - \mathcal{C}_m\|_{\mathcal{B}(H)} \tag{C.1}$$

where $\mathcal{C}_m \in \mathcal{B}(H)$ denotes an operator of rank at most m. We define

$$C = \sigma^2 e^{\frac{|\mathbf{x}-\mathbf{y}|^2}{\gamma^2 \mathrm{diam}(D)^2}} = \sigma^2 \sum_{k=0}^{\infty} \frac{1}{k!} \frac{1}{(-\gamma \mathrm{diam}(D))^{2k}} |\mathbf{x}-\mathbf{y}|^{2k} \tag{C.2}$$

and

$$C_{\bar{m}} = \sigma^2 e^{\frac{|\mathbf{x}-\mathbf{y}|^2}{\gamma^2 \mathrm{diam}(D)^2}} = \sigma^2 \sum_{k=0}^{\bar{m}} \frac{1}{k!} \frac{1}{(-\gamma \mathrm{diam}(D))^{2k}} |\mathbf{x}-\mathbf{y}|^{2k} \tag{C.3}$$

Denote by $\mathcal{C}$ and $\mathcal{C}_{\bar{m}}$ the Carleman operator which is, by means of (2.2), associated to C and $C_{\bar{m}}$, respectively. It follows that

$$\begin{aligned}
\|\mathcal{C} - \mathcal{C}_{\bar{m}}\|_{\mathcal{B}(H)} &\lesssim \|\mathcal{C} - \mathcal{C}_{\bar{m}}\|_{L^\infty(D \times D)} \\
&\lesssim \sigma^2 \sum_{k=\bar{m}+1}^{\infty} \frac{1}{k!} \frac{1}{(\gamma \mathrm{diam}(D))^{2k}} \mathrm{diam}(D)^{2k} \\
&\lesssim \frac{1}{(\bar{m}+1)!} \frac{1}{\gamma^{2(\bar{m}+1)}} e^{1/\gamma^2} \\
&\lesssim \frac{1}{(\bar{m}+1)!} \frac{1}{\gamma^{2(\bar{m}+1)}}
\end{aligned}$$

The rank of the Carleman operator defined by (C.3) can be estimated as

$$\operatorname{rank}(\mathcal{C}_{\bar{m}}) \leq \dim \operatorname{span}\{x_1^{\alpha_1} \cdots x_d^{\alpha_d} : \alpha_1 + \cdots + \alpha_d \leqslant 2\bar{m}\} = \binom{2\bar{m}+d}{d} \tag{C.4}$$

Hence, for a given $m \in \mathbb{N}$ we choose $\bar{m}$ such that

$$\binom{2\bar{m}+d}{d} \leqslant m \leqslant \binom{2(\bar{m}+1)+d}{d}, \tag{C.5}$$

from which it follows that $\bar{m} \sim \frac{1}{2} m^{1/d}$ as $m \to \infty$. This completes the proof.

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