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Research Report No. 2014-19

August 2014
Latest revision: June 2016

Seminar für Angewandte Mathematik
Eidgenössische Technische Hochschule
CH-8092 Zürich
Switzerland

Funding ERC: AdG 247277 STAHDPDE

Noname manuscript No.
(will be inserted by the editor)

Covariance regularity and $\mathcal{H}$-matrix approximation for rough random fields*

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the date of receipt and acceptance should be inserted later

Abstract In an open, bounded domain $\mathrm{D} \subset \mathbb{R}^n$ with smooth boundary $\partial\mathrm{D}$ or on a smooth, closed and compact, Riemannian n-manifold $\mathcal{M} \subset \mathbb{R}^{n+1}$, we consider the linear operator equation $Au = f$ where A is a boundedly invertible, strongly elliptic pseudodifferential operator of order $r \in \mathbb{R}$ with analytic coefficients, covering all linear, second order elliptic PDEs as well as their boundary reductions. Here, $f \in L^2(\Omega; H^t)$ is an H^t-valued random field with finite second moments, with H^t denoting the (isotropic) Sobolev space of (not necessarily integer) order t modelled on the domain D or manifold $\mathcal{M}$, respectively. We prove that the random solution's covariance kernel $K_u = (A^{-1} \otimes A^{-1})K_f$ on $\mathrm{D}\times\mathrm{D}$ (resp. $\mathcal{M}\times\mathcal{M}$) is an asymptotically smooth function provided that the covariance function K_f of the random data is a Schwartz distributional kernel of an analytic, elliptic pseudodifferential operator and that A is a strongly elliptic, analytic (pseudo-) differential operator, including in particular second order, elliptic differential operators with analytic coefficients, and their Calderón-projectors on analytic surfaces (resp. analytic surface pieces). As a consequence, numerical $\mathcal{H}$-matrix calculus allows deterministic approximation of singular covariances K_u of the random solution $u = A^{-1}f \in L^2(\Omega; H^{t-r})$ in $\mathrm{D} \times \mathrm{D}$ with work versus accuracy essentially equal to that for the mean field approximation in D, overcoming the curse of dimensionality in this case.

Keywords Operator Equations · Covariance Kernels · Tensor-Operators

Mathematics Subject Classification (2000) 65N30

* This work was supported in part by the European Research Council AdG grant STAHDPDE 247277 and by the Swiss National Science Foundation (SNF).

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1 Introduction

A key task in uncertainty quantification is the efficient numerical solution of partial differential equations (PDEs) and integral equations with random input data. Specific instances are elliptic diffusion equations with random forcing and boundary data, random diffusion coefficients and random domains. In the latter of these cases, the random solution is, in general, a nonlinear transformation of the random input data. If the fluctuations of the random input data around the statistical mean are large, stochastic Galerkin methods are the methods of choice, which has lead in recent years to a sizeable body of literature on these methods and their numerical analysis. We mention only [31,30,8] and the references there.

For random forcing, and deterministic, linear operators and deterministic domains, the random solution is a linear transformation of the random input data. Statistical moments of the random solution are then deterministic multilinear maps (tensors) for which direct, ie. deterministic, approximations can be designed, see eg. [2,24,36,37]. In cases when the random solution depends nonlinearly on the random input as, for example, in case of random diffusion coefficients or random domains, with small amplitude fluctuations, related moment equations can be derived by perturbation theory. Then, statistical moments are obtained to leading order in the magnitude of the random input data fluctuations about the nominal value; we refer to [5,18,19,21,24] for details.

In the present article, we focus on linear, deterministic operator equations with random loading which take the general form

$$Au(\omega) = f(\omega) \quad \text{in D}, \tag{1.1}$$

where the deterministic operator $A \in OPS^m_{cl}(\mathrm{D})$ is a boundedly invertible, strongly elliptic, classical pseudodifferential operator of order $m \in \mathbb{R}$.

We assume A to be boundedly invertible from $V^\star$ to V, with V being (a closed subspace of) the (Hilbert) Sobolev space $H^{m/2}(\mathrm{D})$, accounting for homogeneous, essential boundary conditions and/or possibly factoring out nontrivial (but finite-dimensional) kernels (strong ellipticity implies that A is, in particular, Fredholm).

For a separable Hilbert space H and a probability space $(\Omega, \mathcal{A}, \mathbb{P})$, we denote by $L^2(\Omega, \mathbb{P}; H)$ the Bochner-space of strongly measurable maps $v : \Omega \mapsto H$ whose norm is square (Bochner) integrable with respect to $\mathbb{P}$. The linearity of (1.1) and the bounded invertibility of the (deterministic) operator $A \in OPS^m_{cl}(\mathrm{D})$ of order $m \in \mathbb{R}$ implies then that for every $f \in L^2(\Omega, \mathbb{P}; V^\star)$, (1.1) admits a unique solution $u \in L^2(\Omega, \mathbb{P}; V)$. If, in particular, $\mathbb{P}$ is a Gaussian measure on $V^\star$, ie. if f is a Gaussian random field on $V^\star$, then u is a Gaussian random field on V. Here, V is a closed subspace of $H^m(\mathrm{D})$, accounting, for example, for homogeneous essential boundary conditions. This is a consequence of linear transformations of Gaussian random fields being again Gaussian; [6, Prop. 1.2.3]. In this case, u being again a Gaussian random field it is completely characterized by its mean $\mathbb{E}[u] \in V$ and by its second moment $\mathbb{E}[u \otimes u] \in V \otimes V$ (cp. [6, Thm. 1.2.1]). Deterministic computational approximation of the second order statistics of the random field u are, therefore, of some interest, in particular in the Gaussian case, but also in linearizations, cp. eg. [24,7,5] and the references there. Two issues arise in the design of efficient algorithms. First, the issue of dimensionality: as indicated above, for (pseudo-) differential equations defined on domains $\mathrm{D} \subset \mathbb{R}^n$, the spatial

two-point correlation is a function of $2n$ variables in $\mathrm{D}\times\mathrm{D}\subset\mathbb{R}^{2n}$ which renders standard approximation schemes prohibitively expensive. Therefore, in [12,36,37], *sparse tensor product approximations* have been proposed and have been shown *to reduce the computational complexity (ie. computational work and memory vs. accuracy) to essentially that of a multilevel approximation of one sample of* (1.1) under *sufficient smoothness (so-called "mix" regularity) of the covariance function* of interest.

This leads to the second issue, and the topic of the present article: since the equation (1.1) is linear and since A is deterministic, taking expectations on both sides of (1.1) immediately yields the deterministic equation

$$A\mathbb{E}[u]=\mathbb{E}[f]\quad\text{in } V^\star\,. \tag{1.2}$$

In a similar manner, deterministic equations for the covariance of $u\in L^2(\Omega,\mathbb{P};V)$ can be derived. Denote by $K_u=\mathbb{E}[(u-\mathbb{E}[u])\otimes(u-\mathbb{E}[u])]$ the centered second moment of $u\in L^2(\Omega,\mathbb{P};V)$, and analogously by K_f the centered second moment (two-point correlation function) for the random forcing f. Then, formally, it holds (cp. [35] for example)

$$(A\otimes A)K_u=K_f\quad\text{in } (V\otimes V)^\star\simeq V^\star\otimes V^\star. \tag{1.3}$$

It was shown in [35–37] that (hypo-) elliptic regularity of A and smoothness of $\mathcal{K}_f$ imply corresponding smoothness of $\mathcal{K}_u$ which, in turn, facilitates efficient sparse tensor product (Galerkin) approximations of the *deterministic* covariance equation (1.3) (eg. [35–37] for details and further references). Equations such as (1.3) also arise from a first-order, second-moment perturbation analysis of nonlinear operator equations with random operators, cp. [5,23] and the references there.

In several applications, however, physical modelling mandates low pathwise regularity of the Gaussian random fields f (cp. eg. [29]). Then, the corresponding regularity of their two-point correlation functions K_f (which, as we shall show here, are closely related to the Schwartz kernel functions of their covariance operators) is low in a vicinity of the diagonal, and the sparse tensor product approximations of [12,36,37] perform poorly. The covariance operators which give rise to such random fields are often a negative power of a strongly elliptic, self-adjoint differential operator, the so-called "precision operator". Pseudodifferential operators and their (distributional) kernels thus naturally arise in the regularity analysis of covariance kernels: the corresponding two-point correlation kernels $K_f(x,y)$ of the random data have singular support on the diagonal set $\Delta=\{(x,y)\in\mathrm{D}\times\mathrm{D}\,|\,x=y\}$ obstructing high approximation rates by sparse tensor approximations (cp. eg. [12, 36,37]). The main point of the present article is to prove that, for large classes of differential or integral operators A in (1.1), $\mathcal{H}$-matrix formatted covariance approximations (cp. eg. [3,15]) afford approximate representation of singular covariance kernels with log-linear complexity $\mathrm{D}\times\mathrm{D}$ with respect to N, the number of degrees of freedom in D (resp. on $\mathcal{M}$). Let us also indicate that in bounded domains D with nonsmooth boundary ∂D (such as, eg., a polygon or polyhedron), there arise additional *boundary singularities* in the covariance function which are concentrated on $\partial\mathrm{D}\times\mathrm{D}\cup\mathrm{D}\times\partial\mathrm{D}$, due to the interaction of the singular support of K_f on Δ. We refer to [32,33] for a detailed discussion of a simple (the domain $\mathrm{D}\subset\mathbb{R}^1$) special case. From these references, we note in particular the local analyticity of $K_u(x,y)$ and the *exponential convergence* of low-rank approximations away from the diagonal $\Delta\subset\mathrm{D}\times\mathrm{D}$ as key ingredients for overcoming the increase in complexity due to

the doubling of the dimension in this case. To generalize [32,33] for the covariance equation (1.3) corresponding to (1.1), with general linear (pseudo-) differential operator A, and on general domains D (resp. on n-Manifolds $\mathcal{M}$) is the purpose of the present arcticle.

This article is organized as follows. In the next section, pseudodifferential operators are introduced and their properties relevant for us collected. Then, in Section 3, the regularity results for covariance function K_u are derived. In Section 4, we show how $\mathcal{H}$-matrices can be used to efficiently compute the unknown covariance K_u given by (1.3). Numerical results are presented in Section 5 to validate and quantify the theory. Conclusions and extensions are indicated in Section 6.

2 Preliminaries

We recapitulate several technical tools from the theory of distributions and pseudodifferential calculus and set notation for the proof of the main results in the next sections.

2.1 Schwartz Kernel Theorem

As the solution of the second moment equations are covariances of random fields, we shall draw extensively on the equivalence of *covariance operators* and *covariance kernels*. The major result here is the (classical) *Schwartz Kernel Theorem*. We present a version of [25, Chap. 5] suitable for our purposes.

We prepare its statement with some definitions. Every function $K \in C(X_1 \times X_2)$ defines an integral operator from $C(X_2)$ to $C(X_1)$ by the formula

$$(\mathcal{K}\phi)(x_1) = \int K(x_1, x_2)\phi(x_2)\mathrm{d}x_2. \tag{2.1}$$

For kernel functions $K \in C(X_1 \times X_2)$, we have (cp. [25, Eq. (5.2.1)])

$$\langle \mathcal{K}\phi, \psi\rangle = K(\psi \otimes \phi) \quad \text{for all } \psi \in C_0^\infty(X_1),\ \phi \in C_0^\infty(X_2). \tag{2.2}$$

The definition (2.2) can be extended to distributions $K \in \mathcal{D}'(X_1 \times X_2)$ if $\mathcal{K}\phi$ is allowed to be a distribution.

Proposition 1 (Schwartz Kernel Theorem [25, Thm. 5.2.1]) *Every distributional kernel $K \in \mathcal{D}'(X_1 \times X_2)$ induces, via* (2.2)*, a continuous, linear map from $C_0^\infty(X_2)$ to $\mathcal{D}'(X_1)$. Conversely, for every linear map $\mathcal{K}$ exists a unique distribution K such that* (2.2) *holds. The distribution K is called* (distributional) kernel *of $\mathcal{K}$.*

2.2 Pseudodifferential Operators

We present basic definitions and terminology from the theory of pseudodifferential operators, in particular elements of the calculus of pseudodifferential operators, going back to R.T. Seeley, and its analytic extension due to L. Boutet de Monvel and P. Kree [4,28]. We refer to [34] for a comprehensive account of this theory,

including subsequent developments. We adopt notation for the statements of results on pseudodifferential operators from the monographs of M.E. Taylor [41], L. Hörmander [26] and, in the analytic case, from [34] indicating precise references and, where applicable, the particular assumptions under which we shall access the (more general than required here) results in these references. The extensions to analytic and Gevrey-class pseudodifferential operators are based on the Gevrey extension of the symbolic calculus for classical pseudodifferential operators developed in [4,28,34].

2.2.1 Symbols

For an order $r \in \mathbb{R}$, the symbol class $S^r(\mathrm{D}\times\mathbb{R}^n)$ consists of functions $a \in C^\infty(\mathrm{D}\times\mathbb{R}^n)$ such that, for any $K \Subset \mathrm{D}$ and for every $\alpha,\beta \in \mathbb{N}_0^n$, there exist constants $C_{\alpha\beta}(K) > 0$ such that

$$\forall x \in K,\ \xi \in \mathbb{R}^n : \quad \left|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)\right| \leq C_{\alpha\beta}(K)\langle\xi\rangle^{r-|\beta|} \tag{2.3}$$

where $\langle\xi\rangle = (1+|\xi|^2)^{1/2}$. The class $S^r(\mathrm{D}\times\mathbb{R}^n)$ is contained in the Hörmander class $S^r_{1,0}$; we shall not require the general classes $S^r_{\rho,\delta}$ (cp. [26]) and, therefore, omit the fine indices. A function $a \in C^\infty(\mathrm{D}\times\mathbb{R}^n\backslash\{0\})$ is called *positively homogeneous of degree* m if

$$\forall t > 0,\ 0 \neq \xi \in \mathbb{R}^n : \quad a_m^0(x,t\xi) = t^m a_m^0(x,\xi).$$

Note that then $\chi(\xi)a_m^0(x,\xi) \in S^m(\mathrm{D}\times\mathbb{R}^n)$ for any smooth, nonnegative cut-off function χ which vanishes identically for $|\xi| < 1/2$ and $\chi(\xi) \equiv 1$ for $|\xi| \geq 1$. For a symbol $a \in S^r(\mathrm{D}\times\mathbb{R}^n)$, the corresponding pseudodifferential operator A is defined for $u \in C_0^\infty(\mathrm{D})$ via the oscillatory integral (cp. [25])

$$A(x,-iD)u(x) = (2\pi)^{-n/2}\int_{\xi\in\mathbb{R}^n} e^{ix\cdot\xi}a(x,\xi)\hat{u}(\xi)\mathrm{d}\xi, \quad x \in \mathrm{D}. \tag{2.4}$$

The set of all pseudodifferential operators A generated via (2.4) from a symbol $a \in S^r(\mathrm{D}\times\mathbb{R}^n)$ is denoted by $OPS^r(\mathrm{D})$.

A symbol $a \in S^r$ is called *classical symbol of order* $r \in \mathbb{R}$ (denoted by S^r_{cl}) if for every $k \in \mathbb{N}_0$ exist functions $a_{r-k}(x,\xi) \in S^{r-k}(\mathrm{D}\times\mathbb{R}^n)$ such that $a \sim \sum_k a_{r-k}$ (in the sense of asymptotic expansions of symbols, cp. [26]), where a_{r-k} is homogeneous of degree $r-k$, ie. it holds that $a_{r-k}(x,t\xi) = t^{r-k}a_{r-k}(x,\xi)$ for every $t > 0$ and for every $\xi \in \mathbb{R}^n$ with $|\xi| > 1$. Denote the subclass of classical symbols of order r by $S^r_{cl}(\mathrm{D}\times\mathbb{R}^n)$. As a consequence of the asymptotic expansion of $a \in S^r_{cl}(\mathrm{D}\times\mathbb{R}^n)$, for every $\alpha,\beta \in \mathbb{N}_0^n$ and for every $K \Subset \mathrm{D}$ exists a constant $c_{\alpha\beta}(K) > 0$ such that for every $N \in \mathbb{N}$ holds

$$\forall x \in K,\ \xi \in \mathbb{R}^n : \quad \left|\partial_x^\alpha \partial_\xi^\beta \left(a(x,\xi) - \sum_{k=0}^{N} a_{r-k}(x,\xi)\right)\right| \leq c_{\alpha\beta}(K)\langle\xi\rangle^{r-N-|\beta|-1}. \tag{2.5}$$

The symbolic calculus in S^r_{cl} is based on equivalences modulo C^∞, ie. in the class of smooth functions. For exponential convergence of separable polynomial approximations, *analyticity* or at least Gevrey class regularity is required. To verify this

for covariance kernels, we consider another subclass of symbols, the so-called *symbols of class* $s \geq 1$ introduced by L. Boutet de Monvel and P. Kree in [4]. It is based on tighter control of dependence of $c_{\alpha\beta}(K)$ in (2.5) on the differentiation orders; the following definition is [4, Def. 1.1] (see also [34, Chap. III.3]).

Definition 1 We say that $a \sim \sum_k a_{r-k} \in S^r_{cl}$ is a (Gevrey) symbol of class $s \geq 1$ if for every $K \Subset \mathrm{D}$ exist constants $c, A > 0$ such that for all $\alpha, \beta \in \mathbb{N}_0^n$

$$\forall x \in K,\ \xi \in \mathbb{R}^n : \quad \left|\partial_x^\alpha \partial_\xi^\beta a_{r-k}(x,\xi)\right| \leq c A^{k+|\alpha+\beta|} |\xi|^{r-k-|\beta|} (k+|\alpha|)!^s \beta!. \tag{2.6}$$

We note that Definition 1 implies that, for $x \in K$, $a_{r-k}(x,\xi)$ is holomorphic with respect to ξ and that for every $K \Subset \mathrm{D}$ exists $\varepsilon > 0$ such that for every $x \in K$ and every $\xi \in C_\varepsilon := \{\xi \in \mathbb{C}^n : |\operatorname{Im}\xi| < \varepsilon |\operatorname{Re}\xi|\}$ the bound

$$\left|\partial_x^\alpha a_{r-k}(x,\xi)\right| \leq A^{k+|\alpha|+1} |\xi|^{r-k} (k+|\alpha|)!^s \tag{2.7}$$

holds. The subclass of S^r_{cl} which satisfies (2.6) or, equivalently, (2.7) is denoted by $S^r_{cl,s}$. It is a subset of the Gevrey symbol class $S^{r,s}_{\rho,\delta}$ (with $\rho = 1$ and $\delta = 0$) introduced in [34, Def. III.3.1]. Notice finally that symbols in $S^r_{cl,s}$ with $s = 1$ depend analytically on $x \in \mathrm{D}$.

2.2.2 Calculus

Pseudodifferential operators admit calculi which are crucial in proving regularity of covariance functions for random field solutions of (1.1). We collect properties of the calculi in S^r_{cl} and in $S^r_{cl,s}$ that will be required ahead.

Proposition 2 *1. For invertible, elliptic $A \in OPS^r_{cl}$ it holds $A^{-1} \in OPS^{-r}_{cl}$.*
2. $A \in OPS^r_{cl}$ (resp. $A \in OPS^r_{cl,s}$) implies $A^\star \in OPS^r_{cl}$ (resp. $A^\star \in OPS^r_{cl,s}$).
3. $A \in OPS^r_{cl}$ and $B \in OPS^t_{cl}$ implies $AB \in OPS^{r+t}_{cl}$.
4. $A \in OPS^r_{cl,s}$ and $B \in OPS^t_{cl,s}$ with at least one of A, B properly supported implies $AB \in OPS^{r+t}_{cl,s}$.
5. For any elliptic $A \in OPS^r_{cl,s}$ with $s \geq 1$ exists $E \in OPS^{-r}_{cl,s}$ such that the operator $AE - I$ has a Schwartz kernel of Gevrey class $s > 1$ (analytic if $s = 1$).

Proof The asserted properties for OPS^r_{cl} are standard properties for this algebra. The properties for the analytic and Gevrey class operators are a consequence of [4, Props. 2.11, 2.12, and 2.14].

2.2.3 Kernels

Via the Schwartz Kernel Theorem (Proposition 1), every classical pseudodifferential operator $A \in OPS^m_{cl}(\mathrm{D})$ with symbol $a \in S^m_{cl}(\mathrm{D})$ can be written as a (distributional) integral operator with (distributional) Schwartz kernel K_A. Early on, development of pseudodifferential operator calculi was based on Fourier analysis. For the analysis of covariances in the present article, the perspective of (distributional) kernel functions associated with pseudodifferential operators is central: Schwartz kernels model two-point correlation functions of random fields with low sample-path regularity in Sobolev and Besov scales, whose covariance operators are compact, self-adjoint on $L^2(\mathrm{D})$.

It was noted early in the development of the calculus of pseudodifferential operators that Schwartz kernels K_A for $A \in OPS^r_{cl}(\mathrm{D})$ can be completely characterized in terms of so-called *pseudohomogeneous functions* (Ψhf for short). The ensuing results date back to R.T. Seeley's work [38,39]; we recapitulate here the main statements, following the presentation in [27, Chap.7.1].

Definition 2 A distributional kernel function $k_q(x,z) \in C^\infty(\mathrm{D} \times \mathbb{R}^n \backslash \{0\})$ is a *pseudohomogeneous kernel (with respect to z) of degree $q \in \mathbb{R}$* if

$$\begin{aligned} \forall t > 0,\ 0 \neq z \in \mathbb{R}^n : \quad & k_q(x,tz) = t^q k_q(x,z), && \text{if } q \in \mathbb{R}\backslash\mathbb{N}_0, \\ & k_q(x,z) = f_q(x,z) + \log(|z|) p_q(x,z), && \text{otherwise,} \end{aligned} \tag{2.8}$$

where $p_q(x,z)$ denotes a homogeneous polynomial in z of degree at most q with $C^\infty(\overline{\mathrm{D}})$-coefficients and the function $f_q(x,z)$ satisfies

$$\forall t > 0,\ 0 \neq z \in \mathbb{R}^n : \quad f_q(x,tz) = t^q f_z(x,z).$$

The class of all pseudohomogeneous functions of degree $q \in \mathbb{R}$ is denoted by $\Psi\mathrm{hf}_q$.

We say that *a Schwartz kernel $k(x,x-y)$, $x,y \in \mathrm{D}$, $x \neq y$, admits a pseudohomogeneous expansion of degree q* if for every $j \in \mathbb{N}_0$ exist $k_{q+j} \in \Psi\mathrm{hf}_{q+j}$ and a constant $0 < \delta < 1$ such that

$$\forall J \in \mathbb{N} : \quad k(x,x-y) - \sum_{j=0}^{J} k_{q+j}(x,x-y) \in C^{q+J-\delta}(\overline{\mathrm{D} \times \mathrm{D}}). \tag{2.9}$$

Note that the partial sums in (2.9) do not converge in general. By $\Psi\mathrm{hk}_q$ we denote the class of all Schwartz kernels $k(x,x-y)$, $x,y \in \mathrm{D}$, $x \neq y$, which admit a pseudohomogeneous expansion (2.9) of degree q in D.

The relevance of the class $\Psi\mathrm{hf}_{-q-n}$ lies in its close connection to the operator class $OPS^q_{cl}(\mathrm{D})$. The following result is [27, Thm. 7.1.1, 7.1.6, 7.1.7], see also [38, p. 279].

Proposition 3 *Let $m \in \mathbb{R}\backslash\mathbb{N}_0$ and let $\mathrm{D} \subset \mathbb{R}^n$ denote a bounded domain with smooth boundary $\partial\mathrm{D}$. Then $A \in OPS^m_{cl}(\mathrm{D})$ iff its Schwartz kernel $K_A(x,x-y) \in \Psi\mathrm{hk}_{-m-n}(\mathrm{D})$. Moreover, for $m \in \mathbb{N}_0$ and for $n \geq 2$, $f_\kappa \in \Psi\mathrm{hf}_\kappa$ with $\kappa = -m-n$ defines the distributional Schwartz kernel K_A of $A \in OPS^m_{cl}(\mathrm{D})$ iff it satisfies the* compatibility conditions

$$\int_{|\Theta|=1} \Theta^\alpha f_\kappa(x,\Theta) \mathrm{d}\omega(\Theta) = 0 \quad \textit{for all } |\alpha| = m. \tag{2.10}$$

We remark that, from the preceding result, it follows for $A \in OPS^m_{cl}(\mathrm{D})$ that the associated Schwartz kernel K_A is absolutely integrable if $m < -n \leq -1$; in this case, the compatibility conditions (2.10) are not required.

In the particular case of analytic symbols $a \in S^r_{cl,1}(\mathrm{D})$, $K_A(x,z)$ is analytic in $\mathrm{D} \times \mathbb{R}^n \backslash \{0\}$. The following result is [4, Prop. 2.5].

Proposition 4 *Let $a \in S^r_{cl,1}(\mathrm{D})$ be an analytic symbol with associated analytic pseudodifferential operator $A \in OPS^r_{cl,1}(\mathrm{D})$. Then, its Schwartz kernel, $K_A(x,x-y)$, $x,y \in \mathrm{D}$, differs from the sum $\sum_{j \geq 0} k_{r+j}(x,x-y)$ only by a function which is analytic in a neighborhood of the diagonal $\Delta \subset \mathrm{D} \times \mathrm{D}$.*

We note in particular that, in the analytic class $S^r_{cl,1}(\mathrm{D})$, the partial sums in the pseudohomogeneous expansions (2.9) converge.

2.3 Matérn Covariances

In the framework of spatially inhomogeneous random fields, it is quite common to assume that the covariance kernels of random fields are *isotropic*, ie. $K(x, y)$ depends only on the distance $r = |x - y|$. Hence, for illustration, we shall present here the Matérn class of kernels as an important example for covariance functions of this kind [29]. They are given by

$$K_\nu(r) := \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu} r}{\ell} \right)^\nu \mathbb{K}_\nu \left(\frac{\sqrt{2\nu} r}{\ell} \right) \tag{2.11}$$

with smoothness parameter $\nu > 0$ and correlation length $\ell > 0$, see [29]. Here, $\mathbb{K}_\nu$ denotes the modified Bessel function of the second kind. For half integer values of ν, ie. for $\nu = p + 1/2$ with $p \in \mathbb{N}_0$, expression (2.11) simplifies to

$$K_{p+1/2}(r) = \exp\left(\frac{-\sqrt{2\nu} r}{\ell} \right) \frac{p!}{(2p)!} \sum_{q=0}^{p} \frac{(p+q)!}{q!(p-q)!} \left(\frac{\sqrt{8\nu} r}{\ell} \right)^{p-q}.$$

The limit case $\nu \to \infty$ formally corresponds to the Gaussian kernel:

$$K_\infty(r) = \exp\left(\frac{-r^2}{2\ell^2} \right).$$

An illustration of the Matérn kernels for $\nu = 1/2, 3/2, 5/2$ and $\nu = \infty$ is given in Figure 1.

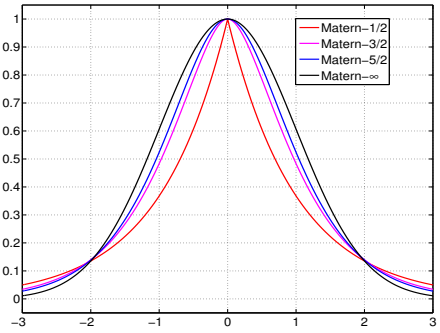

Fig. 1 Matérn kernels $K_\nu(|x|)$ for different values of the smoothness parameter ν for $\nu = 1/2, 3/2, 5/2$ and $\nu = \infty$.

The Fourier transform of the Matérn kernel in $\mathbb{R}^n$ has also been computed in [29]. Since the corresponding Gaussian random fields are stationary, it does not depend on the spatial variable x and is given by

$$a_\nu(\xi) = \alpha \left(1 + \frac{\ell^2}{2\nu} |\xi|^2 \right)^{-\nu - n/2} \tag{2.12}$$

where α is a scaling factor which depends on ν, ℓ and n. Expanding (2.12) asymptotically, as $|\xi| \to \infty$, and comparing with (2.5), we infer readily that the associated covariance kernel function $\mathcal{K}_\nu \in OPS_{cl}^{-2\nu-n}$ and, being independent of x, also that $\mathcal{K}_\nu \in OPS_{cl,1}^{-2\nu-n}$. This also follows from the symbolic calculus in Proposition 2 upon noting that the symbol (2.12) coincides with the symbol of the inverse to the differential operator $A_\nu = \alpha^{-1}(I - \frac{\ell^2}{2\nu}\Delta)^{\nu+n/2}$ which is of order $2\nu + n$ and thus $A_\nu \in OPS_{cl,1}^{2\nu+n}$.

3 Covariance Regularity

We first consider the case when the domain $\mathrm{D} \subset \mathbb{R}^n$ is a bounded, connected subdomain of the euclidean space $\mathbb{R}^n$, $n \geq 2$. We then present two extensions: first, to strongly elliptic pseudodifferential operators on smooth, closed, compact n-manifolds $\mathcal{M} \subset \mathbb{R}^{n+1}$ and second, to classical pseudodifferential operators with Gevrey-class symbols. "Asymptotic smoothness" of covariance functions, in the sense of [3, Chap. 4.3], which is required for log-linear with respect to N $\mathcal{H}$-matrix formatted covariance approximations, is obtained only for the analytic class in Section 3.3 ahead. With a straightforward generalization of the approximation arguments in [3, Chap. 4], analogous results with slightly larger complexity (high powers of $\log N$) hold also for Gevrey regular covariances K_u.

The outline of this section is as follows: we first present a basic regularity result in a bounded domain $\mathrm{D} \subset \mathbb{R}^n$ in Section 3.1. We then generalize it to pseudodifferential operators A on smooth, Riemannian n-manifolds $\mathcal{M}$, using the calculus of (classical) pseudodifferential operators on $\mathcal{M}$ in Section 3.2. Finally, in Section 3.3 we generalize both types of result to the Gevrey and the analytic class, using essentially the same arguments in the calculi of [4] and [34, Chap. III].

3.1 Euclidean Domains

We consider the equation (1.1) in a bounded domain D with smooth boundary $\partial\mathrm{D}$, and with the operator A in (1.1) being a linear, strongly elliptic (pseudo-) differential operator with smooth coefficients.

Theorem 1 *Consider the tensorized equation* (1.3) *with boundedly invertible and properly supported* $A \in OPS_{cl}^{r}(\mathrm{D})$, $r \in \mathbb{R}$, *in the smooth, bounded domain* $\mathrm{D} \subset \mathbb{R}^n$. *Assume further that the covariance kernel* K_f *of the random field* $f \in L^2(\Omega, \mathbb{P}; V^\star)$ *in* (1.1) *belongs to* $\Psi\mathrm{hf}_{-\theta-n}(\mathrm{D})$ *for some* $\theta < -n$. *Then, the covariance kernel* K_u *of the random solution* $u \in L^2(\Omega, \mathbb{P}; V)$ *of* (1.3) *belongs to* $\Psi\mathrm{hf}_{-\theta+2r-n}(\mathrm{D})$.

Moreover, the kernel $K_u(x, y)$ *of the covariance operator* $\mathcal{K}_u$ *is smooth in* $\mathrm{D} \times \mathrm{D}$ *outside of the diagonal* $\Delta := \{(x, y) \in \mathrm{D} \times \mathrm{D} : x = y\}$ *and there hold the pointwise estimates*

$$\begin{aligned} &\forall \alpha, \beta \in \mathbb{N}_0^n \ \exists C_{\alpha\beta} : \\ &\qquad |\partial_x^\alpha \partial_y^\beta K_u(x, y)| \leq C_{\alpha\beta}|x - y|^{-(\theta-2r)-n-|\alpha|-|\beta|}, \quad (x, y) \in (\mathrm{D} \times \mathrm{D})\backslash\Delta. \end{aligned} \tag{3.1}$$

In particular, $\mathcal{K}_u = \mathcal{K}_u^\star$ *and* $\mathcal{K}_u \in OPS_{cl}^{\theta-2r}(\mathrm{D})$.

Proof By the Schwartz Kernel Theorem (Proposition 1), we may identify the kernel K_u in a one-to-one fashion with an operator $\mathcal{K}_u$ as follows: since V is a separable Hilbert space, finite linear combinations of dyads $\varphi_x \otimes \varphi_y$ with components tracing a countable orthonormal basis of V are dense in $V \otimes V$. We may therefore write (1.3) in weak form as

$$\langle (A \otimes A) K_u, \varphi_x \otimes \varphi_y \rangle = \langle K_f, \varphi_x \otimes \varphi_y \rangle.$$

Using Proposition 3, it holds $\mathcal{K}_f \in OPS^{\theta}_{cl}(\mathrm{D})$ for the operator corresponding to K_f. Both, $\mathcal{K}_u$ and $\mathcal{K}_f$, satisfy (we omit tagging φ and ψ with their argument variables)

$$(\mathcal{K}_u \varphi, \psi) = \langle K_u, \varphi \otimes \psi \rangle, \quad (\mathcal{K}_f \varphi, \psi) = (K_f, \varphi \otimes \psi), \quad \varphi, \psi \in C_0^{\infty}(\mathrm{D}).$$

Hence, for every $\varphi, \psi \in C_0^{\infty}(\mathrm{D})$ we may write (1.3) in the form

$$\langle K_u, (A \otimes A)^{\star}(\varphi \otimes \psi) \rangle = \langle K_u, (A^{\star}\varphi) \otimes (A^{\star}\psi) \rangle = (\mathcal{K}_u(A^{\star}\varphi), A^{\star}\psi) = ((A \circ \mathcal{K}_u \circ A^{\star})\varphi, \psi) \,.$$

Since φ and ψ were arbitrary, this implies the *composition equation*

$$A \circ \mathcal{K}_u \circ A^{\star} = \mathcal{K}_f \quad \text{in } OPS^{\theta}_{cl}(\mathrm{D}). \tag{3.2}$$

The bounded invertibility of $A \in OPS^{r}_{cl}(\mathrm{D})$ and the algebra of classical pseudodifferential operators in Proposition 2, implies $A^{-1}, (A^{\star})^{-1} \in OPS^{-r}_{cl}(\mathrm{D})$. Then, the assertion $\mathcal{K}_u \in OPS^{\theta-2r}(\mathrm{D})$ follows from this algebra and from the identity

$$\mathcal{K}_u = A^{-1} \circ \mathcal{K}_f \circ A^{-\star} \quad \text{in } \; OPS^{\theta-2r}_{cl}(\mathrm{D}). \tag{3.3}$$

Since the covariance kernel satisfies $K_f \in \Psi\mathrm{hf}_{-\theta-n}(\mathrm{D})$, it holds $\mathcal{K}_f \in OPS^{\theta}_{cl}(\mathrm{D})$ by Proposition 3. Since $A \in OPS^{r}_{cl}(\mathrm{D})$ was assumed to be boundedly invertible, the algebra of (classical) pseudodifferential operators (precisely, items (1),(2) and (3) of Proposition 2) then implies that expression (3.3) holds in $OPS^{\theta-2r}_{cl}(\mathrm{D})$.

The kernel-to-operator correspondence between $\Psi\mathrm{hf}_{-\theta-n}(\mathrm{D})$ and $OPS^{\theta}_{cl}(\mathrm{D})$ implies $K_u \in \Psi\mathrm{hf}_{-\theta+2r-n}(\mathrm{D})$ from where we obtain (3.1) with Proposition 3.

The self-adjointness of $\mathcal{K}_u$ follows from the assumption that $\mathcal{K}_f = \mathcal{K}_f^{\star}$ by transposing (3.3). □

Remark 1 The assertion on self-adjointness of $\mathcal{K}_u$ does *not* require that A is self-adjoint, as is immediate from the structure of the composition equation (3.2).

Remark 2 The assumption that A be properly supported is not restrictive: each $A \in OPS^{r}(\mathrm{D})$ can be decomposed at $A = A_0 + R$ with $A_0 \in OPS^{r}(\mathrm{D})$ properly supported and a smoothing operator R (cp. [26, Prop. 18.1.22]).

Remark 3 In Theorem 1, we assumed that $\partial\mathrm{D}$ is smooth. In the case when $\partial\mathrm{D}$ is only piecewise smooth, ie. when the domain D exhibits corners (in dimensions $n = 2, 3$) and edges (in dimension $n = 3$), additional singularities may arise. For example, the inverse A^{-1} of *elliptic differential operators* A is well-known to introduce singularities in the solution u which are concentrated at the geometric "singularity set" $\mathrm{S} \subseteq \partial\mathrm{D}$ (see, eg., [13]). Such geometric singularities introduced by the solution operator A^{-1} imply correspondingly larger singular supports for K_u. This is evident from the following argument where we assume that A is a second order, boundedly invertible elliptic differential operator with corresponding

Dirichlet or Neumann boundary conditions. We denote by $G_A(x,\xi)$ the Green's function for the corresponding boundary value problem in D, so that in (1.1) the random solution can be represented formally, for $x \in \mathrm{D}$ and for $\omega \in \Omega$, by the convolution (in the sense of distributions) $u(x;\omega) = G_A(x,\xi) *_\xi f(\xi;\omega)$. Here, the notation $*_\xi$ denotes convolution with respect to the variable ξ. Denote by $G_A^\star(\xi', x')$ the Green's function for the corresponding boundary value problem for the adjoint $A^\star$ of A. Then, given a distributional covariance kernel $K_f(\xi, x')$, we obtain from the composition equation (3.3) the identity

$$K_u(x,x') = G_A^\star(x,\xi) *_\xi K_f(\xi,\xi') *_{\xi'} G_A(\xi', x') \tag{3.4}$$

which holds in the sense of distributions. The theorem on singular supports for convolutions of distributions then implies

$$\operatorname{sing\,supp}(K_u) \subseteq \Delta \cup (\mathrm{S}\times\mathrm{D}) \cup (\mathrm{D}\times\mathrm{S}) \cup (\mathrm{S}\times\mathrm{S}). \tag{3.5}$$

3.2 Operators on Manifolds

We consider next the case that the operator A in (1.1) is a classical pseudodifferential operator on a smooth, closed and compact Riemannian n-manifold $\mathcal{M} \subset \mathbb{R}^{n+1}$. Since $\mathcal{M}$ is assumed closed, $\partial\mathcal{M} = \emptyset$ and in particular $\mathrm{S} = \emptyset$ in Remark 3. This case arises in boundary reduction of elliptic boundary value problems in smooth, bounded domains in $\mathbb{R}^{n+1}$ in which case $\mathcal{M}$ denotes the smooth, compact and Riemannian boundary n-manifold. It is also relevant in first-order second-moment calculus in shape uncertainty quantification of second order, elliptic boundary value problems (cp. [5,24]), where such boundary reduction is, generically, possible (cp. [27]). As function spaces and operators on $\mathcal{M}$ are defined via local coordinates in a suitable atlas of coordinate charts, the precise regularity of kernels of pseudodifferential operators on $\mathcal{M}$ will depend on whether $\mathcal{M}$ is C^∞, Gevrey or analytic.

To state the analog of Theorem 1 for equation (1.1) on $\mathcal{M}$, we invoke definition and calculus of pseudodifferential operators on $\mathcal{M}$ as exposed, eg. in [41, Chap. II.5] or in [26, Chap. 18]. The assumed compactness of $\mathcal{M}$ implies that there exists a finite atlas of $(\mathcal{M}_i, \kappa_i)$ with smooth co-ordinate charts κ_i which parametrize $\mathcal{M}$. By κ, we denote a generic chart. Pseudodifferential operators on $\mathcal{M}$ are defined locally on $\mathcal{M}$ via charts κ with (generic) common compact parameter domain $\mathrm{D} \subset \mathbb{R}^n$.

Definition 3 ([26, Def. 18.1.20]) On the smooth n-manifold $\mathcal{M} \subset \mathbb{R}^{n+1}$, a linear operator $A : C_0^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$ is a pseudodifferential operator of order r on $\mathcal{M}$ if for every chart κ the transported operator $A^\kappa := (\kappa^{-1})^\star A \kappa^\star \in OPS^r(\mathrm{D})$. We write $A \in OPS^r(\mathcal{M})$.

We require $\mathcal{M}$ to be Riemannian in order to avoid technicalities when we identify functions and distributions with their densities via the Schwartz kernel theorem. We call $A \in OPS^r(\mathcal{M})$ *classical* if for each chart $A^\kappa \in OPS^r_{cl}(\kappa(\mathrm{D}))$. In this case, we write $A \in OPS^r_{cl}(\mathcal{M})$.

Theorem 2 *Consider the tensorized equation* (1.3) *with boundedly invertible and properly supported $A \in OPS^r_{cl}(\mathcal{M})$, $r \in \mathbb{R}$, in the smooth, compact Riemannian n-manifold $\mathcal{M} \subset \mathbb{R}^{n+1}$. Assume further that, for every chart κ, the covariance kernel $(\kappa^{-1})^\star K_f \kappa^\star$*

of the random field $f \in L^2(\Omega, \mathbb{P}; V^\star)$ *in* (1.1) *belongs to* $\Psi\mathrm{hf}_{-\theta-n}(\kappa(\mathrm{D}))$ *for some* $\theta < -n$*. Then, for every chart* κ*, the covariance kernel* $(\kappa^{-1})^\star K_u \kappa^\star$ *of the random solution* $u \in L^2(\Omega, \mathbb{P}; V)$ *of* (1.3) *belongs to* $\Psi\mathrm{hf}_{-\theta+2r-n}(\kappa(\mathrm{D}))$*. Moreover, in the parameter domain* $\mathrm{D} \subset \mathbb{R}^n$*, the kernels* $(\kappa^{-1})^\star K_u \kappa^\star$ *of the covariance operator* $\mathcal{K}_u$ *in local coordinates are smooth in* $\mathrm{D} \times \mathrm{D}$ *outside of the diagonal* $\Delta := \{(x, y) \in \mathrm{D} \times \mathrm{D} : x = y\}$ *and there hold the pointwise estimates* (3.1)*. In particular,* $\mathcal{K}_u = \mathcal{K}_u^\star$ *and* $(\kappa^{-1})^\star \mathcal{K}_u \kappa^\star \in OPS_{cl}^{\theta-2r}(\mathrm{D})$*.*

3.3 Analytic Regularity of K_u

The preceding results made strong use of pseudodifferential calculus which is based on statements modulo smooth (ie. C^∞) functions. On the one hand, this allows to use localization arguments via smooth partitions of unity, for example, on the other hand necessarily entails a certain loss of quantitative control of derivatives; in particular, in (3.1) the dependence of the constants $C_{\alpha\beta}$ on the differentation orders α, β remains unspecific. It is well known, however, that to obtain *exponential convergence bounds* for locally piecewise polynomial approximations of $K_u(x, y)$, *analytic or at least Gevrey regularity* of covariance functions is necessary. We refer to [32, 33] for a complete discussion of such approximations, albeit in a rather special setting. There, estimates (3.1) were established with explicit control of the dependence of $C_{\alpha\beta}$ in α and β. It turns out that, in the present rather general setting, an analogous result can be established using an analytic calculus of pseudodifferential operators, from [4], see also [34].

Theorem 3 *In either the euclidean domain* D *with analytic boundary* $\partial\mathrm{D}$ *or on a closed, analytic* n*-manifold* $\mathcal{M} \subset \mathbb{R}^{n+1}$*, assume that the covariance kernel* K_f *of the second order random field* f *in* (1.1) *gives rise to an operator* $\mathcal{K}_f \in OPS_{cl,s}^{\theta}$*, ie. to a classical pseudodifferential operator with symbol* $a_f(x, \xi)$ *of order* θ *and of Gevrey class* $s \geq 1$ *in the sense of [4, Def. 1.1]. Assume further that the operator* $A \in OPS_{cl,s}^{r}$ *is properly supported. Then, the covariance kernel* K_u *of the random field solution* u *of* (1.1) *is the Schwartz kernel of an operator* $\mathcal{K}_u \in OPS_{cl,s}^{\theta-2r}$*. In particular, the constants* $C_{\alpha\beta}$ *which appear in* (3.1) *can be bounded by*

$$\forall \alpha, \beta \in \mathbb{N}_0^n : \quad C_{\alpha\beta} \leq c A^{|\alpha+\beta|} (|\alpha|!)^s \beta! \tag{3.6}$$

for some constants c*,* A *depending only on* D*,* $\mathcal{M}$*, and on* a_f*.*

Proof In either case, the proof is analogous to that of Theorem 1 in the C^ω case. We start from (3.3) and use the corresponding calculus. Specifically, for Gevrey class regular surfaces, $s > 1$, and items (2), (4) and (5) of Proposition 2 imply the result, by (Gevrey-regular) partitions of unity and by transporting (1.1) to an euclidean reference domain via Gevrey-regular coordinate charts. The assertion then follows from the "euclidean" version of the result, Theorem 1.

In the analytic class, ie. when $s = 1$, localization and partitions of unity are not available. Here, we assume a global analytic parametrization, and again rely on items (2), (4) and (5) of Proposition 2; to conclude, we must invoke, however, Proposition 4, whose use entails the requirement that A is properly supported on $\mathcal{M}$ which, by Remark 2 is not restrictive, at least in the smooth class. □

3.4 Spectral Asymptotics

In several applications (polynomial chaos expansions, N-term approximation rates, error analysis of approximate Cholesky factorizations of covariance matrices) spectral asymptotics of $\mathcal{K}_u$ are of interest. This is due to the computational cost of the rank-truncated approximate Cholesky decomposition of discretizations of $\mathcal{K}_u$ is determined by the decay of its eigenvalues, see eg. [22] and the reference therein. Since $\mathcal{K}_u = \mathcal{K}_u^\star$ and $\mathcal{K}_f = \mathcal{K}_f^\star$, general spectral asymptotics for elliptic, self-adjoint pseudodifferential operators (eg. [40]) apply.

Theorem 4 *Assume $\mathcal{K}_f \in OPS^\theta_{cl}$ and $A \in OPS^r_{cl}$ with $\theta < 2r$. Then, either on a smooth and closed, compact n-manifold $\mathcal{M} \subset \mathbb{R}^{n+1}$ or on a bounded domain $\mathrm{D} \subset \mathbb{R}^n$ with smooth boundary $\partial\mathrm{D}$, the covariance operator $\mathcal{K}_u$ of the random field solution u of (1.1) has a discrete spectrum with at most countably many real eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq 0$, enumerated in decreasing order, which may only accumulate at zero. Moreover, there holds the spectral asymptotics*

$$\lambda_k \sim k^{(\theta-2r)/n} \quad \text{as } k \to \infty. \tag{3.7}$$

Proof Consider the case of an operator in the bounded domain D and set $m := \theta - 2r$. By assumption, $m < 0$. We already showed in the proof of Theorem 1 that $\mathcal{K}_u \in OPS^r_{cl}(\mathrm{D})$ and that $\mathcal{K}_u$ is self-adjoint. The mapping properties of OPS^r_{cl} imply $\mathcal{K}_u : L^2(\mathrm{D}) \to H^{-m}(\mathrm{D})$ continuously. Since D is smooth and bounded, the condition $m < 0$ implies in view of Rellich's theorem that the injection $\iota : H^{-m}(\mathrm{D}) \hookrightarrow L^2(\mathrm{D})$ is compact, and therefore the composition $\iota \circ \mathcal{K}_u : L^2(\mathrm{D}) \to L^2(\mathrm{D})$ is a compact, self-adjoint operator. The spectral theorem for such operators implies the existence of a countable family $(\lambda_k, \varphi_k)_{k\geq 1}$ of eigenpairs with real eigenvalues accumulating only at zero, and with the eigenfunctions $\{\varphi_k\}_{k\geq 1} \subset H^{-m}(\mathrm{D})$ forming an orthonormal basis of $L^2(\mathrm{D})$. The spectral asymptotics (3.7) then follows from the Weyl calculus for pseudodifferential operators (cp. eg. [40, Thm. 15.2]). The argument for a smooth, closed and compact Riemannian n-manifold $\mathcal{M} \subset \mathbb{R}^{n+1}$ is analogous. □

4 $\mathcal{H}$-matrix Accelerated Solution of Second Moment Equations

4.1 Galerkin Discretization of the Covariance Equation

We shall discuss the efficient numerical solution of (1.3) by means of a Galerkin scheme. To that end, we introduce a finite element space $V_N = \mathrm{span}\{\varphi_1, \ldots, \varphi_N\} \subset V$. It is assumed that the mesh which underlies this finite element space is quasi-uniform. The basis functions $\{\varphi_i\}$ are assumed to be locally and isotropically supported, so that $\mathrm{diam}(\mathrm{supp}\,\varphi_i) \sim N^{-1/n}$. In particular, we can assign to each degree of freedom $i \in \{1, \ldots, N\}$ a suitable point $x_i \in \mathrm{D}$ or $x_i \in \mathcal{M}$, eg. the barycenter of the support of the corresponding basis function or the corresponding Lagrangian interpolation point if nodal finite element shape functions are used.

The set of tensor product basis functions $\{\varphi_i \otimes \varphi_j\}_{i,j}$ forms a basis of the tensor product finite element space $V_N \otimes V_N \subset V \otimes V$. Thus, making the ansatz

$$K_u(x,y) \approx \sum_{i,j} [\mathbf{K}_u]_{i,j} (\varphi_i \otimes \varphi_j)(x,y) \in V_N \otimes V_N,$$

the Galerkin system for (1.3) reads

$$(\mathbf{A} \otimes \mathbf{A}) \operatorname{vec}(\mathbf{K}_u) = \operatorname{vec}(\mathbf{K}_f) \quad \Longleftrightarrow \quad \mathbf{A}\mathbf{K}_u\mathbf{A}^\star = \mathbf{K}_f, \tag{4.1}$$

where

$$\mathbf{A} := \left[\int_{\mathrm{D}} (A\varphi_j)(x)\varphi_i(x)\mathrm{d}x \right]_{i,j}, \quad \mathbf{K}_f := \left[\int_{\mathrm{D}} \int_{\mathrm{D}} K_f(x,y)\varphi_i(x)\varphi_j(y)\mathrm{d}x\mathrm{d}y \right]_{i,j}.$$

(4.1) is a linear system of equations for N^2 unknowns and thus not directly solvable if N is large due to memory and time consumption.

$\mathcal{H}$-matrices (eg. [3,15]) rely on local low-rank approximations of a given matrix $\mathbf{X} \in \mathbb{R}^{N\times N}$. For suitable index sets $\nu, \nu' \subset \{1,\dots,N\}$, a matrix block $\mathbf{X}|_{\nu\times\nu'}$ can be approximated by a rank-k matrix. This approximation can be represented in factorized form $\mathbf{X}|_{\nu\times\nu'} \approx \mathbf{Y}\mathbf{Z}^\star$ with factors $\mathbf{Y} \in \mathbb{R}^{\#\nu\times k}$ and $\mathbf{Z} \in \mathbb{R}^{\#\nu'\times k}$. Hence, if $k \ll \min\{\#\nu, \#\nu'\}$, the complexity for storing the block is considerably reduced. The construction of the index sets is based on the *cluster tree*.

4.2 Cluster Tree

A *cluster* ν is defined as the nonempty union of indices $\nu = \{i_1,\dots,i_k\} \subset \{1,2,\dots,N\}$. It is called the *father cluster* of ν', which will be denoted by $\nu' \prec \nu$, if $\nu' \subsetneq \nu$ and no further cluster ν'' exists with $\nu' \subsetneq \nu'' \subsetneq \nu$. The cluster ν' is then called a *son cluster* of ν. If we order these clusters hierarchically concerning the father-son relation "$\prec$" we arrive at a tree structure, the so-called cluster tree $\mathcal{T}$.

We shall specify some properties of the cluster tree $\mathcal{T}$ in more detail:

- The set $\{1,\dots,N\}$ is the root of $\mathcal{T}$.
- If the cluster ν is a leaf, then $\#\nu \le C_{\mathrm{leaf}}$, ie. the leaves consist of a relatively small number of indices.
- If the cluster ν is not a leaf, then it is the disjoint union of its two son clusters.
- The cluster ν belongs to the *level* j if there exist j clusters $\{\nu_i\}_{i=0}^{j-1}$ such that

$$\nu \prec \nu_{j-1} \prec \cdots \prec \nu_0 = \{1,\dots,N\}.$$

The root $\{1,\dots,N\}$ of the cluster tree is of the level 0 and J is the maximal level. We denote the k-th cluster of the level j by $\nu_{j,k}$.

The construction of the cluster tree is based on the *support* of the clusters. The support Υ_ν of a cluster ν is defined as the union of the supports of the basis functions corresponding to its elements, that is

$$\Upsilon_\nu = \bigcup_{i\in\nu} \Upsilon_i \quad \text{where } \Upsilon_i := \operatorname{supp}\varphi_i \text{ for all } i \in \{1,\dots,N\}.$$

For computing complexity bounds, the cluster tree should match the following additional requirements, uniformly as N goes to ∞:

- The cluster tree is a balanced binary tree in the sense that the maximal level satisfies $J \sim \log_2 N$ and the number of sons of the clusters $\nu_{j,k}$ is two whenever the cluster is not a leaf.

– The diameter of the support $\Upsilon_{\nu_{j,k}}$ is local with respect to the level j, ie. $\operatorname{diam}\Upsilon_{\nu_{j,k}} \sim 2^{-j/n}$. Moreover, the number $\#\nu_{j,k}$ of indices contained in a cluster $\nu_{j,k}$ on level j scales approximately like 2^{J-j}, ie. $\#\nu_{j,k} \sim 2^{J-j}$.

The cluster tree $\mathcal{T}$ with the indicated terms should be given for our further considerations. A common algorithm for its construction is based on a hierarchical subdivision of the point set which is associated with the basis functions. We begin by embedding the point set $\{x_1, \ldots, x_N\}$ in a top-level cuboid. This cuboid is subsequently subdivided into two cuboids which contain the same number of points and this process is iterated until a cuboid encloses less than a predetermined number of points.

4.3 $\mathcal{H}$-Matrix Approximation

$\mathcal{H}$-matrices have been invented in [14,17] and are a generalization of cluster techniques for the rapid solution of boundary integral equations such as the fast multipole method [11], the mosaic skeleton approximation [42], or the adaptive cross approximation [1]. $\mathcal{H}$-matrix techniques apply to discretized operators whenever the underlying kernel functions are asymptotically smooth (cp. [3, Def. 4.5]).

Definition 4 A kernel function K is called *asymptotically smooth* if there exists $C > 0$ such that for every $(x, y) \in (\mathrm{D} \times \mathrm{D})\backslash\Delta$ and for every $\alpha, \beta \in \mathbb{N}_0^n$ holds

$$\left|\partial_x^\alpha \partial_y^\beta K_u(x,y)\right| \leq C \frac{|\alpha|!|\beta|!}{r^{|\alpha|+|\beta|}} |x-y|^{-|\alpha|-|\beta|} |K(x,y)| \,. \tag{4.2}$$

As an immediate consequence of Theorems 1 and 2, we conclude the following

Proposition 5 *If $X \in OPS^r_{cl,1}(\mathrm{D})$ for some $r \in \mathbb{R}$, then the Schwartz kernel of X is asymptotically smooth in the sense of Definition 4.*

For the discretization of a pseudodifferential operator with asymptotically smooth kernel, we introduce a partition of its domain of definition which separates smooth and non-smooth areas of the kernel function. This is based on the following

Definition 5 Two clusters ν and ν' are called *η-admissible* if

$$\max\{\operatorname{diam}(\Upsilon_\nu), \operatorname{diam}(\Upsilon_{\nu'})\} \leq \eta \operatorname{dist}(\Upsilon_\nu, \Upsilon_{\nu'}) \tag{4.3}$$

holds for some fixed $\eta > 0$.

We shall consider admissible blocks only for cluster-cluster combinations where both clusters are of the same level and thus of similar size. Due to this reasoning, we obtain the list of admissible blocks by means of a recursive algorithm: Starting with the root $(\nu_{0,0}, \nu_{0,0})$, the current cluster pair is checked for admissibility and, if admissible, added to the set $\mathcal{F}$ storing the operator's *farfield*. Otherwise, the admissibility check will be performed on all possible pairs of son clusters of the two original clusters. When we arrive at a pair of inadmissible leaf clusters, it is added to the set $\mathcal{N}$ storing the operator's *nearfield*. This scheme provides us with a so-called *block cluster tree* $\mathcal{B} = \mathcal{F} \cup \mathcal{N}$, cp. [15].

With the definition of the block-cluster tree at hand, we are finally in the position to introduce $\mathcal{H}$-matrices.

Definition 6 The set $\mathcal{H}(\mathcal{B},k)$ of $\mathcal{H}$-matrices of maximal block rank k is defined according to

$$\mathcal{H}(\mathcal{B},k) := \big\{\mathbf{X}\in\mathbb{R}^{N\times N} : \operatorname{rank}(\mathbf{X}|_{\nu\times\nu'})\leq k \text{ for all } (\nu,\nu')\in\mathcal{F}\big\}.$$

Note that all nearfield blocks $\mathbf{X}|_{\nu\times\nu'}$, $(\nu,\nu')\in\mathcal{N}$, are allowed to be full matrices.

In accordance with [15], the storage cost of an $\mathcal{H}$-matrix $\mathbf{X}\in\mathcal{H}(\mathcal{B},k)$ is $\mathcal{O}(kN\log N)$ where for asymptotically smooth kernel functions $K_u(x,y)$ in the sense of eg. [3, Chap. 4] the rank k depends logarithmically on the approximation accuracy and thus on N; this implies in particular that $\mathcal{H}$-matrix formatted approximations of K_u belonging to either the analytic or the Gevrey class achieve accuracy vs. work and memory which is log-linear in N, the number of degrees of freedom used in the physical domain D, even in the presence of the singular support Δ. This, in effect, settles the curse of dimensionality in the approximation of singular covariance kernel functions. These remarks pertain to *covariance approximation* of a given, asymptotically smooth covariance kernel function K, such as K_f in (1.3). A second, more delicate, issue is the *covariance computation* of an implicitly given covariance kernel, such as K_u in (1.3). Approximate, numerical solutions of (1.3) are necessary which account for the asymptotic smoothness of the data and solution at all stages of the computation. To this end, an $\mathcal{H}$-formatted approximate matrix calculus has been developed in [15] and the references there.

4.4 $\mathcal{H}$-Matrix Arithmetic

An important feature of $\mathcal{H}$-matrices is that efficient algorithms for approximate matrix arithmetic operations are available. The approximate matrix-matrix addition in $\mathcal{H}(\mathcal{B},k)$ can be performed in $\mathcal{O}(k^2N\log N)$ operations while the approximate matrix-matrix multiplication can be performed in $\mathcal{O}(k^2N\log^2 N)$ operations. Moreover, employing the recursive block structure, the approximate inversion or the approximate computation of the LU-decomposition within $\mathcal{H}(\mathcal{B},k)$ can also be performed in only $\mathcal{O}(k^2N\log^2 N)$ operations. We refer the reader to [3,10,15,16] for further results and implementation details.

4.5 Fast Solution of Second Moment Equations

Comparing (4.2) with (3.1) and (3.6), we see that verification of asymptotic smoothness for the covariance kernel K_u requires asymptotic smoothness of K_f and an analytic pseudodifferential calculus as reviewed in Section 3.3. More precisely, according to Theorem 3, it follows that $K_u\in OPS^{\theta-2r}_{cl,1}$ if $\mathcal{K}_f\in OPS^{\theta}_{cl,1}$, $A\in OPS^{r}_{cl,1}$ provided that A is properly supported. In particular, it follows from the analytic parametrix construction given in [34, Chap. III] for analytic, elliptic differential operators that strongly elliptic differential operators with constant or analytic coefficients provide asymptotically smooth fundamental solutions which is preserved under boundary reduction on analytic boundary manifolds $\mathcal{M}$. As a consequence, in that case, all matrices in (4.1) can be represented by $\mathcal{H}$-matrices. This reduces the memory consumption to $\mathcal{O}(kN\log N)$ where k depends logarithmically on the approximation accuracy ε. Applying the $\mathcal{H}$-matrix arithmetic, the solution $\mathbf{K}_u$ to (4.1) can thus be computed within $\mathcal{O}(k^2N\log^2 N)$ operations.

A possible realization relies on the solution of the linear system (4.1) of equations by iterative refinement, cp. [9,43]. To that end, let $\hat{\mathbf{A}}^{-1}$ denote an approximate inverse to $\mathbf{A}$. Then, starting with the initial guess $\mathbf{K}_u^{(0)} = \hat{\mathbf{A}}^{-1}\mathbf{K}_f\hat{\mathbf{A}}^{-\star}$, the solution to (4.1) can be approximated via the iteration

$$\boldsymbol{\Theta}^{(i)} = \mathbf{K}_f - \mathbf{A}\mathbf{K}_u^{(i)}\mathbf{A}^\star, \quad \mathbf{K}_u^{(i+1)} = \mathbf{K}_u^{(i)} + \hat{\mathbf{A}}^{-1}\boldsymbol{\Theta}^{(i)}\hat{\mathbf{A}}^{-\star}, \quad i = 0, 1, \dots.$$

For details on the implementaton with $\mathcal{H}$-formatted matrix arithmetic we refer the reader to [7]. There, this approach has been realized for the computation of potentials with random boundary trace.

5 Numerical Results

5.1 Problem Formulation

Given a bounded domain $\mathrm{D} \subset \mathbb{R}^3$ with smooth boundary $\mathcal{M} := \partial\mathrm{D}$ and a probability space $(\Omega, \Sigma, \mathbb{P})$, we consider the Dirichlet problem

$$\left.\begin{aligned} \Delta u(\omega, x) &= 0 && \text{for } x \in \mathrm{D} \\ u(\omega, x) &= f(\omega, x) && \text{for } x \in \mathcal{M} \end{aligned}\right\} \quad \mathbb{P}\text{-almost surely} \tag{5.1}$$

with random Dirichlet data $f \in L^2_{\mathbb{P}}\big(\Omega, H^{1/2}(\mathcal{M})\big) \cong L^2_{\mathbb{P}}(\Omega) \otimes H^{1/2}(\mathcal{M})$ where $\otimes$ denotes the Hilbertian tensor product. For given mean $\mathbb{E}[f]$ and covariance K_f of the Dirichlet data, we shall compute the solution's mean and covariance which satisfy

$$\Delta\mathbb{E}[u] = 0 \text{ in } \mathrm{D} \quad \text{and} \quad \mathbb{E}[u] = \mathbb{E}[f] \text{ on } \mathcal{M} \tag{5.2}$$

and

$$\begin{aligned} (\Delta \otimes \Delta)K_u &= 0 && \text{in } \mathrm{D} \times \mathrm{D}, \\ (\Delta \otimes \mathsf{id})K_u &= 0 && \text{on } \mathrm{D} \times \mathcal{M}, \\ (\mathsf{id} \otimes \Delta)K_u &= 0 && \text{on } \mathcal{M} \times \mathrm{D}, \\ K_u &= K_f && \text{on } \mathcal{M} \times \mathcal{M}. \end{aligned} \tag{5.3}$$

Given a density $\rho \in H^{-1/2}(\mathcal{M})$, the single-layer potential

$$\tilde{S} : H^{-1/2}(\mathcal{M}) \to H^1(\mathrm{D}), \quad (\tilde{S}\rho)(x) := \int_{\mathcal{M}} \frac{\rho(y)}{|x-y|} \mathrm{d}\sigma_y$$

satisfies $\Delta(\tilde{S}\rho) = 0$ in $\mathbb{R}^3 \setminus \mathcal{M}$. For given boundary data $f \in H^{1/2}(\mathcal{M})$, the solution to the corresponding Dirichlet problem is obtained by solving the boundary integral equation

$$(S\rho)(x) := \mathcal{M}_0^{\mathrm{int}}(\tilde{S}\rho)(x) = f(x) \quad \text{for } x \in \mathcal{M}.$$

Here, $\mathcal{M}_0^{\mathrm{int}} : H^1(\mathrm{D}) \to H^{1/2}(\mathcal{M})$ denotes the (interior) trace operator. Hence, the solution $\rho \in L^2_{\mathbb{P}}(\Omega) \otimes H^{-1/2}(\mathcal{M})$ of

$$(\mathsf{id} \otimes S)\rho(\omega, x) = \int_{\mathcal{M}} \frac{\rho(\omega, y)}{|x-y|} \mathrm{d}\sigma_y = f(\omega, x) \tag{5.4}$$

satisfies (5.1). Integrating with respect to the stochastic variable gives, in view of Fubini's theorem, that

$$\int_\Omega (\mathsf{id} \otimes S)\rho(\omega, x)\mathrm{d}\mathbb{P}(\omega) = (S\mathbb{E}[\rho])(x) = \mathbb{E}[f](x) \tag{5.5}$$

and $\mathbb{E}[u] = \tilde{S}\mathbb{E}[\rho]$ is the solution to (5.2). Likewise, by tensorizing (5.4) and by integrating with respect to the stochastic variable, we obtain

$$\int_\Omega (\mathsf{id} \otimes S)\rho(\omega, x)(\mathsf{id} \otimes S)\rho(\omega, y)\mathrm{d}\mathbb{P}(\omega) = (S \otimes S)K_\rho(x, y) = K_f(x, y) \tag{5.6}$$

and $K_u = (\tilde{S} \otimes \tilde{S})K_\rho$ is the solution to (5.3).

The boundary integral equation (5.6) is of the form (1.3) where $A = S$, $K_u = K_\rho$, and $V = H^{-1/2}(\mathcal{M})$. In particular, $S \in OPS^{-1}_{cl,1}(\mathcal{M})$, cp. eg. [27].

5.2 Numerical Computations

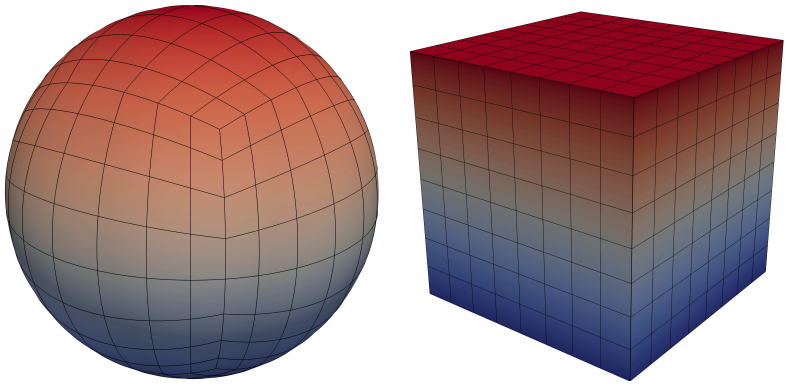

Fig. 2 The surface meshes for the sphere (left) and for the cube (right).

We choose D as the unit ball $\{x \in \mathbb{R}^3 : |x| < 1\}$ and also as the unit cube $(-0.5, 0.5)^3$. To discretize functions on the sphere $\mathcal{M} = \partial\mathrm{D} = \mathbb{S}^2$, we use the space $V_N = \mathrm{span}\{\varphi_1, \dots, \varphi_N\} \subset H^{-1/2}(\mathcal{M})$ of piecewise constant approximations on a regular partition of $\mathcal{M}$. We employ here an exact representation of the particular surface by parametrization via six four-sided patches and do not approximate it by planar panels. The parametrization of the ball's surface is obtained from that of the cube's surface by normalizing each point x by its norm $|x|$, leading again to six patches. The covariance K_f of the Dirichlet data in (5.1) is assumed to be given by the exponential kernel $K_f(x, y) = \exp(-|x - y|)$ which coincides with K_ν in (2.11) for $\nu = 1/2$ In case of the unit ball, the involved operators are all classical pseudodifferential operators. It holds $S \in OPS^{-1}_{cl,1}$ and $\mathcal{K}_f \in OPS^{-3}_{cl,1}$ since $-2\nu - n = 3$ due to $\nu = 1/2$ and $n = 2$, cp. Section 2.3. Hence, we conclude $\mathcal{K}_\rho \in OPS^{-1}_{cl,1}$ in accordance with Theorem 3. Whereas, in case of the unit cube

D, the surface is only piecewise smooth and the regularity theory developed here does not apply, due to singularities concentrated at corners and edges of ∂D, as indicated in Remark 3.

The boundary integral equation (5.6) for the unknown correlation K_ρ is discretized for both surfaces by using $N = 98\,304$ piecewise constant boundary elements on regular, quasiuniform partitions of ∂D into quadrilateral meshes. The mesh on the sphere is obtained from the mesh of the cube's surface by moving a grid point x to the grid point $x/|x|$, see also Figure 2. The Galerkin system (4.1) is solved by the $\mathcal{H}$-matrix arithmetic with very high accuracy as outlined in Section 4.3. Since piecewise constant boundary elements are orthonormal, the matrix $\mathbf{K}_\rho$ is expected to coincide nearly with the directly discretized version of the unknown covariance K_ρ, i.e., with $[(K_\rho\varphi_i, \varphi_j)]_{i,j}$. Next, the matrix $\mathbf{K}_\rho$ is recompressed with different (relative) accuracies ε in order to check its compressibility. This means that we determine an $\mathcal{H}$-matrix $\mathbf{K}_\rho^\varepsilon$ with minimal block rank such that $\|\mathbf{K}_\rho - \mathbf{K}_\rho^\varepsilon\|_F \leq \varepsilon\|\mathbf{K}_\rho\|_F$. The results can be found in Figure 3 for the unit ball on the left hand side and for the unit cube on the right hand side. There, one finds a visualization of the respective $\mathcal{H}$-matrices for $\varepsilon = 10^{-2}$ (top) until $\varepsilon = 10^{-8}$ (bottom), where the rank of the matrix blocks are indicated by color and by the numbers which are inscribed. Notice that the largest blocks are of size $16\,384 \times 16\,384$. The appearance of a self-similar block pattern consisting of six blocks corresponds correspond to the patch-patch interactions of opposite patches of the ball's surface and the cube's surface, respectively. This is clearly visible by the corresponding graph for a square screen, shown in Figure 4.

As expected, the block-ranks increase as ε decreases. Nevertheless, it turns indeed out that $\mathbf{K}_\rho$ can efficiently be approximated by an $\mathcal{H}$-matrix; the slightly larger singular support of K_ρ due to the corners and edges of the cube (cp. Remark 3) causes only marginal increase of ranks.

Finally, we visualize spectra of $\mathcal{H}$-matrix approximations of the involved operators. They are found for the unit ball on the left hand side of Figure 5 and for the unit cube on the right hand side of Figure 5. We observe the expected behaviour $\lambda_k \sim k^{-1/2}$ for the spectrum of the single layer operator and the solution's covariance operator while we observe $\lambda_k \sim k^{-3/2}$ for the input covariance operator $\mathcal{K}_f$. This is validated by the dashed lines which indicate these asymptotics. For the unit ball, the spectra behave thus in agreement with Theorem 4: $S \in OPS^{-1}_{cl,1}$ and $K_f \in OPS^{-3}_{cl,1}$, and Theorem 3 implies $K_u \in OPS^{-1}$. Not covered by the present theory, due to the nonsmoothness of $\partial[0,1]^3$ (cp. Remark 3), the spectra behave nearly the same in this case, indicating that the present results may extend to certain classes of (piecewise analytic) Lipschitz manifolds $\mathcal{M}$.

6 Concluding Remarks

We analyzed $\mathcal{H}$-matrix formatted, deterministic approximations of two-point spatial correlation functions which describe second order statistics of random field solutions of linear operator equations with random forcing, for classical strongly elliptic pseudodifferential operators A, on bounded domains D and on smooth, closed and compact Riemannian n-manifolds $\mathcal{M} \subset \mathbb{R}^{n+1}$ as they arise in boundary reduction of strongly elliptic, linear boundary value problems.

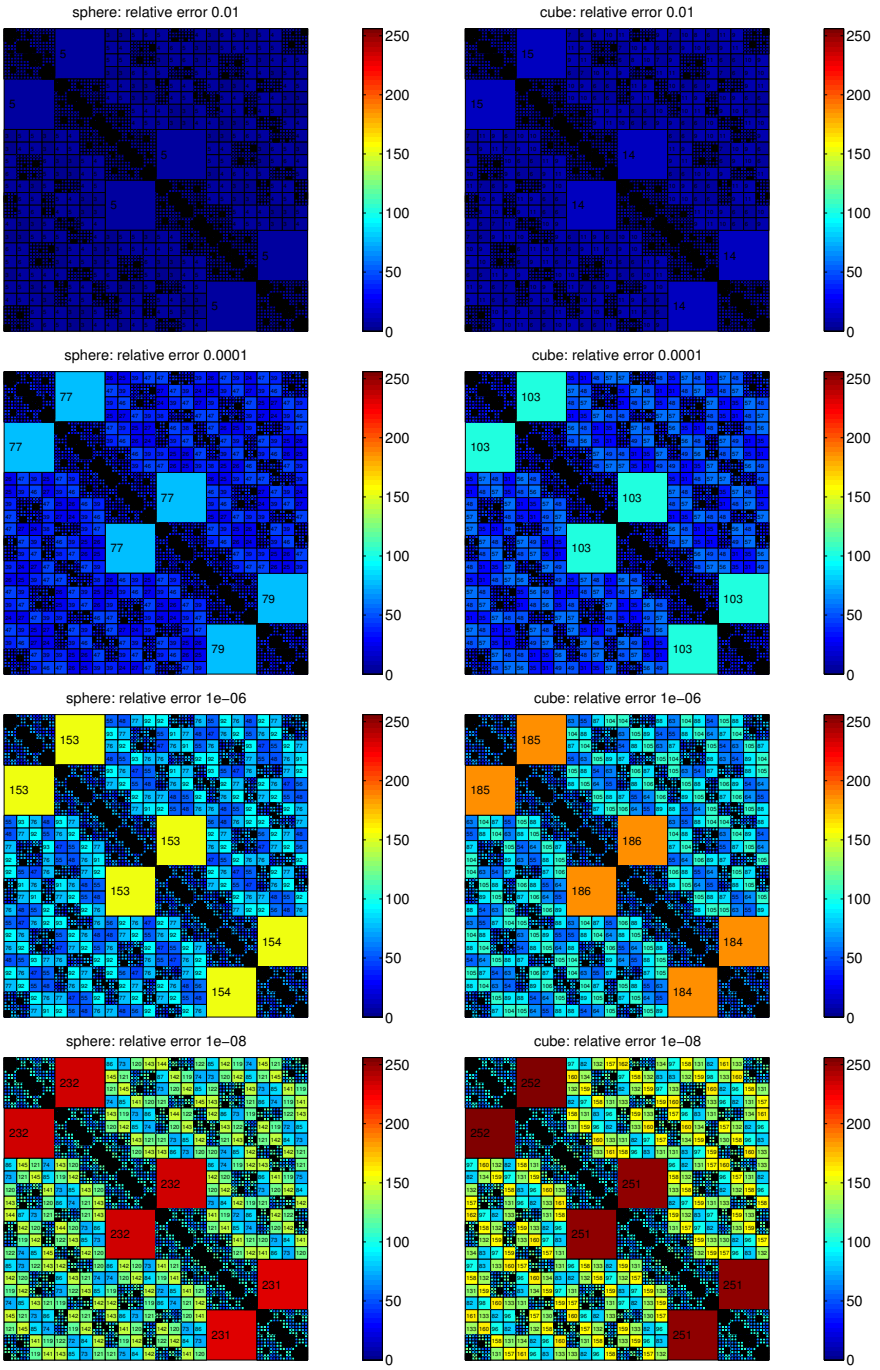

Fig. 3 Ranks of the $\mathcal{H}$-matrix representations of the solution for different relative accuracies for the sphere (left) and for the cube (right).

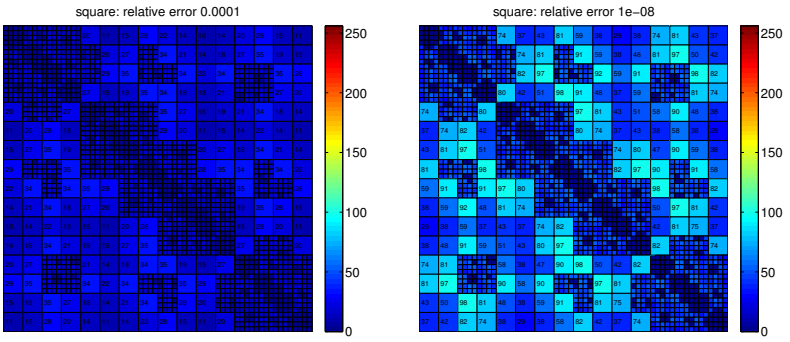

Fig. 4 Ranks of the $\mathcal{H}$-matrix representations of K_ρ for different relative accuracies for the screen. Relative accuracy 10^{-4} (left) and 10^{-8} (right).

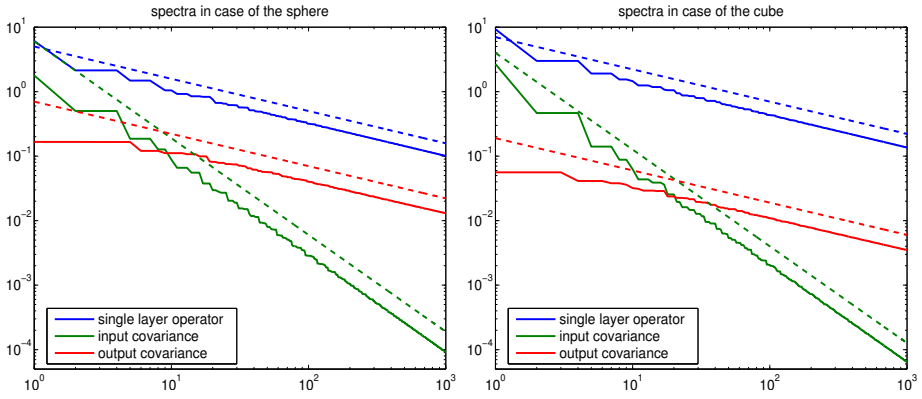

Fig. 5 Spectral decay of the single layer operator, the input covariance operator and the output covariance operator for the sphere (left) and for the cube (right).

Computational efficiency of the direct numerical solution of the deterministic tensor equation (1.3) is hampered by doubling the dimension of the spatial variables. For smooth covariance functions, sparse tensor product approximations were shown in [36,37] to recover log-linear complexity with respect to N, the number of unknowns in D used to discretize A. In many applications, however, there arise random fields with low spatial path regularity which, in turn, entail two-point correlation functions which are singular on the diagonal $\{x = y\}$ of $\mathrm{D} \times \mathrm{D}$ (resp. of $\mathcal{M} \times \mathcal{M}$), but which are smooth (even Gevrey regular) on $(\mathrm{D} \times \mathrm{D})\backslash\{x = y\}$. For such functions, $\mathcal{H}$-matrix formatted, deterministic approximations are known to converge again in essentially linear complexity. We proved that two-point correlation functions in second order statistics of random field solutions of pseudodifferential equations generically exhibit the same regularity. We also provide a sharp estimate on the singularity strength with respect to the order of the operator and space dimension. The spectral asymptotics of the covariance operators of the implicitly (via operator equation (1.1)) defined random field u was characterized in Theorem 4 likewise in terms of these parameters; this result, apart from being

interesting in itself, is the basis for the numerical analysis of rank truncations and approximate Cholesky covariance factorizations which arise in fast simulation methods (see, eg., [20]). The use of pseudodifferential calculus implies that our results apply to boundary value problems for all linear, elliptic systems of partial differential equations with analytic data as well as to their boundary reductions, as well as to more general, hypoelliptic operators A. The scope of our results is more general: covariances with kernels which have only Gevrey class regularity are covered since proofs of $\mathcal{H}$-matrix rank bounds in [3, Chap. 4] extend to Gevrey regular functions.

Numerical experiments with a strongly elliptic pseudodifferential operator of order -1 confirmed the theoretical results; they indicated, moreover, that the smoothness requirements imposed by the use of pseudodifferential calculus are, most likely, excessive, and could be considerably weakened. Detailed theoretical justification of these observations is beyond the scope of the present article.

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