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Karhunen–Loève approximation of random fields by generalized fast multipole methods ☆

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Dedicated to W.L. Wendland to his 70th anniversary.

Abstract

KL approximation of a possibly instationary random field $a(\omega,x)\in L^2(\Omega,\mathrm{d}P;L^\infty(D))$ subject to prescribed meanfield $E_a(x)=\int_\Omega a(\omega,x)\,\mathrm{d}P(\omega)$ and covariance $V_a(x,x')=\int_\Omega(a(\omega,x)-E_a(x))(a(\omega,x')-E_a(x'))\,\mathrm{d}P(\omega)$ in a polyhedral domain $D\subset\mathbb{R}^d$ is analyzed. We show how for stationary covariances $V_a(x,x')=g_a(|x-x'|)$ with $g_a(z)$ analytic outside of $z=0$, an M-term approximate KL-expansion $a_M(\omega,x)$ of $a(\omega,x)$ can be computed in log-linear complexity. The approach applies in arbitrary domains D and for nonseparable covariances C_a. It involves Galerkin approximation of the KL eigenvalue problem by discontinuous finite elements of degree $p\geqslant 0$ on a quasiuniform, possibly unstructured mesh of width h in D, plus a generalized fast multipole accelerated Krylov-Eigensolver. The approximate KL-expansion $a_M(x,\omega)$ of $a(x,\omega)$ has accuracy $\mathrm{O}(\exp(-bM^{1/d}))$ if g_a is analytic at $z=0$ and accuracy $\mathrm{O}(M^{-k/d})$ if g_a is C^k at zero. It is obtained in $\mathrm{O}(MN(\log N)^b)$ operations where $N=\mathrm{O}(h^{-d})$.

1. Introduction

Accurate numerical prediction of properties for mass produced specimens requires accounting for uncertainties in their components. Testing procedures (destructive or nondestructive) that are limited to sample specimens allow only to collect statistical data of mass-manufactured components. They can, in general, not ascertain material properties for any particular specimen.

This mandates statistical modelling of, for example, spatially inhomogeneous material and solution characteristics in finite element simulations.

To this end, we employ a probability space (Ω,Σ,P) and assume that the material property of interest is a spatially inhomogeneous random field, i.e., a P-measurable map $a(\cdot,\omega)\colon\Omega\to L^\infty(D)$. To be able to speak about mean and variances of $a(x,\omega)$ we *assume*

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$$a \in L^2(\Omega, \mathrm{d}P; L^\infty(D)). \tag{1.1}$$

Random fields (1.1) arise in two broad classes of applications:

1. Measurements $\mathcal{M}_N = \{a_j(x) : j = 1, \ldots, N\}$ of a can be considered as realization of N independent random variables $\{a_j(\cdot, \omega)\}_{j=1}^N$ distributed identically to the underlying random field $a(x, \omega)$. For example, in digitized light microscopy or computer tomography, samples $a(\cdot, \omega_j)$ correspond to (pixel or voxel) datasets that are too large as input data for continuum mechanical simulations. Besides accounting for measurement uncertainty, statistical modelling of $a(x, \omega)$ serves the purpose of data reduction, i.e., description of the random field's statistics in terms of a finite, preferably small, number of parameters.
2. In subsurface flow and reservoir simulation, there is only one "specimen" with given, deterministic $a(x)$. Information about $a(x)$ can only be gathered in a few points, so that here $\mathcal{M}_N = \{a(x_j) : j = 1, \ldots, N\}$, and the uncertainty in spatial variation of $a(x)$ in between x_j is modelled by statistical procedures (see, e.g. [2,3,13,16,25] for more on this). The uncertainty in $a(x)$ is once more described by a random field (1.1).

Given a random diffusion coefficient $a(x, \omega)$, prediction of, say, concentration $u(x, \omega)$ requires solution of a stochastic partial differential equation such as

$$f(x) + \mathrm{div}(a(x, \omega)\nabla u(x, \omega)) = 0 \quad \text{in } D. \tag{1.2}$$

The simplest approach to solution of (1.2) is Monte-Carlo (MC) simulation. Here, samples $a(x, \omega_j)$ of $a(x, \omega)$ with prescribed statistical properties are generated and, for each sample, a deterministic problem (1.2) is solved for $u(x, \omega_j)$. From a sufficiently large set of solution samples, moments of the random solution $u(x, \omega)$ can be estimated.

An alternative to MC simulation is the *Stochastic Galerkin Method*. Proposed originally by Ghanem and Spanos [10], one selects a basis in (and thereby introduces coordinates into) $L^2(\Omega, \mathrm{d}P)$. Then $a(x, \omega)$ is approximated by separating deterministic and stochastic variables, i.e., by

$$a_M(x, \omega) = \sum_{m=1}^{M} \phi_m(x) Y_m(\omega), \tag{1.3}$$

where Y_m: $\Omega \to \Omega_m$ are suitably chosen random variables with ranges $\Omega_m \subseteq \mathbb{R}$ and probability measures $\pi_m(\mathrm{d}y_m) = \pi_m(y_m)\,\mathrm{d}y_m$.

The random solution $u(x, \omega) \in L^2(\Omega, \mathrm{d}P; V)$ (with V denoting a suitable Hilbert space of finite energy solutions) of (1.2) is projected onto some suitable finite dimensional space $(\Pi_{m=1}^M \Omega_m, \Sigma_M, P_M)$ where Σ_M is the σ-algebra of Borel subsets of $\Pi_{m=1}^M \Omega_m$ and $P_M = \pi_1(\mathrm{d}y_1) \otimes \cdots \otimes \pi_M(\mathrm{d}y_M)$.

The computational efficiency of the stochastic Galerkin approach strongly depends on judicious selection of the "coordinates" Y_m in $L^2(\Omega, \mathrm{d}P)$ [8,15]. Wiener introduced and many investigators afterwards (e.g. [7,10,26] and the references there) used so-called random field "chaos" expansions (of $u(x, \omega)$) in Hermite polynomials of Gaussian random variables Y_m which are orthogonal with respect to the Gaussian probability density. They are dense in $L^2(\Omega, \mathrm{d}P)$ but not problem-adapted. Analogous polynomial systems which are orthogonal with respect to more general probability measures were proposed recently [22,27].

Due to the high cost of the stochastic Galerkin FEM for large M [5,8,23], considerable computational work could (and should) be spent on finding 'optimal' (with respect to an error measure for $a - a_M$) separated approximations (1.3) of a.

In this paper, we address this issue under assumption (1.1), if $a - a_M$ is measured in $L^2(\Omega, \mathrm{d}P; L^2(D))$. In this case, an approximation (1.3) with certain optimality properties is obtained by truncating the Karhunen–Loéve (KL) expansion of $a(x, \omega)$. To define the KL-expansion, we *assume* that the known information on $a(x, \omega)$ includes mean field and two-point correlation, i.e., that

$$E_a(x) := \int_\Omega a(x, \omega)\,\mathrm{d}P(\omega) \quad \text{and} \quad C_a(x, x') := \int_\Omega a(x, \omega) a(x', \omega)\,\mathrm{d}P(\omega) \tag{1.4}$$

are known. An equivalent assumption is that the mean field E_a and its covariance V_a are known, since by definition,

$$V_a(x,x') := C_a(x,x') - E_a(x)E_a(x'). \tag{1.5}$$

Due to (1.1), the 2-point correlation of $a(x,\omega)$ is well-defined and belongs to $L^\infty(D\times D)$. Associate with V_a a compact, self-adjoint operator $\mathscr{V}_a : L^2(D) \to L^2(D)$ via

$$(\mathscr{V}_a u)(x) = \int_{x'\in D} V_a(x,x')u(x')\,\mathrm{d}x' \tag{1.6}$$

and denote by $(\lambda_m, \phi_m(x))_{m=1}^\infty$ the sequence of its eigenpairs, with $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_m \searrow 0$ and with $(\phi_m(x))_{m=1}^\infty$ constituting an orthonormal basis of $L^2(D)$. Then the KL expansion of the random field (1.1) takes the form

$$a(x,\omega) = E_a(x) + \sum_{m=1}^{\infty} \sqrt{\lambda_m}\phi_m(x)X_m(\omega), \tag{1.7}$$

where $X_m(\omega)$ are centered at 0, pairwise uncorrelated random variables on probability spaces $(\Omega_m, \Sigma_m, P_m)_{m\in\mathbb{N}}$. They relate to $a(x,\omega)$ via

$$\sqrt{\lambda_m}X_m(\omega) = \int_{x\in D} (a(x,\omega) - E_a(x))\phi_m(x)\,\mathrm{d}x \quad m = 1,2,\ldots \tag{1.8}$$

Note that, in order to allow a proper parametrization of the uncertainty space (independence of the coordinates), the family $(X_m)_{m=1}^\infty$ of random variables in the Karhunen–Loève expansion is often *assumed* to be independent. This might not be the case in general for an arbitrary random field a, so that the independence assumption could in fact introduce an additional data representation error.

We *compute* a KL-*approximation of* $a(x,\omega)$ based on $\mathscr{M}_N$ by *truncation* of (1.7) after M terms and by *Galerkin approximation* of the first M KL-eigenpairs, *for given covariance kernel* V_a: if $(\lambda_m^h, \phi_m^h(x))_{m=1}^M$ denote approximate eigenpairs of $\mathscr{V}_a$ in (1.6) based on a one-parameter family of subspaces $S_h \subset L^2(D)$, the corresponding approximate KL-expansion $a_M^h(x,\omega)$ of the random field $a(x,\omega)$, based on $\mathscr{M}_N$, is given by

$$a_M^h(x,\omega) = E_a(x) + \sum_{m=1}^{M} \sqrt{\lambda_m^h}\phi_m^h(x)X_m^h(\omega), \tag{1.9}$$

where the laws π_m^h of the random variables $X_m^h : \Omega \to \mathbb{R}$ can be *determined from experiments* $\mathscr{M}_N$ *and from* $(\lambda_m^h, \phi_m^h(x))_{m=1}^M$ by a maximum likelihood estimate

$$\min_{Y_m^h(\omega)} \sum_{a(x)\in\mathscr{M}_N} \left\| a(x,\omega) - \left\{ E_a(x) + \sum_{m=1}^{M} \sqrt{\lambda_m^h}\phi_m^h(x)Y_m^h(\omega) \right\} \right\|^2_{L^2(\Omega\times D)}. \tag{1.10}$$

The laws π_m^h of Y_m^h are *constrained* such that the product measures $P_M(\omega) := \otimes_{m=1}^M \pi_m^h(\omega)$ are probability measures which approach, as $M\to\infty$ and $h\to 0$, the law of $a(x,\omega)$, i.e., measure P. Since the decay of $a - a_M^h$ with a_M^h in (1.9) as $M\to\infty$ is essential for the complexity of the stochastic Galerkin approximation of (1.2), we analyze the decay of λ_m and the regularity of $\phi_m(x)$ in dependence on the smoothness of $V_a(x,x')$. We show that the M-term KL truncation error behaves, asymptotically as $M\to\infty$, as the best approximation error of $a(x,\omega)$ from the usual FE-spaces in D. However, for any finite and, particularly, small values of M, the KL-expansion is the best possible M-term approximation of $a(x,\omega)$ in $L^2(\Omega\times D)$.

The efficient computation of approximate Karhunen–Loève expansions (1.9) of a possibly nonstationary random field $a(x,\omega)$ in a polyhedral domain $D\subset\mathbb{R}^d$ for given mean field $E_a(x)$ and subject to arbitrary, prescribed spatial covariance function $V_a(x,x')$ is the purpose of the present paper. Our approach is based on a Ritz–Galerkin approximation of the KL-eigenvalue problem

$$\mathscr{V}_a\varphi = \lambda\varphi. \tag{1.11}$$

Since the covariance operator $\mathscr{V}_a$ in (1.6) is nonlocal, the matrix of its Galerkin discretization is fully populated.

We approximate the leading M eigenpairs of $\mathscr{V}_a$ by a Krylov subspace iteration [9] requiring only matrix–vector multiplies. The fully populated moment matrix of the discretized covariance V_a need never be formed explicitly, since an approximate matrix vector multiplication can be realized in linear complexity by a generalized fast multipole method (gFMM) in D.

This algorithm extends the Greengard–Rokhlin method (e.g. [12] and the references there) which was developed and highly optimized for the Coulomb potential to most covariances $V_a(x,x')$ used in statistical modelling of spatially inhomogeneous random fields (e.g. [2,3,20]), trading generality for efficiency in replacing spherical harmonic expansions with tensorized polynomial interpolants, but retaining fast shift operations.

To ensure well-posedness of (1.2), we assume in addition to (1.1) that $a \in L^\infty(D\times\Omega)$ is strictly positive, with lower and upper bounds a_- and a_+, respectively,

$$0 < a_- \leqslant a(x,\omega) \leqslant a_+ < \infty, \quad \lambda\times P\text{-a.e.} \qquad (x,\omega)\in D\times\Omega. \tag{1.12}$$

Note that the existence of C_a and V_a is ensured by (1.1) and by (1.12).

The outline of the paper is as follows: in Section 2, we present formal definitions and properties of the KL-expansion of random fields. We then give estimates on the rate of decay of the KL eigenvalues λ_m. These estimates are crucial in determining the approximation rate of truncated, M-term KL-expansions. In Section 3, we discuss the Galerkin approximation of truncated M-term KL-expansions, for given kernel $V_a(x,x')$. Section 4 addresses the generalized fast multipole method, gives algorithmic details such as kernel interpolation and the realization of the shift operations, and establishes exponential convergence with respect to the expansion order of the multipole error.

2. Karhunen–Loève expansion

We introduce the definitions and basic properties of KL expansions of random fields $a(x,\omega)$ which are of second order, i.e., which satisfy (1.1). The basic reference is [17], Chapter XI. We analyze the rate of decay of the KL eigenvalues and regularity of the KL eigenfunctions.

2.1. Correlation, KL expansion

Let $(H_1,\langle,\rangle_{H_1}),(H_2,\langle,\rangle_{H_2})$ and $(S,\langle,\rangle_S)$ be separable Hilbert spaces. If $(s_m)_{m\in\Lambda}$ is an orthonormal basis (ONB) in S (Λ is either finite or $\mathbb{N}_+$), any element $f\in H_1\otimes S$ can be uniquely represented as a convergent series

$$f=\sum_{m\in\Lambda} f_m\otimes s_m. \tag{2.1}$$

It is then easy to prove

Proposition 2.1. *The mapping*

$$H_1\otimes S\times H_2\otimes S\ni(f,g)\to C_{fg}:=\sum_{m\in\Lambda} f_m\otimes g_m\in H_1\otimes H_2 \tag{2.2}$$

is well-defined, bilinear and bounded with norm 1, *and it does not depend on the choice of the basis* $(s_m)_{m\in\Lambda}$ *in* S.

Based on Proposition 2.1 we give the following:

Definition 2.2. For $f\in H_1\otimes S$ and $g\in H_2\otimes S$, we call $C_{fg}\in H_1\otimes H_2$ defined in Proposition 2.1 the correlation of the pair (f,g).

If $H_1=H_2=H$ and the corresponding scalar products also coincide, we show next that the set $\{C_f:=C_{ff}: f\in H\otimes S\}$ of all correlation kernels is in one-to-one correspondence with a certain class of operators on H.

We denote by $\mathscr{B}_{\mathrm{sym}}(H)$ the space of symmetric bounded linear operators in a Hilbert space $(H,\langle,\rangle_H)$, while for $p>0$, $\mathscr{B}_{\mathrm{sym},p}(H)$ will be the space of symmetric compact linear operators in H whose eigenvalue sequence belongs to ℓ^p. The operators in $\mathscr{B}_{\mathrm{sym},1}(H)$ are termed trace class.

Theorem 2.3. *If* $(H,\langle,\rangle_H)$ *and* $(S,\langle,\rangle_S)$ *are separable Hilbert spaces of the same dimension and* $(s_m)_{m\in\Lambda}$ *is an ONB in* S, *the correlations of elements in* $H\otimes S$ *are in a one-to-one correspondence with the positive definite trace class operators in* H, *via*

$$\sum_{m\in\Lambda} f_m \otimes f_m = C_f \to \mathscr{C}_f : H \ni x \to \sum_{m\in\Lambda} \langle f_m, x\rangle_H \cdot f_m \in H \tag{2.3}$$

for $f = \sum_{m\in\Lambda} f_m \otimes s_m$.

Proof. Obviously, the operator $\mathscr{C}_f$ defined on the r.h.s. of (2.3) is compact as a norm limit of finite rank operators obtained by truncating the series. The positivity of $\mathscr{C}_f$ is also clear, so it remains to check that its trace is finite. Choosing $(e_m)_{m\in\Lambda}$ ONB in H, we have

$$\mathrm{Tr}\,\mathscr{C}_f = \sum_{m\in\Lambda} \langle \mathscr{C}_f e_m, e_m\rangle_H = \sum_{m\in\Lambda}\sum_{n\in\Lambda} \langle f_m, e_n\rangle_H^2 = \sum_{m\in\Lambda} \|f_m\|_H^2 = \|f\|_{H\otimes S}^2 < \infty. \tag{2.4}$$

The mapping (2.3) is therefore well-defined. From the identity

$$\langle \mathscr{C}_f x, y\rangle_H = \langle C_f, x\otimes y\rangle_{H\otimes H} \quad \forall x, y \in H, \tag{2.5}$$

it follows that the definition of $\mathscr{C}_f$ does not depend on the basis $(s_m)_{m\in\Lambda}$ and that the mapping (2.3) is injective.

We check the surjectivity of (2.3). To this end, let $\mathscr{C}$ be a positive definite trace class operator in H. $\mathscr{C}$ is in particular compact and has an eigenpair sequence $(\lambda_m, \phi_m)_{m\in\Lambda}$,

$$\mathscr{C}\phi_m = \lambda_m \phi_m \quad \forall m \in \Lambda. \tag{2.6}$$

The eigenvalues $(\lambda_m)_{m\in\Lambda}$ have finite multiplicity, their sequence is nonincreasing and may accumulate only in 0. Moreover, the trace class condition reads

$$\sum_{m\in\Lambda} \lambda_m < \infty. \tag{2.7}$$

Then the series

$$\sum_{m\in\Lambda} \sqrt{\lambda_m}\cdot \phi_m \otimes s_m \tag{2.8}$$

converges due to (2.7) to an element $f \in H\otimes S$ for which we clearly have

$$C_f = \sum_{m\in\Lambda} \lambda_m \cdot \phi_m \otimes \phi_m. \tag{2.9}$$

From (2.5), (2.6) and (2.9) it follows that $\mathscr{C}_f$ has the same spectral decomposition as $\mathscr{C}$, i.e., $\mathscr{C}_f = \mathscr{C}$. □

As a consequence of Theorem 2.3 it is easily seen that

Corollary 2.4. *Let* $(H,\langle,\rangle_H)$ *be a separable Hilbert space and* $C \in H\otimes H$ *be a correlation kernel. Then in terms of the spectral decomposition* (2.6) *of* $\mathscr{C} \in \mathscr{B}_{\mathrm{sym},1}(H)$ *defined as in* (2.5), C *can be represented as*

$$C = \sum_{m\in\Lambda} \lambda_m \cdot \phi_m \otimes \phi_m. \tag{2.10}$$

We next give a description of all the elements in $H\otimes S$ with a given correlation kernel.

Theorem 2.5. *Consider* $(H,\langle,\rangle_H)$, $(S,\langle,\rangle_S)$ *separable Hilbert spaces and* $C \in H\otimes H$ *a correlation kernel, together with its representation* (2.10). *Then* $f \in H\otimes S$ *satisfies* $C_f = C$ *iff there exists an orthonormal family* $(X_m)_{m\in\Lambda} \subset S$, *such that*

$$f = \sum_{m\in\Lambda} \sqrt{\lambda_m}\phi_m \otimes X_m. \tag{2.11}$$

Proof. The 'if' part follows by the arguments used to conclude the proof of Theorem 2.3, after completing the family $(X_m)_{m\in\Lambda}$ to an ONB.

Conversely, if $C_f = C$, then we expand

$$f = \sum_{m\in\Lambda} \phi_m \otimes Y_m \tag{2.12}$$

with $(Y_m)_{m\in\Lambda} \subset S$, from which it follows via Proposition 2.1

$$C_f = \sum_{m,m'\in\Lambda} \langle Y_m, Y_{m'}\rangle_S \cdot \phi_m \otimes \phi_{m'}. \tag{2.13}$$

Comparing (2.13) and (2.10), it follows that

$$\langle Y_m, Y_{m'}\rangle_S = \lambda_m \delta_{mm'} \tag{2.14}$$

and (2.11) holds with $X_m := Y_m/\sqrt{\lambda_m}$. □

Definition 2.6. The expansion (2.11) of f in terms of the spectral decomposition of $\mathscr{C}_f$ is called the Karhunen–Loève expansion of f.

Partial sums of the KL expansion of $f \in H \otimes S$ are optimal approximations of f in subspaces of $H \otimes S$ which are finite dimensional in the first argument.

Theorem 2.7. *If $f \in H \otimes S$ has the KL expansion (2.11), then for any $M \in \mathbb{N}$ it holds*

$$\inf_{\substack{U\subset H\\ \dim U = M}} \|f - P_{U\otimes S} f\|^2_{H\otimes S} = \sum_{m\geqslant M+1} \lambda_m \tag{2.15}$$

and is attained only for $U = \mathrm{Span}\{\phi_1, \phi_2, \ldots, \phi_M\}$ (and g consequently the Mth truncate of (2.11)).

Proof. It is clear that the equality holds for $U = \mathrm{Span}\{\phi_1, \phi_2, \ldots, \phi_M\}$, since $P_{U\otimes S} f$ is then the Mth truncate of (2.11). It is also clear that (2.15) holds for $M = 0$. It suffices therefore to prove that the infimum in (2.15) cannot be smaller than the r.h.s. of (2.15). We argue by induction on M.

Note first that w.l.o.g. we can assume the family $(X_m)_{m\in\Lambda}$ to be an ONB of S. Consider now $U \subset H$ of dimension M and $g \in U \otimes S$. g can be written as

$$g = \sum_{m\in\Lambda} u_m \otimes X_m \tag{2.16}$$

with $u_m \in V$. Then we have

$$\|f - g\|^2 = \sum_{m\in\Lambda} \lambda_m \|\phi_m - u_m\|^2. \tag{2.17}$$

Define now $N \in \mathbb{N}$ to be the largest integer such that for $W := \mathrm{Span}\{u_1, u_2, \ldots, u_N\}$ it holds $\dim W = M - 1$. Clearly, $N \leqslant M - 1$ and from (2.17) we deduce

$$\begin{aligned}
\|f - g\|^2 &= \sum_{m\leqslant N} \lambda_m \|\phi_m - u_m\|^2 + \sum_{m\geqslant N+1} \lambda_m \|\phi_m - u_m\|^2 \\
&= \sum_{m\in\Lambda} \lambda_m \|\phi_m - P_W u_m\|^2 - \sum_{m\geqslant N+1} \lambda_m (\|\phi_m - P_W u_m\|^2 - \|\phi_m - u_m\|^2) \\
&\geqslant \sum_{m\in\Lambda} \lambda_m \|\phi_m - P_W u_m\|^2 - \sum_{m\geqslant N+1} \lambda_m \|P_{U\ominus W}(\phi_m - P_W u_m)\|^2 \\
&= \sum_{m\in\Lambda} \lambda_m \|\phi_m - P_W u_m\|^2 - \sum_{m\geqslant N+1} \lambda_m \|P_{U\ominus W}\phi_m\|^2 \geqslant \sum_{m\in\Lambda} \lambda_m \|\phi_m - P_W u_m\|^2 - \lambda_M,
\end{aligned} \tag{2.18}$$

since $U \ominus W$ is one-dimensional and $N \geqslant M - 1$. W being $M - 1$ dimensional, (2.17) and (2.18) show that

$$\|f - g\|^2 \geqslant \inf_{\substack{U\subset H\\ \dim U = M-1}} \inf_{h\in U\otimes S} \|f - h\|^2 - \lambda_M. \tag{2.19}$$

Taking the infimum over g and U in (2.19), the conclusion follows by induction on M. □

As an example, let us specialize now Theorem 2.5 by choosing as in Section 1 $H := L^2(D)$ and $S := L^2(\Omega, \mathrm{d}P)$ and obtain (see also [17]).

Proposition 2.8. *If $a \in L^2(D \times \Omega)$, then there exists a sequence of random variables $(X_m)_{m \geqslant 1} \subset L^2(\Omega, \mathrm{d}P)$ satisfying*

$$\int_\Omega X_m(\omega)\,\mathrm{d}P(\omega) = 0, \quad \int_\Omega X_n(\omega)X_m(\omega)\,\mathrm{d}P(\omega) = \delta_{nm} \quad \forall n, m \geqslant 1 \tag{2.20}$$

and such that the random field a can be expanded in $L^2(D \times \Omega)$ as

$$a(x,\omega) = E_a(x) + \sum_{m=1}^{\infty} \sqrt{\lambda_m}\phi_m(x)X_m(\omega), \tag{2.21}$$

where $(\lambda_m, \phi_m)_{m \geqslant 1}$ is the eigenpair sequence of the Carleman operator

$$\mathscr{V}_a : L^2(D) \to L^2(D), \quad (\mathscr{V}_a\phi)(x) := \int_D V_a(x,x')\phi(x')\,\mathrm{d}x' \qquad \forall \phi \in L^2(D) \tag{2.22}$$

and $V_a := C_{a-E_a}$. Moreover, for $\lambda_m \neq 0$,

$$X_m(\omega) := \frac{1}{\sqrt{\lambda_m}} \int_D (a(x,\omega) - E_a(x))\phi_m(x)\,\mathrm{d}x \quad \forall m \geqslant 1. \tag{2.23}$$

Definition 2.9. The r.h.s. of (2.21) is called the Karhunen–Loève expansion (KL expansion for short) of the random field $a \in L^2(D \times \Omega)$.

Let us briefly discuss the optimality result Theorem 2.7 in this context. The (mean square) approximability of $a(x,\omega)$ by its KL truncates via Theorem 2.7 relies on the knowledge of the exact eigenfunctions (which are not available in practice), and on modeling the random variables given by (2.23) (achievable by testing the measurements $\mathscr{M}_N$ against the eigenfunctions, assumed to be known). Thus in general the optimal approximations of the random field $a(x,\omega)$ cannot be found, unless the covariance kernel and the domain D have simple structure (as, e.g. when V_a is separable and D of tensor product type; cf. e.g. [10]). However, nearly optimal approximations can be constructed using computed (necessarily inexact) eigenfunctions of $\mathscr{V}_a$, that is, exact eigenfunctions of $P_U\mathscr{V}_aP_U$, where $U \subset L^2(D)$ is a finite element space and P_U is a suitable (quasi-)interpolation operator. We formulate the corresponding result in the abstract setting of Theorem 2.7.

Theorem 2.10. *If $f \in H \otimes S$ and U is a closed subspace of H, we denote by $(\lambda_m, \phi_m)_{m \geqslant 1}$ and $(\lambda_{U,m}, \phi_{U,m})_{m \geqslant 1}$ the eigenpair sequences of $\mathscr{C}_f$ and $P_U\mathscr{C}_fP_U$, respectively. For any $M \in \mathbb{N}_+$ we define $W_M := \mathrm{span}\{\phi_{U,m} | 1 \leqslant m \leqslant M\}$. Then*

$$\dim W_M = M, \quad \|f - P_{W_M \otimes S} f\|^2_{H\otimes S} = \sum_{m=1}^{M}(\lambda_m - \lambda_{U,m}) + \sum_{m=M+1}^{\infty} \lambda_m. \tag{2.24}$$

Proof. Denote further by $(\lambda_{W_M^\top,m})_{m \geqslant 1}$ the eigenvalue sequence of $P_{W_M^\top}\mathscr{C}_fP_{W_M^\top}$, where $W_M^\top$ is the orthogonal complement of W_M in H. We have successively

$$\|f - P_{W_M\otimes S} f\|^2_{H\otimes S} = \|P_{W_M^\top \otimes S} f\|^2_{H\otimes S} = \sum_{m=1}^{\infty} \lambda_{W_M^\top,m} = \mathrm{Tr}\, P_{W_M^\top}\mathscr{C}_fP_{W_M^\top} = \mathrm{Tr}\,\mathscr{C}_f - \mathrm{Tr}\, P_{W_M}\mathscr{C}_fP_{W_M}$$

$$= \sum_{m=1}^{\infty} \lambda_m - \sum_{m=1}^{M} \lambda_{U,m}. \quad \square$$

Definition 2.11. If $f \in H \otimes S$, U is a closed subspace of H and $M \in \mathbb{N} \cup \{\infty\}$, we denote by $(\lambda_{U,m}, \phi_{U,m})_{m \geqslant 1}$ the eigenpair sequence of $P_U\mathscr{C}_fP_U \in \mathscr{B}_{\mathrm{sym},\infty}(U)$ and by W_M the space spanned by $(\phi_{U,m})_{1 \leqslant m \leqslant M}$. Then there exists an orthonormal family $(X_{U,m})_{1 \leqslant m \leqslant M} \subset S$ such that

$$P_{W_M\otimes S} f = \sum_{m\geqslant 1} \sqrt{\lambda_{U,m}}\phi_{U,m}\otimes X_{U,m} \tag{2.25}$$

and we call the expansion (2.25) the (U,M)-quasi Karhunen–Loève (KL) expansion of f.

Note that the (H,∞)-quasi KL expansion coincides with the KL expansion of f constructed in Theorem 2.5.

Remark 2.12. In our applications below, the subspace U will be a finite element (FE) subspace of dimension $N = \dim(U) < \infty$ much larger than M. The projection (2.25) can be understood as projection of f onto the principal components of U.

If no eigensolver is available, the random field $a(x,\omega)$ still can be approximated by an expansion separating the deterministic and stochastic parts and obtained by testing $a(x,\omega)$ against a basis of an arbitrary space $U \subset L^2(D)$. The accuracy of this approximation is just as high as that of the $U\otimes U$ Galerkin approximation of V_a. We further note that, although weaker than the approximation method presented in Theorem 2.7, (2.25) can become (e.g., in the case of an analytic covariance V_a) asymptotically, i.e., as $M\to\infty$, optimal.

Proposition 2.13. *Consider H,S separable Hilbert spaces and $(U_m)_{m\geqslant 1}$ a nested, dense sequence of closed subspaces of H. If $f\in H\otimes S$, define for any $m\geqslant 1$*

$$\varepsilon_m := \|C_f - P_{U_m\otimes U_m} C_f\|_{H\otimes H}. \tag{2.26}$$

Then for any $M\geqslant 1$ it holds

$$\|f - P_{U_M\otimes S} f\|^2_{H\otimes S} \leqslant \sum_{m=M}^{\infty} (\dim U_{m+1} - \dim U_m)^{1/2}\varepsilon_m. \tag{2.27}$$

Proof. For $m\geqslant 1$ let us denote by N_m the dimension of U_m and choose $(\phi_m)_{m\geqslant 1}$ ONB in H such that $U_m = \operatorname{span}\{\phi_1,\phi_2,\ldots,\phi_{N_m}\}$ for any $m\geqslant 1$. Then there exists a family $(X_m)_{m\geqslant 1}\subset S$ such that

$$f = \sum_{m\geqslant 1}\phi_m\otimes X_m, \quad C_f = \sum_{m,m'\geqslant 1}\langle X_m, X_{m'}\rangle_S \phi_m\otimes\phi_{m'}. \tag{2.28}$$

Clearly then,

$$\|f - P_{U_M\otimes S} f\|^2_{H\otimes S} = \left\|\sum_{m>N_M}\phi_m\otimes X_m\right\|^2_{H\otimes S} = \sum_{m>N_M}\|X_m\|^2_S. \tag{2.29}$$

But, using (2.28),

$$\sum_{m>N_M}\|X_m\|^4_S \leqslant \sum_{\max\{m,m'\}>N_M} |\langle X_m, X_{m'}\rangle_S|^2 = \|C_f - P_{U_M\otimes U_M} C_f\|^2_{H\otimes H} = \varepsilon_M^2,$$

from which we deduce via the Cauchy–Schwarz inequality and for any $M\geqslant 1$

$$\sum_{N_M<m\leqslant N_{M+1}}\|X_m\|^2_S \leqslant (N_{M+1}-N_M)^{1/2}\left(\sum_{N_M<m\leqslant N_{M+1}}\|X_m\|^4_S\right)^{1/2} \leqslant (N_{M+1}-N_M)^{1/2}\varepsilon_M. \tag{2.30}$$

The conclusion follows inserting (2.30) in (2.29). □

Since we are interested in the KL expansion of stochastic coefficients $a(x,\omega)$ of partial differential equations such as the diffusion equation (1.2), a sufficient condition for P-a.s., pointwise a.e. in D convergence of (2.21) is of interest.

Proposition 2.14. *The KL series (2.21) converges P-a.s. in $L^\infty(D)$ if*

$$\sum_{m=1}^{\infty}\lambda_m(\log m)^2\|\phi_m\|^2_{L^\infty(D)}\operatorname{Var}(X_m) < \infty. \tag{2.31}$$

Follows from [17] Theorem 36.B (i), applied to $\sqrt{\lambda_m}\|\phi_m\|_{L^\infty(D)}X_m(\omega)$ if we note the X_m in (2.21) satisfy (2.20), i.e., have mean zero and are pairwise uncorrelated.

2.2. KL eigenvalue decay

From Proposition 2.14, the pointwise convergence of the KL expansion (2.21) is related to eigenvalue decay and to pointwise eigenfunction bounds. We now prove such decay rates for the KL eigenvalues in terms of regularity of the covariance kernel V_a (pointwise eigenfunction bounds will be considered in the following section).

Definition 2.15. A correlation function $V_a : D \times D \to \mathbb{R}$ is said to be piecewise analytic/smooth/$H^{p,q}$ on $D \times D$ ($p, q \in [0, \infty[$) if there exists a partition $\mathscr{D} = \{D_j\}_{j=1}^J$ of D into a finite sequence of simplices D_j and a finite family $\mathscr{G} = \{G_j\}_{j=1}^J$ of open sets in $\mathbb{R}^d$ such that

$$\overline{D} = \bigcup_{j=1}^{J} \overline{D_j}, \quad \overline{D_j} \subset G_j \qquad \forall 1 \leqslant j \leqslant J, \tag{2.32}$$

and such that $V_a|_{D_j \times D_{j'}}$ has an extension to $G_j \times G_{j'}$ which is analytic in $G_j \times G_{j'}$ /is smooth in $G_j \times G_{j'}$/ is in $H^{p,q}(G_j \times G_{j'}) := H^p(G_j) \otimes H^q(G_{j'})$, for any pair (j,j'). We denote by $\mathscr{A}_{\mathscr{D},\mathscr{G}}(D^2)/\mathscr{C}^\infty_{\mathscr{D},\mathscr{G}}(D^2)/H^{p,q}_{\mathscr{D},\mathscr{G}}(D^2)$ the corresponding regularity spaces. Similarly we introduce spaces of piecewise regular functions defined on D, which we denote by $\mathscr{A}_{\mathscr{D},\mathscr{G}}(D)/\mathscr{C}^\infty_{\mathscr{D},\mathscr{G}}(D)/H^p_{\mathscr{D},\mathscr{G}}(D)$.

To prove decay estimates for the eigenvalues of a piecewise analytic kernel (in the sense of Definition 2.15) we need the following auxiliary result.

Lemma 2.16. *Let $(H,\langle\cdot,\cdot\rangle)$ be a Hilbert space and $\mathscr{C} \in \mathscr{B}(H)$ be symmetric, nonnegative and compact operator whose eigenpair sequence is denoted by $(\lambda_m,\phi_m)_{m\geqslant 1}$.*

If $m \in \mathbb{N}$ and $\mathscr{C}_m \in \mathscr{B}(H)$ is an operator of rank at most m, then

$$\lambda_{m+1} \leqslant \|\mathscr{C} - \mathscr{C}_m\|_{\mathscr{B}(H)}. \tag{2.33}$$

Proof. Straightforward application of the minimax principle,

$$\lambda_{m+1} = \min_{\substack{V \subset H \\ \dim V^\perp \leqslant m}} \max_{\substack{\phi \in V \\ \|\phi\|_H = 1}} \langle \mathscr{C}\phi, \phi\rangle \leqslant \max_{\substack{\phi \in (\mathrm{Ran}\mathscr{C}_m)^\perp \\ \|\phi\|_H = 1}} \langle \mathscr{C}\phi, \phi\rangle = \max_{\substack{\phi \in (\mathrm{Ran}\mathscr{C}_m)^\perp \\ \|\phi\|_H = 1}} \langle (\mathscr{C} - \mathscr{C}_m)\phi, \phi\rangle \leqslant \|\mathscr{C} - \mathscr{C}_m\|_{\mathscr{B}(H)}. \quad \square$$

We require approximation properties of the FE-spaces $S^p_h(D)$. By $H^k(\mathscr{D})$ we denote the functions which belong to $H^k(D_j)$ for every $D_j \in \mathscr{D}$. Then we have

Proposition 2.17. *Let $S^p_h(D)$ denote the space of discontinuous, piecewise polynomial functions of total degree $p \geqslant 0$ on a quasiuniform triangulation $\mathscr{M}_h$ of mesh width h subordinate to the partition $\mathscr{D}$ of D and denote by $N = \dim S^p_h(D)$ its dimension. Denote by $P_h : L^2(D) \to S^p_h$ the $L^2(D)$ projection. Then for every $\varphi \in H^k(\mathscr{D})$ it holds, as $h/(p+1) \to 0$,*

$$\|\varphi - P_h\varphi\|_{L^2(D)} \leqslant C(k)(h/(p+1))^{\min\{p+1,k\}} \leqslant C(k)N^{-\min\{p+1,k\}/d} \tag{2.34}$$

and, if φ is analytic in each $\overline{D}_j, D_j \in \mathscr{D}$, there are $b,C > 0$ such that, as $p \to \infty$ on a fixed triangulation $\mathscr{M}$ of D subordinate to $\mathscr{D}$,

$$\|\varphi - P_h\varphi\|_{L^2(D)} \leqslant C\exp(-bp) \leqslant C\exp(-bN^{1/d}). \tag{2.35}$$

2.2.1. Piecewise analytic covariance

For piecewise analytic kernels in the sense of Definition 2.15 we have

Proposition 2.18. *Let $V \in L^2(D\times D)$ be a symmetric kernel defining the compact and nonnegative integral operator*

$$\mathscr{V} : L^2(D) \to L^2(D), \quad (\mathscr{V}u)(x) = \int_D V(x,x')u(x')\,\mathrm{d}x'. \tag{2.36}$$

If V is piecewise analytic on $D\times D$ and $(\lambda_m)_{m\geqslant 1}$ is the eigenvalue sequence of its associated operator (2.36), then there exist constants $c_{1,V}, c_{2,V} > 0$ depending only on V such that

$$0 \leqslant \lambda_m \leqslant c_{1,V}\mathrm{e}^{-c_{2,V}m^{1/d}} \quad \forall m \geqslant 1. \tag{2.37}$$

Proof. Under the assumption of piecewise analyticity of the kernel $V(x,x')$ (in the sense of Definition 2.15), the operator $\mathscr{V}$ maps $L^2(D)$ into the set of piecewise analytic functions. Define $\mathscr{V}_m := P_h\mathscr{V}$. Then $N := \operatorname{rank}\mathscr{V}_m = \mathrm{O}(1/(p+1)^d)$, and, by Proposition 2.17, (2.35) we get $\|\mathscr{V}-\mathscr{V}_m\|_{\mathscr{B}(H)} \leqslant C\exp(-bp) \leqslant C\exp(-bN^{1/d})$. Lemma 2.16 then implies (2.37). □

One is often interested in Gaussian covariance kernels of the form

$$V_a(x,x') := \sigma^2\exp(-|x-x'|^2/(\gamma^2\Lambda^2)) \quad \forall (x,x') \in D\times D, \tag{2.38}$$

where σ, $\gamma > 0$ are real parameters and Λ is the diameter of the domain D. Note that σ and γ are in this case referred to as the standard deviation and the correlation length of a, respectively. Since this kernel admits an analytic continuation to the whole complex space $\mathbb{C}^d$, the eigenvalues decay is in this case even faster than in (2.37).

Proposition 2.19. *If $a \in L^2(D\times\Omega)$ and V_a is given by (2.38), then for the eigenvalue sequence $(\lambda_m)_{m\geqslant 1}$ of $\mathscr{V}_a$ it holds*

$$0 \leqslant \lambda_m \lesssim \sigma^2\frac{(1/\gamma)^{m^{1/d}+2}}{\Gamma(0.5m^{1/d})} \quad \forall m \geqslant 1, \tag{2.39}$$

where Γ is the gamma function interpolating the factorial.

Proof. A repetition of the argument in the proof of Proposition 2.18 using as approximations for $\mathscr{V}_a$ the integral operators given by the Taylor truncates of V_a. □

Remark 2.20. Note that the decay estimates (2.37) and (2.39) are subexponential in dimension $d > 1$. The exponent $1/d$ accounts for higher multiplicity of the eigenvalues in the presence of symmetries in V_a and D and cannot be removed, in general.

2.2.2. Finitely differentiable covariance

So far, we assumed that the kernel function $V(x,x')$ is piecewise analytic which implied exponential decay of the KL-eigenvalues. If the requirement of analyticity of $V(x,x')$ is weakened to finite Sobolev regularity, only algebraic decay holds true.

Proposition 2.21. *Let $D \subset \mathbb{R}^d$ be a bounded domain and $V \in L^2(D\times D)$ be the symmetric kernel of the compact, nonnegative integral operator*

$$\mathscr{V} : L^2(D) \to L^2(D), \quad (\mathscr{V}u)(x) = \int_D V(x,x')u(x')\,\mathrm{d}x'. \tag{2.40}$$

If V is piecewise $H^{k,0} := H^k \otimes L^2$ on $D\times D$ with $k > 0$ and $(\lambda_m)_{m\geqslant 1}$ denotes the eigenvalue sequence of $\mathscr{V}$, there exists a constant $c_{3,V} > 0$ such that

$$\lambda_m \leqslant c_{3,V}m^{-k/d} \quad \forall m \geqslant 1. \tag{2.41}$$

Proof. Analogous to Proposition 2.18, using (2.34) in place of (2.35). □

Corollary 2.22. *Let $D \subset \mathbb{R}^d$ be a bounded domain and $V \in L^2(D \times D)$ be a symmetric kernel defining a compact, nonnegative integral operator via (2.40). If V is piecewise smooth on $D \times D$ and $(\lambda_m)_{m \geqslant 1}$ denotes the eigenvalue sequence of its associated operator $\mathscr{V}$, then for any $s > 0$ there exists a constant $c_{V,s} > 0$ such that*

$$0 \leqslant \lambda_m \leqslant c_{V,s} m^{-s} \quad \forall m \geqslant 1. \tag{2.42}$$

2.3. KL eigenfunction regularity

The regularity of the covariance kernel implies corresponding regularity of the KL eigenfunctions. The following result follows immediately from the KL-eigenvalue problem (1.11).

Proposition 2.23. *Assume that the covariance kernel $V_a(x, x')$ is piecewise analytic/ is $H^{p,q}$ on $D \times D$, in the sense of Definition 2.15. Then the KL eigenfunctions φ_m are analytic/ H^p in every $\overline{D_j} \in \mathscr{D}$.*

Pointwise control of KL eigenfunctions is important to establish pointwise convergence of the KL expansion, i.e., convergence in $L^2(\Omega, \mathrm{d}P; L^\infty(D))$. This in turn is important to ensure the ellipticity and stable solvability of problems like (1.2) when $a(x, \omega)$ is replaced by a finite KL-approximation.

Theorem 2.24. *For $D \subset \mathbb{R}^d$ a bounded domain and V piecewise smooth on $D \times D$, such that the domains D_j in Definition 2.15 all have the uniform cone property, we denote by $(\lambda_m, \phi_m)_{m \geqslant 1}$ the eigenpair sequence of the associated integral operator $\mathscr{V}$ via (2.36), such that $\|\phi_m\|_{L^2(D)} = 1 \ \forall\ m \geqslant 1$. Then for any $s > 0$ and any multiindex $\alpha \in \mathbb{N}^d$ there exists $c_{V,s,\alpha} > 0$ such that*

$$\|\partial^\alpha \phi_m\|_{L^\infty(D_j)} \leqslant c_{V,s,\alpha} |\lambda_m|^{-s} \qquad \forall m \geqslant 1, \quad \forall 1 \leqslant j \leqslant J. \tag{2.43}$$

Remark 2.25. Under the regularity assumptions of Theorem 2.24 the estimate (2.43) is optimal in the sense that for any α it fails to hold with $s = 0$. This can be seen for instance on $D :=]0,1[$ by taking

$$V := \sum_{m \geqslant 1} \lambda_m \cdot \phi_m \otimes \phi_m,$$

where $\lambda_m := e^{-m}$ and $\phi_m(x) := m \cdot \phi(m^2 x - m) \quad \forall x \in]0,1[, \quad \forall m \geqslant 1,$ with $\phi \in C_0^\infty(]0,1[)$ satisfying $\|\phi\|_{L^2(]0,1[)} = 1$.

Remark 2.26. Further assumptions (like stationarity of $a(x, \omega)$) lead to the uniform L^∞ boundedness of the eigenfunctions, but not of their derivatives.

For the proofs of the results presented in this section we refer the reader to Appendix A and to [24].

3. Approximate KL expansion

In order to use the (truncated) KL expansion (2.21) in practice, we must be able to compute efficiently and accurately approximations to the first M KL-eigenpairs in arbitrary domains D. In one dimension, for particular kernels, explicit eigenfunctions are known (see, e.g. [10]). These can be used to obtain explicit eigenpairs also for multidimensional tensor product domains D, if the covariance $V_a(x, x')$ is separable. This is often the case in subsurface flow problems, where D is a box and the covariance kernel V_a is Gaussian as in (2.38). To deal with random coefficients in arbitrary geometries, however, an efficient numerical approximation of the eigenpairs of the covariance operator (2.36) is an essential step in the efficient numerical solution of problem (1.2).

3.1. Galerkin discretization of the KL eigenvalue problem

Let $h \in \mathfrak{H}$ be a discretization parameter and let $S_h \subset L^2(D)$ denote the corresponding finite element space. The variational formulation of the eigenvalue problem reads, in discretized form.

Find $(\lambda_{h,m}, \phi_{h,m})_{m\geqslant 1} \subset \mathbb{R} \times S_h$ such that

$$\int_{D\times D} V_a(x,x')\phi_{h,m}(x')\psi(x)\,dx'\,dx = \lambda_{h,m}\int_D \phi_{h,m}(x)\psi(x)\,dx \quad \forall \psi \in S_h. \tag{3.1}$$

Eq. (3.1) shows that the sequence $(\lambda_{h,m}, \phi_{h,m})_{m\geqslant 1}$ is nothing but the eigenvalue sequence of the compact, self-adjoint operator $P_h \mathscr{K} P_h$ in $L^2(D)$. Theorem 2.10 implies then (with $U = S_h$) that an important contribution to the error introduced by a quasi-KL expansion of the random field $a(x,\omega)$ comes from the difference between the traces of the continuous and discretized operator. In order to control the trace discretization error we make the following.

Assumption 3.1. The eigenpair sequence $(\lambda_m, \phi_m)_{m\geqslant 1}$ of the integral operator $\mathscr{V}$ has the property that for any $s > 0$ there exists $c_{V,\mathscr{S},s} > 0$ such that

$$\|\phi_m - P_h\phi_m\|_{L^2(D)} \leqslant c_{V,\mathscr{S},s}\lambda_m^{-s}\Phi(h) \qquad \forall m \geqslant 1, \quad \forall h \in \mathfrak{H} \tag{3.2}$$

where the function $\Phi : \mathbb{R} \to \mathbb{R}$ describes the approximation property of the finite element spaces $\mathscr{S} := (S_h)_{h\in\mathfrak{H}}$.

Assumption 3.1 is satisfied again in the case of a piecewise regular kernel K for the standard h finite element method (piecewise polynomials of degree at most p) with $\Phi(h) = h^{p+1}$ (see, e.g. [24]).

Based on Assumption 3.1 we prove the main result of this section.

Theorem 3.2. *If $V \in L^2(D\times D)$ is piecewise smooth on $D\times D$, defining a nonnegative self-adjoint operator $\mathscr{V}$ via (2.36) such that Assumption 3.1 is satisfied, there exists a constant $c_{V,\mathscr{S}} > 0$ such that*

$$0 \leqslant \operatorname{Tr}\mathscr{V} - \operatorname{Tr}P_h\mathscr{V}P_h \leqslant c_{V,\mathscr{S}}\Phi(h)^2 \quad \forall h \in \mathfrak{H}. \tag{3.3}$$

Proof. Fix $h \in \mathfrak{H}$. From the minimax principle we immediately deduce $\lambda_{h,m} \leqslant \lambda_m\ \forall m \geqslant 1$, so that

$$\operatorname{Tr}P_h\mathscr{V}P_h \leqslant \operatorname{Tr}\mathscr{V}. \tag{3.4}$$

Further, the obvious identity

$$\mathscr{V} - P_h\mathscr{V}P_h = (I-P_h)\mathscr{V} + \mathscr{V}(I-P_h) - (I-P_h)\mathscr{V}(I-P_h)$$

together with the fact that $\mathscr{V}$ is nonnegative ensure that $(H := L^2(D))$

$$\langle(\mathscr{V} - P_h\mathscr{V}P_h)u, u\rangle_H \leqslant 2|\langle\mathscr{V}u, (I-P_h)u\rangle_H| \quad \forall u \in H. \tag{3.5}$$

Using (3.5) and Assumption 3.1 it follows

$$\begin{aligned}\operatorname{Tr}\mathscr{V} - \operatorname{Tr}P_h\mathscr{V}P_h &= \sum_{m\geqslant 1}\langle(\mathscr{V} - P_h\mathscr{V}P_h)\phi_m, \phi_m\rangle_H \leqslant 2\sum_{m\geqslant 1}|\langle\mathscr{V}\phi_m, (I-P_h)\phi_m\rangle_H| \\ &\leqslant 2\sum_{m\geqslant 1}\lambda_m\|(I-P_h)\phi_m\|_H^2 \leqslant c_{V,\mathscr{S},s}\Phi(h)^2\sum_{m\geqslant 1}\lambda_m^{1-2s}.\end{aligned} \tag{3.6}$$

By Corollary 2.22 the series on the r.h.s. of (3.6) converges absolutely, which concludes the proof. □

3.2. Convergence of the discretized KL expansion

From Theorems 2.10 and 3.2 we immediately deduce.

Proposition 3.3. *Consider $a \in L^2(D\times\Omega)$ such that $V_a \in L^2(D\times D)$ is piecewise smooth on $D\times D$, defining a nonnegative self-adjoint operator $\mathscr{V}_a$ via (2.36). If Assumption 3.1 holds, then there exists a constant $c_{V,\mathscr{S}} > 0$ such that for any $h \in \mathfrak{H}$ and $M \geqslant 1$ the (S_h,M)-quasi KL expansion of a, defined by*

$$a_{h,M}(x,\omega) = E_a(x) + \sum_{m=1}^{M}\sqrt{\lambda_{h,m}}\phi_{h,m}(x)X_{h,m}(\omega) \tag{3.7}$$

satisfies

$$\|a - a_{h,M}\|^2_{L^2(D\times\Omega)} \leqslant c_{V,\mathscr{S}}\Phi(h)^2 + \sum_{m=M+1}^{\infty}\lambda_m \quad \forall h \in \mathfrak{H}. \tag{3.8}$$

In applications to partial differential equations with random coefficients, it is necessary to ensure that the approximate, truncated KL expansion satisfies sign conditions pointwise in $x \in D$ an P-a.s. in $\omega \in \Omega$. Using the pointwise eigenfunction bounds Theorem 2.24, it is possible to establish pointwise convergence of the KL expansion.

Assumption 3.4. The family $(X_m)_{m=1}^{\infty}$ of random variables the KL expansion (1.7) is uniformly bounded, i.e.,

$$\exists c_X > 0 \quad \|X_m\|_{L^\infty(\Omega,\mathrm{d}P)} \leqslant c_X \quad \forall m \geqslant 1. \tag{3.9}$$

We then have

Theorem 3.5. *If V_a is piecewise analytic on $D \times D$ and if Assumption 3.4 holds, then the KL expansion (1.7) converges pointwise exponentially. More precisely, there exists $c_2 > 0$ such that for every $s > 0$ there exists $C > 0$ with the property that for all $M \geqslant 1$ it holds*

$$\|a - a_M\|_{L^\infty(D\times\Omega)} \leqslant C \exp(-c_2(1/2 - s)M^{1/d}). \tag{3.10}$$

4. Fast multipole covariance approximation

Computation of an approximate KL-expansion requires numerical solution of the matrix eigenproblem corresponding to (3.1), i.e., of

$$\mathbf{V}\underline{\phi} = \lambda \mathbf{M}\underline{\phi}. \tag{4.1}$$

If $S_h^p(D) = \mathrm{span}\{b_i(x) : i = 1, \ldots, N\}$, we have

$$V_{ii'} = \int_D \int_D b_i(x) V_a(x,x') b_{i'}(x')\,\mathrm{d}x\,\mathrm{d}x', \quad M_{ii'} = \int_D \int_D b_i(x) b_{i'}(x')\,\mathrm{d}x\,\mathrm{d}x'. \tag{4.2}$$

Both matrices $\mathbf{V}$ and $\mathbf{M}$ are symmetric and positive definite, with $\mathbf{M}$ being diagonal if we choose as basis of S_h^p polynomials which are $L^2(D)$-orthogonal and supported on the elements $\pi \in \mathscr{M}_h$. The size N of the KL eigenproblem (4.1) can be as large as 10^6 and dense eigensolvers are not applicable. We compute KL eigenpairs corresponding to the largest eigenvalues of (4.1) by an iterative Krylov subspace eigensolver [9] which requires only matrix–vector multiplies.

If $a(x,\omega)$ is stationary, its covariance is translation invariant, i.e., $V_a(x,x') = V_a(x - x')$. If, moreover, D is an axiparallel cube and the triangulation $\mathscr{M}_h$ is uniform and axiparallel, fast Fourier techniques can be used to realize $\underline{x} \to \mathbf{V}\underline{x}$ in $\mathrm{O}(N)$ operations (e.g. [11]).

For polyhedra in dimension $d = 3$ and unstructured meshes $\mathscr{M}_h$, Fourier techniques can no longer be applied. We show in certain situations that for large N the matrix–vector multiplication $\underline{\phi} \to \mathbf{V}\underline{\phi}$ can be done approximately in $\mathrm{O}(N \log N)$ operations and memory using a generalized fast multipole method (gFMM) applicable to general, piecewise analytic correlation kernels $V_a(x,x')$. It generalizes the Greengard–Rokhlin [6,12,19] method for the Coulomb potential. Using this cluster approximation of the far field yields a perturbed matrix $\widetilde{\mathbf{V}}$ and, consequently, perturbed KL-eigenpairs. We estimate the error due to clustering the far field and show that an expansion order $m = \mathrm{O}(|\log h|)$ is sufficient to preserve the consistency of the Galerkin approximation of the eigenpairs.

4.1. Covariance kernel expansions

Assumption 4.1. Given a separation constant $0 \leqslant \eta < 1$, $V_a : D \times D \to \mathbb{C}$ a kernel function and $\mathscr{I}$ an index set, for all $x_0, y_0 \in D$, $x_0 \neq y_0$, and expansion orders $m \in \mathbb{N}_0$ there exists a degenerate covariance kernel V_a^m

$$V_a(x,y) \approx V_a^m(x,y;x_0,y_0) := \sum_{(\mu,\nu)\in\mathscr{I}_m} \kappa_{(\mu,\nu)}(x_0,y_0) X_\mu(x;x_0) Y_\nu(y;y_0) \tag{4.3}$$

for $\mathscr{I}_m \subset \mathscr{I} \times \mathscr{I}$ such that for all $x,y \in D$ satisfying

$$|y - y_0| + |x - x_0| \leqslant \eta |y_0 - x_0|, \tag{4.4}$$

the error $V_a - V_a^m$ in (4.3) is bounded by

$$|V_a(x,y) - V_a^m(x,y;x_0,y_0)| \leqslant \Phi(m;\eta,V)|y-x|^s \tag{4.5}$$

with the convergence rate $\Phi(m;\eta,V)$ exponentially decreasing with respect to the expansion order m and with $s > 0$ denoting the singularity order at $x = y$.

Note we admit covariance kernels V_a which are singular on the diagonal $x = y$; $s \geqslant 0$ is required due to (1.1) – the following assertions are actually valid for $s > -d$.

The purpose of the expansion (4.3) is to decouple the source points y from the field points x. The simplest example of such a decoupling is Taylor expansion.

If the random field $a(s,\omega)$ is stationary, the covariance V_a is translation invariant:

$$V_a(x,y) = V_a(y-x). \tag{4.6}$$

We expand $V_a(y-x)$ formally into a Taylor series centered at $y_0 - x_0$ with $x_0, y_0 \in \mathbb{R}^d$:

$$V_a(y-x) = \sum_{(\nu,\mu)\in\mathbb{N}_0^d\times\mathbb{N}_0^d} (D^{\mu+\nu}V_a)(y_0-x_0)\frac{(x_0-x)^\mu}{\mu!}\frac{(y-y_0)^\nu}{\nu!}.$$

With this we get an approximation (4.3) where:

$$\begin{aligned} &\mathcal{I} := \mathbb{N}_0^d, \quad \mathcal{I}_m := \{(\mu,\nu)\in\mathcal{I}\times\mathcal{I} : |\mu+\nu| < m\},\\ &\kappa_{(\mu,\nu)}(x_0,y_0) := (D^{\mu+\nu}V_a)(y_0-x_0),\\ &X_\mu(x;x_0) := \frac{(x_0-x)^\mu}{\mu!}, \quad Y_\nu(y;y_0) := \frac{(y-y_0)^\nu}{\nu!}. \end{aligned} \tag{4.7}$$

Applying the binomial formula the expansion (4.3) can be shifted from x_0 to x_1 and from y_0 to y_1 by:

$$\begin{aligned} X_\mu(x;x_1) &= \frac{(x_1-x)^\mu}{\mu!} = \sum_{\substack{\nu\in\mathbb{N}_0^d\\ \nu\leqslant\mu}} \frac{(x_1-x_0)^{\mu-\nu}}{(\mu-\nu)!}X_\nu(x;x_0),\\ Y_\nu(y;y_1) &= \frac{(y-y_1)^\nu}{\nu!} = \sum_{\substack{\mu\in\mathbb{N}_0^d\\ \mu\leqslant\nu}} \frac{(y_0-y_1)^{\nu-\mu}}{(\nu-\mu)!}Y_\mu(y;y_0). \end{aligned} \tag{4.8}$$

The Taylor expansion coefficients have to be calculated by differentiation of the covariance kernel V_a. To avoid this we interpolate $V_a(x,y)$ by Čebyšev polynomials so that only the kernel has to be evaluated at $O(m^d)$ different points and no derivatives come into play. Let $I := [-1,1]$, $m \in \mathbb{N}_0$ and $T_\mu(x) = \cos(\mu\arccos(x))$, $\mu \in \mathbb{Z}$, denote the Čebyšev polynomials of the first kind. For any function f, defined on I, we consider the formal Čebyšev expansion

$$f(x) = \sum_{\mu\in\mathbb{Z}} \widehat{f}(\mu)T_\mu(x), \quad \widehat{f}(\mu) := \frac{1}{\pi}\int_{-1}^{1} \frac{f(\xi)T_\mu(\xi)}{\sqrt{1-\xi^2}}\,\mathrm{d}\xi \tag{4.9}$$

and the Čebyšev interpolant

$$f_m(x) := \sum_{\substack{\mu\in\mathbb{Z}\\ |\mu|<m}} \widehat{f}_\mu T_\mu(x), \quad \widehat{f}_\mu := \frac{1}{m}\sum_{0\leqslant i<m} f(x_i)T_\mu(x_i), \tag{4.10}$$

where we assume f to be known at the m Čebyšev-points $x_i := \cos((i+1/2)\pi/m) \in I$, i.e., the m roots of T_m. Employing tensor products,

$$T_\mu(x) := \prod_{1\leqslant i\leqslant d} T_{\mu_i}(x_i), \quad \mu\in\mathbb{Z}^d,\ x\in I^d, \tag{4.11}$$

we extend expansion and interpolation to the d-dimensional case with x_i denoting the ith component of $x \in I^d$. This yields

$$f(x) = \sum_{\mu\in\mathbb{Z}^d} \widehat{f}(\mu) T_\mu(x), \quad \widehat{f}(\mu) := \pi^{-d} \int_{I^d} \frac{f(\xi) T_\mu(\xi)}{\prod_{1\leqslant i\leqslant d} \sqrt{1-((\xi)_i)^2}}\, \mathrm{d}\xi \tag{4.12}$$

and

$$f_m(x) := \sum_{\substack{\mu\in\mathbb{Z}^d \\ |\mu|<m}} \widehat{f}_\mu T_\mu(x), \quad \widehat{f}_\mu := m^{-d} \sum_{\substack{v\in\mathbb{N}_0^d \\ v_i<m}} f(x_v) T_\mu(\underline{x}_v), \tag{4.13}$$

where $\underline{x}_v := (x_{v_i})_{1\leqslant i\leqslant d} \in I^d$.

Remark 4.2. Note that $T_{\mu_i}(x) = T_{-\mu_i}(x)$, $\sum_{\substack{\mu\in\mathbb{Z}^d \\ |\mu|<m}} \widehat{f}_\mu T_\mu(x) = \sum_{\substack{\mu\in\mathbb{N}_0^d \\ |\mu|<m}} 2^{d-|\delta_{\mu 0}|} \widehat{f}_\mu T_\mu(x)$.

For the fast multipole algorithms, we require the following connection between interpolation and expansion from [21]: Suppose $f : I^d \to \mathbb{R}$ to be a continuous function that admits a Čebyšev expansion. Then interpolation (4.13) and expansion (4.12) are related by

$$\widehat{f}_\mu = \sum_{\zeta\in\mathbb{Z}^d} (-1)^{|\zeta|} \widehat{f}(2m\zeta + \mu) \tag{4.14}$$

for all $\mu \in \mathbb{Z}^d$ with $|\mu| < m$. In particular, the Čebyšev interpolant of T_v, $v \in \mathbb{Z}^d$, is given by $(-1)^{|v-\mu|/(2m)} T_\mu$ where $v \equiv \mu \bmod 2m$. In the following result from [14,21], sufficient conditions on $V_a(x,x')$ are given for the validity of Assumption 4.1 with *exponential convergence with respect to the expansion order m*.

Theorem 4.3. *For sufficiently small separation parameter $0 < \eta < 1$, singularity order $s \geqslant 0$ and a kernel function*

$$V_a : D \times D \to \mathbb{R}; \quad V_a(x,y) := K(y-x)|y-x|^s, \tag{4.15}$$

where K admits an analytic extension into $\mathbb{C}^d \setminus \{0\}$. Suppose χ denotes for any $x_0, y_0 \in D$, $x_0 \neq y_0$, the affine transformation

$$\chi : \mathbb{R}^d \to \mathbb{R}^d; \quad \chi(\xi) := \eta \|y_0 - x_0\|_\infty \xi + y_0 - x_0. \tag{4.16}$$

Then, the approximation of the stationary covariance V_a given by the Čebyšev interpolant of $f(\cdot; x_0, y_0) := (K \circ \chi)|\chi|^s$ on I^d,

$$V_a^m(x,y;x_0,y_0) := \sum_{\substack{\mu\in\mathbb{Z}^d \\ |\mu|<m}} \widehat{f}_\mu(x_0,y_0) T_\mu(\chi^{-1}(y-x)), \tag{4.17}$$

satisfies the error bound (4.5) with $\Phi(m;\eta,V) = C\exp(-b(\eta)m)$. In addition, V_a^m admits the representation (4.3) with

$$\begin{aligned} &\mathscr{I}_m := \{(\mu,v) \in \mathbb{N}_0^d \times \mathbb{N}_0^d : |\mu + v| < m\}, \\ &\kappa_{(\mu,v)}(x_0,y_0) := (\mu+v)! c_{\mu+v}(x_0,y_0), \end{aligned} \tag{4.18}$$

where the c_μ, $\mu \in \mathbb{N}_0^d$, are the coefficients of the interpolation polynomial defined by

$$\sum_{\substack{\mu\in\mathbb{Z}^d \\ |\mu|<m}} \widehat{f}_\mu(x_0,y_0) T_\mu\left(\frac{z}{\eta\|y_0-x_0\|_\infty}\right) = \sum_{\substack{\mu\in\mathbb{N}_0^d \\ |\mu|<m}} c_\mu(x_0,y_0) z^\mu. \tag{4.19}$$

Remark 4.4. If the kernel V_a belongs to C^k, approximation properties of the Chebysev polynomials and the L^∞ stability bounds for the interpolation operator in the Chebysev points imply that V_a^m admits the representation (4.3) with $\mathscr{I}_m$ as in (4.18), but only with the algebraic convergence rate $\Phi(m;\eta,V) = Cm^{-k}$.

Remark 4.5. Theorem 4.3 implies exponential convergence of the Čebyšev-interpolated covariance V_a^M for covariance kernels (4.15) which possibly are singular on the diagonal $x = y$ with singularity order $s > -d/2$. An important example is

$$V_a(x,x') = C\exp(-\gamma|x-x'|^{\delta}), \quad 1 \leqslant \delta \leqslant 2. \tag{4.20}$$

For $\delta = 2$, the kernel is analytic and Galerkin approximations to KL eigenpairs converge exponentially as $p \to \infty$, requiring therefore a small, dense matrix $\mathbf{V}$ and, in the gFMM, the (mandatory!) choice $m = p$ will yield no gain in complexity over a dense matrix approach. For $\delta < 2$, such kernels exhibit only very low regularity in the sense of Definition 2.15. Therefore, the Galerkin approximation (3.1) will use subspaces $S_h^p(D)$ of low, fixed polynomial degree p, and convergence by h-refinement. The resulting low, algebraic convergence rates mean that very large matrix eigenvalue problems (4.1) must be solved to obtain accurate KL eigenpairs. The exponential error bound $\exp(-bm)$ of the FMM implies in this case that m grows polynomially in $\log N$. The gFMM reduced, in this case, the work of a matrix vector multiply from N^2 to a polylogarithmic bound in N.

To compute (4.18) we interpolate the kernel function by Čebyšev polynomials

$$V_a^m(x,y;x_0,y_0) = \sum_{\substack{\mu\in\mathbb{Z}^d \\ |\mu|<m}} \widehat{f}_\mu(x_0,y_0) T_\mu(\chi^{-1}(y-x)), \tag{4.21}$$

where the m^d expansion coefficients are given by

$$\widehat{f}_\mu(x_0,y_0) = m^{-d} \sum_{\substack{v\in\mathbb{N}_0^d \\ v_i<m}} (K\circ\chi)(x_v)|\chi(x_v)|^s T_\mu(x_v). \tag{4.22}$$

Expanding the interpolant by Taylor we get

$$\begin{aligned} V_a^m(x,y;x_0,y_0) &= \sum_{\substack{\zeta\in\mathbb{Z}^d \\ |\zeta|<m}} \widehat{f}_\zeta(x_0,y_0) T_\zeta(\chi^{-1}(y-x)) = \sum_{\substack{\zeta\in\mathbb{Z}^d \\ |\zeta|<m}} \widehat{f}_\zeta(x_0,y_0) T_\zeta\left(\frac{y-x-y_0+x_0}{\eta\|y_0-x_0\|_\infty}\right) \\ &= \sum_{\substack{\zeta\in\mathbb{N}_0^d \\ |\zeta|<m}} c_\zeta(x_0,y_0)(y-x-y_0+x_0)^\zeta = \sum_{(v,\mu)\in\mathbb{N}_0^d\times\mathbb{N}_0^d} \sum_{\substack{\zeta\in\mathbb{N}_0^d \\ |\zeta|<m}} c_\zeta(x_0,y_0) D^{\mu+v}(z^\zeta)(0) \frac{(x_0-x)^\mu}{\mu!}\frac{(y-y_0)^v}{v!} \\ &= \sum_{\substack{(v,\mu)\in\mathbb{N}_0^d\times\mathbb{N}_0^d \\ |\mu+v|<m}} \frac{(x_0-x)^\mu}{\mu!}\frac{(y-y_0)^v}{v!}(\mu+v)! c_{\mu+v}(x_0,y_0). \end{aligned}$$

Remark 4.6. The coefficients $\widehat{f}_\mu(x_0,y_0)$ in (4.19)–(4.22) require $O(m^d)$ kernel evaluations at the Čebyšev points of order m.

4.2. Cluster expansions

Assumption 4.1 provides an approximation of the covariance kernel which is in general not valid for all $(x,y) \in D\times D$. In order to define a global approximation on $D\times D$, a collection of local approximations is used, where each local approximation is associated with an appropriate block of a given partition of $D\times D$. We call the blocks clusters and the combination of local approximations cluster expansion.

More precisely, let $\mathscr{P}(D)$ denote the set of all subsets of D, $\check{r}_A := \inf_{x\in\mathbb{R}^d}\sup_{y\in A}|y-x| \in \mathbb{R}$ the Čebyšev radius of a set $A \subset \mathbb{R}^d$ and $\check{c}_A \in \mathbb{R}^d$ with $\check{r}_A = \sup_{y\in A}|y-\check{c}_A|$ its Čebyšev center.

Definition 4.7. Suppose $\mathscr{C} \subset \mathscr{P}(D)\times\mathscr{P}(D)$ to be a finite partition of $D\times D$ which is subordinate to $\mathscr{D}$ in Definition 2.15 and let $0<\eta<1$ be a separation constant. An element $(\sigma,\tau) \in \mathscr{C}$ is called η-cluster iff

$$\check{r}_\sigma + \check{r}_\tau \leqslant \eta|\check{c}_\sigma - \check{c}_\tau|. \tag{4.23}$$

The set of all η-clusters in $\mathscr{C}$,

$$\mathscr{F} := \mathscr{F}(\mathscr{C}, \eta) = \{(\sigma, \tau) \in \mathscr{C} : (\sigma, \tau) \text{ is } \eta\text{-cluster}\}, \tag{4.24}$$

is called *far field of grain* η and its complement $\mathscr{N} := \mathscr{N}(\mathscr{C}, \eta) = \mathscr{C} \setminus \mathscr{F}(\mathscr{C}, \eta)$ the *near field of grain* η. Moreover, let the kernel $V_a(x,y)$ satisfy Assumption 4.1. Then

$$V_a^m(x,y) := \begin{cases} V_a^m(x,y;\check{c}_\sigma,\check{c}_\tau) & \text{if } (x,y) \in \sigma \times \tau \text{ and } (\sigma,\tau) \in \mathscr{F}, \\ V_a(x,y) & \text{otherwise} \end{cases} \tag{4.25}$$

for all $(x,y) \in D \times D$, $x \neq y$, defines a cluster expansion of the correlation kernel $V_a(x,y)$.

Replacing the covariance kernel $V_a(x,y)$ in the definition of the matrix $\mathbf{V}$ in (4.1) by its cluster expansion V_a^m introduces, for $u,v \in L^2(D)$, an approximate matrix $\widetilde{\mathbf{V}}$:

$$(\widetilde{\mathbf{V}})_{ij} = \int_D \int_D V_a^m(x,y) b_i(x) b_j(y)\, \mathrm{d}y\, \mathrm{d}x. \tag{4.26}$$

The matrix $\widetilde{\mathbf{V}}$ may be decomposed according to

$$\widetilde{\mathbf{V}} = \mathbf{N} + \sum_{(\sigma,\tau)\in\mathscr{F}} \mathbf{X}_\sigma^{\mathrm{T}} \mathbf{F}_{\sigma\tau} \mathbf{Y}_\tau \tag{4.27}$$

with

$$(\mathbf{N})_{i,j} := \sum_{(\sigma,\tau)\in\mathscr{N}} \int_\sigma \int_\tau V_a(x,y) b_i(x) b_j(y)\, \mathrm{d}y\, \mathrm{d}x, \quad (\mathbf{F}_{\sigma\tau})_{\mu,\nu} := \kappa_{(\mu,\nu)}(\check{c}_\sigma, \check{c}_\tau),$$

$$(\mathbf{X}_\sigma)_{\mu,i} := \int_\sigma X_\mu(x;\check{c}_\sigma) b_i(x)\, \mathrm{d}x, \quad (\mathbf{Y}_\tau)_{\nu,j} := \int_\tau Y_\nu(y;\check{c}_\tau) b_j(y)\, \mathrm{d}y$$

for $(\sigma,\tau) \in \mathscr{F}$ and $(\mu,\nu) \in \mathscr{I}_m$. In (4.27), the matrix $\mathbf{N}$ represents the near field part of $\widetilde{\mathbf{V}}$ whereas the sum of matrices describes the influence of the far field. If the partition $\mathscr{C}$ is chosen as discussed in the following section, $\mathbf{N}$ is a sparse matrix. In addition, the matrix vector multiplication related to the far field part can be evaluated in essentially linear complexity.

Remark 4.8. The matrices $\mathbf{F}_{\sigma\tau}$ are never formed explicitly. Typically, their entries $(\mathbf{F}_{\sigma\tau})_{\mu\nu}$ only depend on $\mu + \nu$ with $|\nu + \mu| < m$. Therefore, $\mathrm{O}(m^d)$ rather than $\mathrm{O}(m^{2d})$ expansion coefficients have to be evaluated and stored [6,12].

Remark 4.9. The expansions in the previous section preserve symmetry of the kernel V_a, i.e., $V_a^m(x,y) = V_a^m(y,x)$. If, in addition, the given partition $\mathscr{C}$ exhibits symmetry, i.e., $(\sigma,\tau) \in \mathscr{C} \Rightarrow (\tau,\sigma) \in \mathscr{C}$, then $\widetilde{\mathbf{V}}$ is symmetric.

Remark 4.10. (Collocation) For continuous covariances $V_a(x,x')$, we may allow in definitions (4.2) and (4.26) of $\mathbf{V}_{ij}$ and $\widetilde{\mathbf{V}}_{ij}$, respectively, the choice $b_i(x) = \delta(x_i)$, the Dirac delta function at x_i, the barycenter of element $\pi_i \in \mathscr{M}_h$. Then all integrals in (4.2) and (4.27) become point evaluations and, with the choice $M = \mathbf{1}$, the matrix eigenvalue problem (4.1) becomes a collocation approximation of (1.11). The components of $\underline{\phi}$ correspond to point values of piecewise constant approximations of the eigenfunctions.

4.3. Cluster algorithm

Eq. (4.27) specifies an approximation $\widetilde{\mathbf{V}}$ of the matrix $\mathbf{V}$ which allows to control the approximation error (see Section 4.4). To reduce the complexity of assembly and storage of $\mathbf{V}$ we must choose the partition $\mathscr{C}$ appropriately. An efficient way which also provides the desired complexity reduction from N^2 to $\mathrm{O}(N \log N)$ is to start with a recursive hierarchical decomposition of the mesh $\mathscr{M}_h$ represented by a tree $\mathscr{T} := (\mathscr{V}, \mathscr{E})$. An algorithm similar to Algorithm 4.1 might be used to generate such a decomposition, i.e., $\mathscr{T} := \mathrm{tree}(\mathscr{M}_h)$.

Algorithm 4.1 $((\mathscr{V},\mathscr{E}) := \mathrm{tree}(A))$.

if $|A| < c$ then
  return $(\{A\},\emptyset)$;
else
  $(A_0,A_1) := \mathrm{split}(A)$
  $(\mathscr{V}_0,\mathscr{E}_0) := \mathrm{tree}(A_0)$; $(\mathscr{V}_1,\mathscr{E}_1) := \mathrm{tree}(A_1)$;
  return $(\mathscr{V}_0 \cup \mathscr{V}_1 \cup \{A\}, \mathscr{E}_0 \cup \mathscr{E}_1 \cup \{(A,A_0),(A,A_1)\})$.

The function split(A) bisects a set of elements A into two disjoint sets A_0 and A_1 such that the Čebyšev radius of both sets is reduced. This, for example, could be achieved by splitting the bounding box of A along the longest side and distribute the elements with respect to the two parts.

Given a hierarchical decomposition $\mathscr{T}$ of $\mathscr{M}_h$, it is straightforward to construct a partition $\mathscr{C}$ as outlined in Algorithm 4.2. The decomposition $\mathscr{T}$ serves two purposes during the construction process: (i) it defines the pool $\mathscr{V}$ of subsets available for the construction of clusters and (ii) it defines the sets $\mathrm{children}(A) := \{A' \in \mathscr{V} : \exists (A,A') \in \mathscr{E}\}$. Calling $\mathrm{partition}(\mathscr{M}_h,\mathscr{M}_h)$ generates a partition $\mathscr{C}$ by specifying its far field $\mathscr{F}$ and near field $\mathscr{N}$. The resulting partition is symmetric in the sense of Remark 4.9.

Note that in Algorithm 4.2 $\mathscr{N}$ and $\mathscr{F}$ are given in terms of sets of elements π of the triangulation $\mathscr{M}$ of D.

Algorithm 4.2 $((\mathscr{N},\mathscr{F}) := \mathrm{partition}(A,B))$.

if $(\cup_{\pi\in A}\pi, \cup_{\pi\in B}\pi)$ is an η-cluster then
  return $(\emptyset,\{(A,B)\})$;
else
  $A' := \mathrm{children}(A)$; $B' := \mathrm{children}(B)$;

$$\text{return} \begin{cases} \bigcup_{a\in A', b\in B'} \mathrm{partition}(a,b) & \text{if } A' \neq \emptyset \text{ and } B' \neq \emptyset \text{ and } |A| = |B|, \\ \bigcup_{a\in A'} \mathrm{partition}(a,B) & \text{if } A' \neq \emptyset \text{ and } (|A| > |B| \text{ or } B' = \emptyset), \\ \bigcup_{b\in B'} \mathrm{partition}(A,b) & \text{if } (|A| < |B| \text{ or } A' = \emptyset) \text{ and } B' \neq \emptyset, \\ (\{(A,B)\},\emptyset) & \text{otherwise.} \end{cases}$$

The approximate matrix vector product $\vec{v} = \widetilde{\mathbf{V}}\vec{u}$ is evaluated in five steps:

(i) compute $\vec{v}_{\mathscr{N}} := \mathbf{N}^L\vec{u}$,
(ii) for all τ compute $\vec{u}_\tau := \mathbf{Y}_\tau^L\vec{u}$,
(iii) for all σ compute $\vec{v}_\sigma := \sum_{(\sigma,\tau)\in\mathscr{F}} \mathbf{F}_{\sigma\tau}\vec{u}_\tau$,
(iv) compute $\vec{v}_{\mathscr{F}} := \sum_\sigma \mathbf{X}_\sigma^{L^{\mathrm{T}}}\vec{v}_\sigma$,
(v) compute $\vec{v} = \vec{v}_{\mathscr{N}} + \vec{v}_{\mathscr{F}}$.

Steps (ii) and (iv) can be accelerated using the hierarchical decomposition as it is possible to represent the matrices $\mathbf{X}_\sigma$ and $\mathbf{Y}_\tau$ by the corresponding matrices related to children of σ and τ:

$$\mathbf{X}_\sigma = \sum_{\sigma'\in\mathrm{children}(\sigma)} \mathbf{C}_{\sigma\sigma'}\mathbf{X}_{\sigma'}, \tag{4.28}$$

$$\mathbf{Y}_\tau = \sum_{\tau'\in\mathrm{children}(\tau)} \mathbf{D}_{\tau\tau'}\mathbf{Y}_{\tau'}, \tag{4.29}$$

where the matrices $\mathbf{C}_{\sigma\sigma'}$ and $\mathbf{D}_{\tau\tau'}$ represent so-called shift operators as, e.g., in (4.8). These relationships are exploited in Algorithms 4.3 and 4.4 which replace steps (ii) and (iv) above, i.e., by $\mathrm{scatter}(\mathscr{M},u)$ and $\vec{v}_{\mathscr{F}} := \mathrm{gather}(\mathscr{M},0)$. Note that only the matrices $\mathbf{Y}_\tau$ and $\mathbf{X}_\sigma$, where τ and σ are leafs of the decomposition, are necessary. By Remark 4.8, these matrices contain $\mathrm{O}(m^d)$ entries.

Algorithm 4.3 (scatter$(A,\vec{u})$).

$\tau := \cup_{\pi\in A}$; $A' :=$ children(A);
if $A' = \emptyset$ then
  $\vec{u}_\tau := \mathbf{Y}_\tau^L u$;
else
  $\vec{u}_\tau := \sum_{a\in A'} \mathbf{D}_{\tau\tau'}$scatter$(a,\vec{u})$ with $\tau' := \cup_{\pi\in a}\pi$;
return $\vec{u}_\tau$.

Algorithm 4.4 (gather$(A,\vec{w}_A)$).

$\sigma := \cup_{\pi\in A}\pi$; $A' :=$ children(A);
if $A' = \emptyset$ then
  return $\mathbf{X}_\sigma^{L\,\mathrm{T}}(\vec{v}_\sigma + \vec{w}_A)$;
else
  return $\sum_{a\in A'}$gather$(a, \mathbf{C}_{\sigma\sigma'}^{\mathrm{T}}(\vec{v}_\sigma + \vec{w}_A))$ with $\sigma' := \cup_{\pi\in a}\pi$.

4.4. Cluster error

By construction, the local error bound (4.5) remains valid for a cluster expansion:

Theorem 4.11. *If the covariance $V_a(x,x')$ satisfies Assumption 4.1, there are $C_0, C_1 > 0$ independent of $x,y \in D$ and of m such that for all $(x,y) \in D_j \times D_{j'}$, $x \neq y$ and all m it holds*

$$|V_a(x,y) - V_a^m(x,y)| \leqslant C_0(C_1\eta)^m |V_a(x,y)|. \tag{4.30}$$

The replacement (4.3) of $V_a(x,y)$ by the global cluster expansion V_a^m in the far field introduces an approximate bilinear form via

$$\widetilde{V}^m(u,v) = \int_D \int_D v(x) V_a^m(x,x') u(x')\,\mathrm{d}x'\,\mathrm{d}x \quad \forall u,v \in L^2(D). \tag{4.31}$$

We associate the perturbed form $\widetilde{V}^m(\cdot,\cdot)$ with the matrix $\widetilde{\mathbf{V}}$ and approximate eigenpairs via the perturbed variational problem:

$$\widetilde{\phi}_h \in S_h^p : \widetilde{V}^m(\widetilde{\phi}_h, v) = \widetilde{\lambda}(\widetilde{\phi}_h, v) \quad \forall v \in S_h^p(D). \tag{4.32}$$

Our purpose is to estimate the error $\|\phi_m - \widetilde{\phi}_{m,h}\|_{L^2(D)}$. To apply the classical theory [18], we estimate the error in the Carlemann operators corresponding to the cluster expansions:

Theorem 4.12. *Let a cluster approximation V_a^m of the two point correlation V_a be given which satisfies Assumption 4.1 with sufficiently small η. Then the corresponding covariance operators $\mathscr{V}_a$ and $\mathscr{V}_a^m$ satisfy for all $m \in \mathbb{N}$ for any $0 < \eta < 1$ the error bounds*

$$\|\mathscr{V}_a - \mathscr{V}_a^m\|_{L^2(D)\to L^2(D)} \leqslant C_0(C_1\eta)^m |D|^2, \tag{4.33}$$

$$\|\mathscr{V}_a - \mathscr{V}_a^m\|_{L^\infty(D)\to L^\infty(D)} \leqslant C_0(C_1\eta)^m. \tag{4.34}$$

Proof. To show (4.33) we estimate for arbitrary $f \in L^2(D)$

$$\|\mathscr{V}_a f - \mathscr{V}_a^m f\|_{L^2(D)}^2 = \int_{x\in D} \left(\int_{y\in D} (V_a(x,y) - V_a^m(x,y)) f(y)\,\mathrm{d}y \right)^2 \mathrm{d}x \leqslant \|V_a - V_a^m\|_{L^\infty(D\times D)}^2 |D|^2 \|f\|_{L^2(D)}^2$$

and refer to (4.30). The proof of (4.34) is analogous. □

As an immediate consequence, we obtain

Corollary 4.13. *If Assumption 3.1 holds, the family* $\{\mathscr{V}_a^m\}_{m\in\mathbb{N}}$ *of operators converges as* $m\to\infty$ *in* $\mathscr{B}(L^2(D))$ *and* $\mathscr{B}(L^\infty(D))$ *with rate* $\Phi(m;\eta,V)=\exp(-b(\eta)m)$ *to* $\mathscr{V}_a$. *The approximate covariance operators* $\{\mathscr{V}_a^m\}_{m\in\mathbb{N}}$ *are, in particular, collectively compact in these spaces.*

Corollary 4.14. *Let* $P_h: L^2(D)\to S_h^p(D)$ *denote the* $L^2(D)$ *projection. If Assumption 3.1 holds, the family* $\{P_h\mathscr{V}_a^m P_h\}_{m\in\mathbb{N}}$ *of operators obtained from the cluster approximation with expansion order* m *converges as* $m\to\infty$ *and* $h\to 0$ *in* $\mathscr{B}(L^2(D))$ *and* $\mathscr{B}(L^\infty(D))$ *to* $\mathscr{V}_a$.

The approximate covariance operators $\{P_h\mathscr{V}_a^m P_h\}_{m\in\mathbb{N}}$ *are, in particular, collectively compact approximations in the sense of* [4] *of* $\mathscr{V}_a$ *in these spaces.*

Corollary 4.14 implies that the abstract error analysis of [18] is applicable to assess the impact of the cluster-approximation on the approximate KL eigenpairs obtained from $P_h\mathscr{V}_a^m P_h$.

5. Conclusion

Computation of approximate KL expansions in general domains $D\subset\mathbb{R}^d$ for given covariance function $V_a(x,x')$ with gFMM accelerated matrix–vector multiplication is only advised if

(i) the accuracy of the Galerkin eigenpairs of $P_h\mathscr{V}_a P_h$ is preserved and
(ii) the complexity of the cluster-approximated matrix–vector multiplication of $P_h\mathscr{V}_a^m P_h$ with the order m chosen to satisfy (i) is substantially lower than for the full matrix–vector multiplication.

In the case that V_a is piecewise analytic in $D\times D$ and a p-FEM is used to approximate the KL-eigenfunctions, the gFMM will not yield significant speed up, since the expansion order m must grow proportionally to the polynomial degree p of the FE subspace in order for the cluster error to match the exponential gFMM convergence rate.

In the case that V_a belongs to C^k in the sense of Definition 2.15, the convergence rate of the Galerkin approximated KL eigenpairs is at best algebraic, but so is the convergence rate $\Phi(m;\eta,V)$ of the cluster-approximated operator $\mathscr{V}_a^m$ (see Remark 4.5).

Computation of approximate KL-approximations using gFMM is thus preferable over dense matrix eigensolvers of the KL EVP only for covariances V_a with low regularity in the sense of Definition 2.15 which satisfy Assumption 4.1.

We mention that for all discrete eigenproblems the solver [9] yielded approximations accurate to about 14 decimals to the first 20 eigenpairs in about 70 iterations, independent of δ in (4.20). The results are presented in Figs. 4.1 and 4.2.

Appendix A. Proof of Theorem 2.24

The proof of Theorem 2.24 is based on the Ehrling–Nirenberg–Gagliardo inequalities (see [1]) to which we refer the reader for the following result.

Theorem A.1. *Let* $D\subset\mathbb{R}^d$ *be a bounded domain having the uniform cone property and* $\varepsilon_0\in(0,\infty)$, $n\in\mathbb{N}$, $p\in[1,\infty)$. *Then there exists* $c_{\varepsilon_0,n,p,D}>0$ *such that* $\forall\varepsilon\in(0,\varepsilon_0]$ $\forall j\in\{0,1,\ldots,n-1\}$ *and* $\forall u\in W^{n,p}(D)$,

$$|u|_{j,p}\leqslant c_{\varepsilon_0,n,p,D}\{\varepsilon|u|_{n,p}+\varepsilon^{-j/(n-j)}|u|_{0,p}\},\tag{A.1}$$

where

$$|u_{j,p}|^p:=\int_D\sum_{|\alpha|=j}|\partial^\alpha u|^p.\tag{A.2}$$

We note now that piecewise regularity of eigenfunctions follows from that of the kernel V.

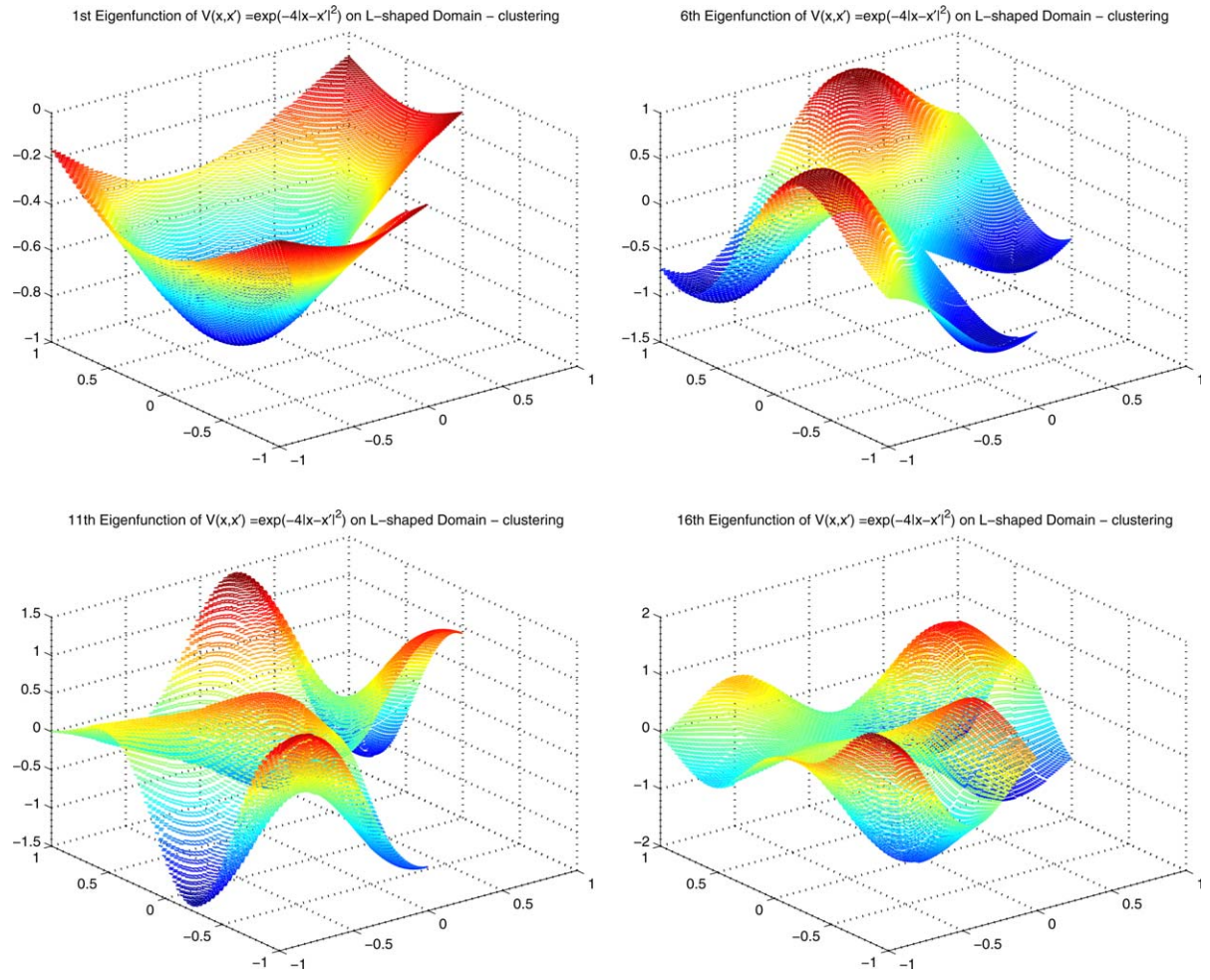

Fig. 4.1. Eigenfunctions No. 1, 6, 11, 16 of Gaussian covariance kernel ((4.20) with $\delta = 2$, $C = 1$) on L-shaped domain $D =]-1,1[^2 \setminus ([0,1] \times [-1,0])$ for correlation length 0.5, computed using clustering on a regular triangulation of D with 16,384 triangular elements. PC w. 1GB RAM, generalized FMM and [9] was used.

Proposition A.2. *If $V \in \mathscr{A}_{\mathscr{D},\mathscr{G}}(D^2)/\mathscr{C}^{\infty}_{\mathscr{D},\mathscr{G}}(D^2)/H^{p,q}_{\mathscr{D},\mathscr{G}}(D^2)$, then the eigenfunctions of the associated Carleman operator $\mathscr{V}$ given by (2.36) corresponding to nontrivial eigenvalues belong to $\mathscr{A}_{\mathscr{D},\mathscr{G}}(D)/\mathscr{C}^{\infty}_{\mathscr{D},\mathscr{G}}(D)/H^{p}_{\mathscr{D},\mathscr{G}}(D)$.*

Proof. The conclusion follows at once from the eigenvalue equation

$$\phi_m(x) = \frac{1}{\lambda_m} \sum_{j' \in \mathscr{J}} \int_{D_{j'}} V(x,x')\phi_m(x')\,\mathrm{d}x' \quad \forall x \in D_j, \tag{A.3}$$

which can be naturally extended to G_j by replacing V by its regular continuation on $G_j \times G_{j'}$. □

Proof of Theorem 2.24. We first note that the eigenvalue Eq. (A.3) implies (by differentiating and applying the Cauchy–Schwarz inequality to estimate the resulting integrals) for any $\alpha \in \mathbb{N}^d$ the existence of a constant $c_{K,\alpha} > 0$ such that

$$\|\partial^{\alpha}\phi_m\|_{L^{\infty}(D_j)} \leqslant c_{K,\alpha}|\lambda_m|^{-1} \qquad \forall m \geqslant 1, \quad \forall 1 \leqslant j \leqslant J. \tag{A.4}$$

We apply now Theorem A.1 on D_j with $p = 2$, $\varepsilon_0 := \max_{m \in \mathbb{N}_+}|\lambda_m|$ and choose in (A.1) $\varepsilon = \lambda_m$, $u = \phi_m$ for an arbitrary $m \geqslant 1$ (we assume w.l.o.g. $\lambda_m \neq 0$). It follows that for any $n \in \mathbb{N}$ there exists $c_{\varepsilon_0,n,D_j} > 0$ such that for all $l \in \{0,1,\ldots,n-1\}$

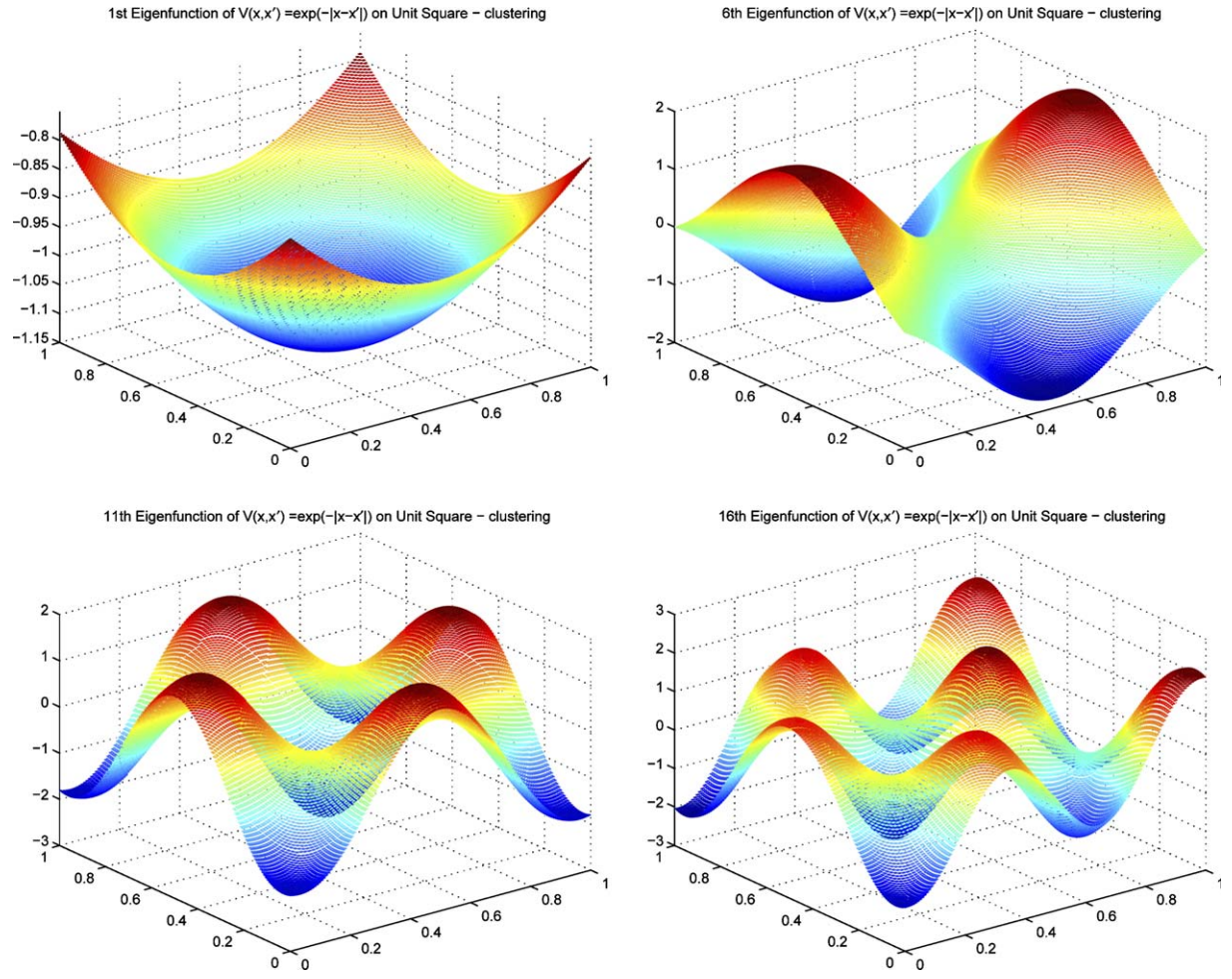

Fig. 4.2. Eigenfunctions No. 1, 6, 11, 16 of exponential covariance kernel ((4.20) with $\delta = 1$, $C = 1$) on unit square $D =]0,1[^2$ for correlation length 1, computed using clustering on a regular triangulation of D with 32,768 triangular elements. PC w. 1GB RAM, generalized FMM and [9] was used.

$$|\phi_m|_{D_j,l,2} \leqslant c_{\varepsilon_0,n,D_j}\{\lambda_m|\phi_m|_{n,2} + \lambda_m^{-l/(n-l)}|\phi_m|_{0,2}\} \leqslant c_{\varepsilon_0,n,D_j,K}\{1 + \lambda_m^{-l/(n-l)}\} \leqslant c_{\varepsilon_0,n,D_j,K}\lambda_m^{-l/(n-l)}, \tag{A.5}$$

due to (A.4).

Now, for any $s > 0$ and $\alpha \in \mathbb{N}^d$ we choose $l = \lceil d/2 \rceil + |\alpha|$ and $n > l$ such that $l/(n-l) < s$. From (A.5) and the Sobolev embedding theorems we deduce then

$$\|\partial^\alpha \phi_m\|_{L^\infty(D_j)} \leqslant c_{\alpha,D_j}\|\phi_m\|_{H^l(D_j)} \leqslant c_{\alpha,D_j}\sum_{k=0}^{l}|\phi_m|_{D_j,k,2} \leqslant c_{\varepsilon_0,n,D_j,K,\alpha}\sum_{k=0}^{l}\lambda_m^{-k/(n-k)} \leqslant c_{\varepsilon_0,n,D_j,K,\alpha}\lambda_m^{-l/(n-l)}$$
$$\leqslant c_{\varepsilon_0,n,D_j,K,\alpha}\lambda_m^{-s}$$

for all $m \geqslant 1$, and the proof is concluded. □

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