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Hierarchical Matrix Approximation for the Uncertainty Quantification of Potentials on Random Domains[☆]

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Abstract

Computing statistical quantities of interest of the solution of PDE on random domains is an important and challenging task in engineering. We consider the computation of these quantities by the perturbation approach. Especially, we discuss how third order accurate expansions of the mean and the correlation can numerically be computed. These expansions become even fourth order accurate for certain types of boundary variations. The correction terms are given by the solution of correlation equations in the tensor product domain, which can efficiently be computed by means of \mathcal{H} -matrices. They have recently been shown to be an efficient tool to solve correlation equations with rough data correlations, that is, with low Sobolev smoothness or small correlation length, in almost linear time. Numerical experiments in three dimensions for higher order ansatz spaces show the feasibility of the proposed algorithm. The application to a non-smooth domain is also included.

Keywords: uncertainty quantification, perturbation approach, random domains, hierarchical matrices, boundary element method

2010 MSC: 60H35, 65C30, 65N12, 65N15, 65N38

1. Introduction

The numerical solution of strongly elliptic linear partial differential equations (PDEs) is an important task in science and engineering. It is nowadays well understood and can be accomplished up to high accuracy, provided that the input data are known exactly. Motivated by tolerances in manufacturing processes and measurement errors, the computation of statistical output functionals of the solution of PDEs on objects with uncertain shapes has recently gained a lot of interest. The domain mapping approach, see e.g. [1, 2, 3], is well suited for modelling large variations in the domain, but usually leads to high-dimensional and costly integration problems, which suffer from the curse of dimensionality. The perturbation approach, see e.g. [4, 5, 6, 7], is motivated by small disturbances in manufacturing processes and models uncertain small deformations under the following view point. Notice that both approaches have recently been combined in [8].

Given a reference domain D_0 , the random domains $D_\varepsilon(\omega)$ are defined by the perturbation of the reference domain's boundary in some ε tube, leading to the model problem

$$\begin{aligned}\Delta u_\varepsilon(\omega) &= 0 && \text{in } D_\varepsilon(\omega), \\ u_\varepsilon(\omega) &= g && \text{on } \partial D_\varepsilon(\omega).\end{aligned}$$

Using shape calculus, cf. [9], and under some smoothness assumptions, the non-linear dependence of the solution $u_\varepsilon(\omega)$ on $D_\varepsilon(\omega)$ can, in a suitable compact subdomain K , be expanded in a Taylor

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expansion in ε , i.e.,

$$u_\varepsilon(\omega) = u_0 + \varepsilon \delta u(\omega) + \frac{\varepsilon^2}{2} \delta^2 u(\omega) + \mathcal{O}(\varepsilon^3) \quad \text{in } K. \quad (1)$$

The zero order term u_0 can directly be computed by solving the deterministic PDE

$$\begin{aligned} \Delta u_0 &= 0 \quad \text{in } D_0, \\ u_0 &= g \quad \text{on } \partial D_0, \end{aligned}$$

on the unperturbed domain. The first and second order correction terms can be computed by solving the very same equation as for the zero order term, but with different boundary conditions.

Based on the Taylor expansion (1), statistical quantities of the solution like the mean

$$\mathbb{E}[u_\varepsilon] = u_0 + \varepsilon \mathbb{E}[\delta u] + \frac{\varepsilon^2}{2} \mathbb{E}[\delta^2 u] + \mathcal{O}(\varepsilon^3) \quad \text{in } K,$$

the covariance

$$\text{Cov}[u_\varepsilon] = \varepsilon^2 \text{Cor}[\delta u] + \mathcal{O}(\varepsilon^3) \quad \text{in } K,$$

and the correlation

$$\text{Cor}[u_\varepsilon] = u_0 \otimes u_0 + \varepsilon^2 \text{Cor}[\delta u] + \frac{\varepsilon^2}{2} \left(u_0 \otimes \mathbb{E}[\delta^2 u] + \mathbb{E}[\delta^2 u] \otimes u_0 \right) + \mathcal{O}(\varepsilon^3) \quad \text{in } K$$

can be expanded into asymptotic expansions in ε . It has already been shown in [7] that the second order correction term $\text{Cor}[\delta u]$ is the solution to a correlation equation in the higher-dimensional product domain $D_0 \times D_0$. While the first and second order correction terms $\mathbb{E}[\delta u]$ and $\mathbb{E}[\delta^2 u]$ of the mean are given as the solution of PDEs on D_0 , the computation of the boundary values for $\mathbb{E}[\delta^2 u]$ has not been investigated yet. We show that they can likewise be obtained by the solution of a correlation equation, but in the product domain $\partial D_0 \times \partial D_0$. As this equation lives solely on the domain boundary, the boundary element method is an obvious discretization method for its solution. Hence, we will use it as a discretization scheme for all occurring equations, omitting the meshing of D_0 . We provide the full convergence analysis for the proposed discretization scheme and slightly relax the assumptions from [7] on the boundary perturbations on our way. Additionally, we remark that the asymptotics can even be up to fourth order accurate, if the law of the prescribed boundary variations behaves in a specific way.

We therefore have to solve two correlation equations in the tensor product domain in order to compute third order accurate approximations in the perturbation amplitude ε . As a naive discretization of these higher dimensional problems, also referred to as the full tensor approach, is prohibitively expensive, the solution of such correlation equations has been the topic of several articles, cf. [5, 7, 10, 11, 12, 13, 14, 15] for example. Except for [5, 11], where a low-rank approximation of the underlying correlation is employed, all of the mentioned approaches rely in some sense on a sparse tensor approximation. Both, low-rank approximations and sparse tensor discretizations, are best suitable if the prescribed correlation is sufficiently smooth, compare [16, 17] for the behaviour of low-rank approximations in dependence of the smoothness, and are known to struggle for ‘‘rough’’ correlations. This means that the prescribed correlation exhibits only minor smoothness assumptions or has a high concentration of measure. While rough correlations do not necessarily have an influence on the convergence rates ([18] discusses an specific example where the rate is reduced), they may have a huge influence on the constants involved in the complexity estimates.

Recently, the hierarchical matrix approach (in short \mathcal{H} -matrix approach) to correlation equations, cf. [18, 19, 20], has been shown to be a promising approach to cope with rough correlations. In the context of correlation equations, \mathcal{H} -matrices provide an alternative compression scheme to represent the full tensor approach and allow the solution of correlation equations in almost linear time. Being introduced in [21, 22], \mathcal{H} -matrices are feasible for the data-sparse representation of (block-) matrices which can be approximated block-wise with low-rank. They have originally been

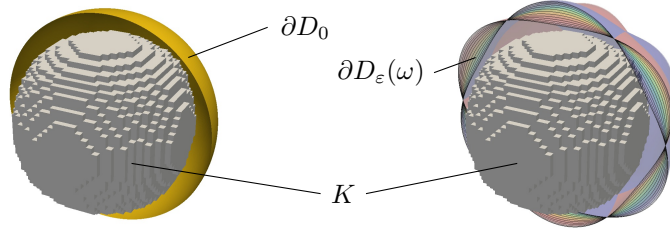


Figure 1: The boundary of the reference domain ∂D_0 , a family of perturbed domains $\partial D_\varepsilon(\omega)$, and the compactum K .

employed for the efficient treatment of boundary integral equations, as they arise in the boundary element method. Nonetheless, they also provide an arithmetic which can be employed for the solution of matrix equations, as they occur from the discretization of correlation equations.

The rest of this article is organized as follows. In Section 2, we derive expansions of the mean, the covariance, and the correlation with respect to the perturbation's amplitude via shape calculus. Section 3 is concerned with the necessary boundary integral equations to allow for a natural treatment of the random perturbations of the boundary. In Section 4, we introduce the corresponding Galerkin discretization, whereas Section 5 is concerned with its error estimation. Section 6 is concerned with the efficient treatment of the derived equations with \mathcal{H} -matrices. We demonstrate the feasibility of the proposed approach by numerical experiments in three spatial dimensions in Section 7. Finally, in Section 8, we draw our conclusions.

2. Random Domains

2.1. Basic definitions

For the following considerations, let $D_0 \subset \mathbb{R}^n$ be a reference domain with, in order to ensure $C^{3,1}$ -continuity of its outer normal, a $C^{4,1}$ -boundary. On a separable, complete probability space $(\Omega, \Sigma, \mathbb{P})$, consider a random vector field $\mathbf{V} \in L^2_{\mathbb{P}}(\Omega; C^{3,1}(\partial D_0, \mathbb{R}^n))$ with $\|\mathbf{V}(\omega, \cdot)\|_{C^{3,1}(\partial D_0)} \lesssim 1$ uniformly for all $\omega \in \Omega$, which perturbs the boundary of the reference domain ∂D_0 in accordance with $\partial D_\varepsilon(\omega) := \partial D_0 + \varepsilon \mathbf{V}(\omega, \partial D_0)$ for some given $\varepsilon > 0$. A new *random domain* $D_\varepsilon(\omega)$ is then given by the interior of the perturbed boundary $\partial D_\varepsilon(\omega)$. For later considerations, we also introduce a compact set K , which is contained in all possible boundary variations and in particular the reference domain, i.e.

$$K \Subset D_0 \cap D_\varepsilon^{\cap \Omega}, \quad D_\varepsilon^{\cap \Omega} := \bigcap_{\omega \in \Omega} D_\varepsilon(\omega).$$

The complete setting of the introduced sets is illustrated in Figure 1.

Note that, in contrast to the domain mapping approach, which requires a vector field on the whole reference domain, the perturbation approach only requires a vector field on the boundary. A correspondence between the two approaches is given by the fact that every vector field on the boundary ∂D_0 can smoothly be extended into the interior of D_0 in such a way that it vanishes on the compactum K .

For all further considerations, let $g \in H^3(D_0 \cup D_\varepsilon^{\cup \Omega})$, where $D_\varepsilon^{\cup \Omega}$ denotes the hold-all domain

$$D_\varepsilon^{\cup \Omega} := \bigcup_{\omega \in \Omega} D_\varepsilon(\omega).$$

Then, it follows $u_0 \in H^3(D_0)$ for the unique solution u_0 of the unperturbed problem

$$\begin{aligned} \Delta u_0 &= 0 && \text{in } D_0, \\ u_0 &= g && \text{on } \partial D_0, \end{aligned} \tag{2}$$

see [23, Theorem 20.4] for example. Here and in the following, the Dirichlet data have to be understood in the trace sense.

2.2. Shape Calculus for Parametrized Domains

We look at the randomly perturbed problem

$$\begin{aligned}\Delta u_\varepsilon(\omega) &= 0 && \text{in } D_\varepsilon(\omega), \\ u_\varepsilon(\omega) &= g && \text{on } \partial D_\varepsilon(\omega),\end{aligned}\tag{3}$$

which is posed on the random domain $D_\varepsilon(\omega)$. Given the reference domain D_0 , one can expand u_ε into a *local shape Taylor expansion*

$$u_\varepsilon(\omega, \mathbf{x}) = u_0(\mathbf{x}) + \varepsilon \delta u[\mathbf{V}(\omega)](\mathbf{x}) + \frac{\varepsilon^2}{2} \delta^2 u[\mathbf{V}(\omega), \mathbf{V}(\omega)](\mathbf{x}) + \mathcal{O}(\varepsilon^3), \quad \mathbf{x} \in K \Subset D_0 \cap D_\varepsilon(\omega),\tag{4}$$

which holds for all $0 < \varepsilon \leq \varepsilon_0$ for some $\varepsilon_0 > 0$ small enough. Here, the *first order local shape derivative* $\delta u[\mathbf{V}(\omega)] \in H^2(D_0)$ is given by

$$\begin{aligned}\Delta \delta u[\mathbf{V}(\omega)] &= 0 && \text{in } D_0, \\ \delta u[\mathbf{V}(\omega)] &= \langle \mathbf{V}(\omega), \mathbf{n} \rangle \frac{\partial(g - u_0)}{\partial \mathbf{n}} && \text{on } \partial D_0,\end{aligned}\tag{5}$$

cf. [9, Chapter 3.1]. Given a second vector field $\mathbf{V}' \in L^2_{\mathbb{P}}(\Omega; C^{3,1}(D_0, \mathbb{R}^n))$ with $\|\mathbf{V}'(\omega, \cdot)\|_{C^{3,1}(D_0)} \lesssim 1$ uniformly for all $\omega \in \Omega$, the *second order local shape derivative* $\delta^2 u[\mathbf{V}(\omega), \mathbf{V}'(\omega)] \in H^1(D_0)$ is given, cf. [24, Theorem 1], by

$$\begin{aligned}\Delta \delta^2 u[\mathbf{V}(\omega), \mathbf{V}'(\omega)] &= 0 && \text{in } D_0, \\ \delta^2 u[\mathbf{V}(\omega), \mathbf{V}'(\omega)] &= \langle \mathbf{H}(g - u_0) \mathbf{V}'(\omega), \mathbf{V}(\omega) \rangle \\ &\quad - \langle \mathbf{V}(\omega), \mathbf{n} \rangle \frac{\partial \delta u[\mathbf{V}'(\omega)]}{\partial \mathbf{n}} \\ &\quad - \langle \mathbf{V}'(\omega), \mathbf{n} \rangle \frac{\partial \delta u[\mathbf{V}(\omega)]}{\partial \mathbf{n}} && \text{on } \partial D_0,\end{aligned}\tag{6}$$

where $\mathbf{H}(\varphi) = [\partial^2 \varphi / \partial x_i \partial x_j]_{i,j}$ denotes the Hessian of φ .

Of course, according to (4), we only need the second order local shape derivative in case of identical fields, i.e., $\mathbf{V} = \mathbf{V}'$. Hence, in order to compute the boundary conditions of the aforementioned equation (6) for $\mathbf{V} = \mathbf{V}'$, it remains to explain how to compute $\langle \mathbf{H}(g - u_0) \mathbf{V}(\omega), \mathbf{V}(\omega) \rangle$ on ∂D_0 . It holds on a C^2 -boundary and for $\varphi \in H^3(D)$, cf. [9, Proposition 2.68],

$$\Delta \varphi = \Delta_\Gamma \varphi + 2\mathcal{H} \frac{\partial \varphi}{\partial \mathbf{n}} + \frac{\partial^2 \varphi}{\partial \mathbf{n}^2} \quad \text{on } \partial D_0,\tag{7}$$

where Δ_Γ denotes the *Laplace-Beltrami operator* and \mathcal{H} denotes the *mean curvature* of ∂D_0 given by $2\mathcal{H} = -\nabla \cdot \mathbf{n}$. Since $u_0 = g$ on ∂D_0 , see (2), we have $\Delta_\Gamma(g - u_0) = 0$, and, since

$$\langle \mathbf{H}(\varphi) \mathbf{V}(\omega), \mathbf{V}(\omega) \rangle = \frac{\partial^2 \varphi}{\partial \mathbf{n}^2} \langle \mathbf{V}(\omega), \mathbf{n} \rangle^2 \quad \text{on } \partial D_0,$$

it holds

$$\langle \mathbf{H}(g - u_0) \mathbf{V}(\omega), \mathbf{V}(\omega) \rangle = \left(\Delta g - 2\mathcal{H} \frac{\partial(g - u_0)}{\partial \mathbf{n}} \right) \langle \mathbf{V}(\omega), \mathbf{n} \rangle^2 \quad \text{on } \partial D_0\tag{8}$$

by the use of (7).

2.3. Statistical Moments on Random Domains

For the following considerations, we can assume without loss of generality that the boundary perturbations are centered, i.e.

$$\mathbb{E}[\mathbf{V}] = \mathbf{0}, \quad \text{and thus formally } \mathbb{E}[D_\varepsilon] = D_0,$$

which is not a restriction, since one can easily recenter the random field by considering $\mathbf{V}' = \mathbf{V} - \mathbb{E}[\mathbf{V}]$. This especially means that the expectation of first order local shape derivative (5) vanishes, which implies

$$\mathbb{E}[u_\varepsilon](\mathbf{x}) = u_0(\mathbf{x}) + \frac{\varepsilon^2}{2}\mathbb{E}[\delta^2 u](\mathbf{x}) + \mathcal{O}(\varepsilon^3), \quad \mathbf{x} \in K \Subset D_\varepsilon^{\cap\Omega}. \quad (9)$$

By tensorizing (4) and integrating over Ω , we further obtain

$$\begin{aligned} \text{Cor}[u_\varepsilon](\mathbf{x}, \mathbf{y}) &= u_0(\mathbf{x})u_0(\mathbf{y}) + \varepsilon^2 \text{Cor}[\delta u](\mathbf{x}, \mathbf{y}) \\ &+ \frac{\varepsilon^2}{2} \left(u_0(\mathbf{x})\mathbb{E}[\delta^2 u](\mathbf{y}) + \mathbb{E}[\delta^2 u](\mathbf{x})u_0(\mathbf{y}) \right) + \mathcal{O}(\varepsilon^3), \quad \mathbf{x}, \mathbf{y} \in K \Subset D_\varepsilon^{\cap\Omega}. \end{aligned} \quad (10)$$

Finally, subtracting (9) from both sides in (4), tensorizing and integrating over Ω yields

$$\text{Cov}[u_\varepsilon](\mathbf{x}, \mathbf{y}) = \varepsilon^2 \text{Cor}[\delta u](\mathbf{x}, \mathbf{y}) + \mathcal{O}(\varepsilon^3), \quad \mathbf{x}, \mathbf{y} \in K \Subset D_\varepsilon^{\cap\Omega}. \quad (11)$$

In order to compute the quantities $\mathbb{E}[u_\varepsilon]$, $\text{Cor}[u_\varepsilon]$, and $\text{Cov}[u_\varepsilon]$, appearing in (9), (10), and (11), we have to solve for $\mathbb{E}[\delta^2 u]$ and $\text{Cor}[\delta u]$. To this end, we combine (6) and (8) to arrive at, see also [7],

$$\begin{aligned} \Delta \mathbb{E}[\delta^2 u[\mathbf{V}, \mathbf{V}]] &= 0 && \text{in } D_0, \\ \mathbb{E}[\delta^2 u[\mathbf{V}, \mathbf{V}]] &= \left(\Delta g - 2\mathcal{H} \frac{\partial(g - u_0)}{\partial \mathbf{n}} \right) \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \Big|_{\mathbf{x}=\mathbf{y}} - 2\mathbb{E} \left[\langle \mathbf{V}, \mathbf{n} \rangle \frac{\partial \delta u[\mathbf{V}]}{\partial \mathbf{n}} \right] && \text{on } \partial D_0. \end{aligned} \quad (12)$$

Next, tensorizing (5) and integrating over Ω yields

$$\begin{aligned} (\Delta \otimes \Delta) \text{Cor}[\delta u] &= 0 && \text{in } D_0 \times D_0, \\ (\Delta \otimes \text{Id}) \text{Cor}[\delta u] &= 0 && \text{on } D_0 \times \partial D_0, \\ (\text{Id} \otimes \Delta) \text{Cor}[\delta u] &= 0 && \text{on } \partial D_0 \times D_0, \\ \text{Cor}[\delta u] &= \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \left(\frac{\partial(g - u_0)}{\partial \mathbf{n}} \otimes \frac{\partial(g - u_0)}{\partial \mathbf{n}} \right) && \text{on } \partial D_0 \times \partial D_0. \end{aligned} \quad (13)$$

The asymptotic expansions for $\mathbb{E}[u_\varepsilon]$, $\text{Cor}[u_\varepsilon]$, and $\text{Cov}[u_\varepsilon]$ can under certain circumstances be improved to fourth order accuracy with help of the following lemma, which is inspired by [6, Lemma 2.3].

Lemma 2.1. *Assume that the boundary perturbations in normal direction are given by an expansion*

$$\langle \mathbf{V}(\omega, \mathbf{x}), \mathbf{n} \rangle = \sum_{i=1}^M \kappa_i(\mathbf{x}) Y_i(\omega),$$

where Y_i , $i = 1, \dots, M$, are i.i.d random variables. Then, it holds

$$\begin{aligned} \delta u_0[\mathbf{V}(\omega)] &= \sum_{i=1}^M \delta u_0[\kappa_i \cdot \mathbf{n}] Y_i(\omega), \\ \delta^2 u_0[\mathbf{V}(\omega), \mathbf{V}(\omega)] &= \sum_{i,j=1}^M \delta^2 u_0[\kappa_i \cdot \mathbf{n}, \kappa_j \cdot \mathbf{n}] Y_i(\omega) Y_j(\omega), \end{aligned}$$

and

$$\delta^3 u_0[\mathbf{V}(\omega), \mathbf{V}(\omega), \mathbf{V}(\omega)] = \sum_{i,j,k=1}^M \delta^3 u_0[\kappa_i \cdot \mathbf{n}, \kappa_j \cdot \mathbf{n}, \kappa_k \cdot \mathbf{n}] Y_i(\omega) Y_j(\omega) Y_k(\omega),$$

provided the third local shape derivative $\delta^3 u$ exists.

Proof. The first two expressions have already been provided in [6, Lemma 2.3], whereas the third one is analogously derived by exploiting the trilinearity of $\delta^3 u_0$. \square

Obviously, due to the independence of the random variables $(Y_i)_{i=1}^M$, it holds

$$\mathbb{E}[\delta^3 u] = \sum_{i=1}^M \delta^3 u_0[\kappa_i \cdot \mathbf{n}, \kappa_i \cdot \mathbf{n}, \kappa_i \cdot \mathbf{n}] \mathbb{E}[Y_i^3] = 0,$$

if the underlying law is symmetric. The expansion of the mean $\mathbb{E}[u_\varepsilon]$ (9) is thus fourth order accurate. Similarly, it holds under the same assumptions

$$\text{Cor}[\delta^2 u, \delta u] = \sum_{i=1}^M \delta^2 u_0[\kappa_i \cdot \mathbf{n}, \kappa_i \cdot \mathbf{n}] \delta u_0[\kappa_i \cdot \mathbf{n}] \mathbb{E}[Y_i^3] = 0.$$

Hence, the expansion for $\text{Cor}[u_\varepsilon]$ (10) becomes fourth order accurate, and, likewise, also the expansion for $\text{Cov}[u_\varepsilon]$ (11) becomes fourth order accurate.

3. Boundary Integral Equations

We shall derive boundary integral equations in this section to compute the asymptotic expansions (9), (10), and (11) for the statistics of the random solution. To this end, observe that the boundary conditions for the PDEs of $\mathbb{E}[\delta^2 u]$ and $\text{Cor}[\delta u]$, (12) and (13), depend on the Neumann data $t^{(u_0)} = \partial u_0 / \partial \mathbf{n}$ of the solution u_0 of the unperturbed problem (2). Having the Dirichlet data g of u_0 at hand, the corresponding Neumann data are given by the *Dirichlet-to-Neumann map*,

$$\mathcal{S}: H^{1/2}(\partial D_0) \rightarrow H^{-1/2}(\partial D_0), \quad \mathcal{S} := \mathcal{V}^{-1} \left(\frac{1}{2} + \mathcal{K} \right), \quad g \mapsto t^{(u_0)}, \quad (14)$$

where the *single layer operator* is given by

$$\mathcal{V}: H^{-1/2}(\partial D_0) \rightarrow H^{1/2}(\partial D_0), \quad (\mathcal{V}\rho)(\mathbf{x}) = \int_{\partial D_0} \frac{\rho(\mathbf{y})}{4\pi\|\mathbf{x} - \mathbf{y}\|} d\sigma_{\mathbf{y}}, \quad \mathbf{x} \in \partial D_0, \quad (15)$$

and the *double layer operator* is given by

$$\mathcal{K}: H^{1/2}(\partial D_0) \rightarrow H^{1/2}(\partial D_0), \quad (\mathcal{K}\rho)(\mathbf{x}) = \int_{\partial D_0} \frac{\langle \mathbf{x} - \mathbf{y}, \mathbf{n}_{\mathbf{y}} \rangle \rho(\mathbf{y})}{4\pi\|\mathbf{x} - \mathbf{y}\|^3} d\sigma_{\mathbf{y}}, \quad \mathbf{x} \in \partial D_0, \quad (16)$$

cf. e.g. [25].

To obtain the second term of the Dirichlet data of $\mathbb{E}[\delta^2 u]$ in (12), we employ that it can be rewritten as the trace of a correlation, call it A ,

$$\mathbb{E} \left[\langle \mathbf{V}, \mathbf{n} \rangle \frac{\partial \delta u[\mathbf{V}]}{\partial \mathbf{n}} \right] = \mathbb{E} \left[\langle \mathbf{V}(\cdot, \mathbf{x}), \mathbf{n}_{\mathbf{x}} \rangle \frac{\partial \delta u[\mathbf{V}(\cdot, \mathbf{y})]}{\partial \mathbf{n}_{\mathbf{y}}} \right] \Big|_{\mathbf{x}=\mathbf{y}} =: A(\mathbf{x}, \mathbf{y}) \Big|_{\mathbf{x}=\mathbf{y}}. \quad (17)$$

The Dirichlet-to-Neumann map and the definition of the first order local shape derivative (5) then yield

$$\begin{aligned} A(\mathbf{x}, \mathbf{y}) &:= \mathbb{E} \left[\langle \mathbf{V}(\cdot, \mathbf{x}), \mathbf{n}_{\mathbf{x}} \rangle \frac{\partial \delta u[\mathbf{V}(\cdot, \mathbf{y})]}{\partial \mathbf{n}_{\mathbf{y}}} \right] \\ &= \mathbb{E} \left[\langle \mathbf{V}(\cdot, \mathbf{x}), \mathbf{n}_{\mathbf{x}} \rangle \mathcal{S} \left(\langle \mathbf{V}(\cdot, \mathbf{y}), \mathbf{n}_{\mathbf{y}} \rangle \left(\frac{\partial g}{\partial \mathbf{n}_{\mathbf{y}}} - t^{(u_0)} \right) \right) \right] \\ &= (\text{Id} \otimes \mathcal{S}) \left(\mathbb{E} \left[\langle \mathbf{V}(\cdot, \mathbf{x}), \mathbf{n}_{\mathbf{x}} \rangle \langle \mathbf{V}(\cdot, \mathbf{y}), \mathbf{n}_{\mathbf{y}} \rangle \right] \left(\mathbb{1} \otimes \left(\frac{\partial g}{\partial \mathbf{n}_{\mathbf{y}}} - t^{(u_0)} \right) \right) \right) \\ &= (\text{Id} \otimes \mathcal{S}) \left(\left(\mathbb{1} \otimes \left(\frac{\partial g}{\partial \mathbf{n}_{\mathbf{y}}} - t^{(u_0)} \right) \right) \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \right). \end{aligned} \quad (18)$$

Given the Dirichlet data of $\mathbb{E}[\delta^2 u]$,

$$g^{\mathbb{E}[\delta^2 u]} = \left(\Delta g - 2\mathcal{H} \frac{\partial(g - u_0)}{\partial \mathbf{n}} \right) \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \Big|_{\mathbf{x}=\mathbf{y}} - 2A \Big|_{\mathbf{x}=\mathbf{y}}, \quad (19)$$

and the corresponding Neumann data

$$t^{\mathbb{E}[\delta^2 u]} = \mathcal{S}g^{\mathbb{E}[\delta^2 u]}$$

of $\mathbb{E}[\delta^2 u]$, the solution $\mathbb{E}[\delta^2 u]$ of (12) can be represented by the representation formula

$$\mathbb{E}[\delta^2 u](\mathbf{x}) = \tilde{\mathcal{V}}\left(t^{\mathbb{E}[\delta^2 u]}\right)(\mathbf{x}) - \tilde{\mathcal{K}}\left(g^{\mathbb{E}[\delta^2 u]}\right)(\mathbf{x}), \quad \mathbf{x} \in D_{\Omega}. \quad (20)$$

Here, the *single layer potential* is given by

$$\tilde{\mathcal{V}}: H^{-1/2}(\partial D_0) \rightarrow H^1(D_0), \quad (\tilde{\mathcal{V}}\rho)(\mathbf{x}) = \int_{\partial D_0} \frac{\rho(\mathbf{y})}{4\pi\|\mathbf{x} - \mathbf{y}\|} d\sigma_{\mathbf{y}}, \quad \mathbf{x} \in D_{\Omega},$$

and the *double layer potential* is given by

$$\tilde{\mathcal{K}}: H^{1/2}(\partial D_0) \rightarrow H^1(D_0), \quad (\tilde{\mathcal{K}}\rho)(\mathbf{x}) = \int_{\partial D_0} \frac{\langle \mathbf{x} - \mathbf{y}, \mathbf{n}_{\mathbf{y}} \rangle \rho(\mathbf{y})}{4\pi\|\mathbf{x} - \mathbf{y}\|^3} d\sigma_{\mathbf{y}}, \quad \mathbf{x} \in D_{\Omega},$$

cf. e.g. [25].

Similarly, given the Dirichlet data of $\text{Cor}[\delta u]$,

$$g^{\text{Cor}[\delta u]} = \left(\frac{\partial(g - u_0)}{\partial \mathbf{n}} \otimes \frac{\partial(g - u_0)}{\partial \mathbf{n}} \right) \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle],$$

and solving

$$(\mathcal{V} \otimes \mathcal{V})\rho^{\text{Cor}[\delta u]} = g^{\text{Cor}[\delta u]}, \quad (21)$$

the second order correction term $\text{Cor}[\delta u]$ can be represented as solution of (13) by the representation formula

$$\text{Cor}[\delta u](\mathbf{x}, \mathbf{y}) = (\tilde{\mathcal{V}} \otimes \tilde{\mathcal{V}})\left(\rho^{\text{Cor}[\delta u]}\right)(\mathbf{x}, \mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in D_{\Omega}. \quad (22)$$

4. Galerkin Discretization

For the following discussion of the Galerkin discretizations, let S_h^d be the space of piecewise polynomial ansatz functions of order d on ∂D_0 , generated from a quasi-uniform mesh on ∂D_0 . Since the Neumann data $t^{(u_0)}$ of the solution u_0 of the unperturbed problem (2) are needed for the computation of both of the correction terms $\mathbb{E}[\delta^2 u]$ and $\text{Cor}[\delta u]$, we will first consider the discretization of the Dirichlet-to-Neumann map (14). Although the discretization is pretty standard in boundary element methods, cf., e.g., [25], we believe its repetition will help to establish notation and will help the reader to understand the following more involved steps.

4.1. Dirichlet-to-Neumann Map

The variational formulation of the Dirichlet-to-Neumann map (14) is given as follows:

Find $t^{(u_0)} \in H^{-1/2}(\partial D_0)$ such that

$$(\mathcal{V}t^{(u_0)}, v)_{L^2(\partial D_0)} = \left(\left(\frac{1}{2} + \mathcal{K} \right) g, v \right)_{L^2(\partial D_0)}$$

for all $v \in H^{-1/2}(\partial D_0)$.

Replacing the energy space $H^{-1/2}(\partial D_0)$ by the finite dimensional space $S_h^d \subset H^{-1/2}(\partial D_0)$, choosing a basis $(\psi_i)_{i=1}^N$ of S_h^d , and replacing g with its L^2 -projection $\Pi_h g$, we end up with the linear system of equations

$$\mathbf{V} \mathbf{t}^{(u_0)} = \left(\frac{1}{2} \mathbf{M} + \mathbf{K} \right) \mathbf{M}^{-1} \mathbf{g}. \quad (23)$$

The corresponding system matrices are given by

$$\mathbf{V} = [(\mathcal{V} \psi_j, \psi_i)_{L^2(\partial D_0)}]_{i,j=1}^N, \quad \mathbf{K} = [(\mathcal{K} \psi_j, \psi_i)_{L^2(\partial D_0)}]_{i,j=1}^N, \quad \mathbf{M} = [(\psi_j, \psi_i)_{L^2(\partial D_0)}]_{i,j=1}^N,$$

while the vectors are given by

$$\mathbf{g} = \left[(g, \psi_i)_{L^2(\partial D_0)} \right]_{i=1}^N, \quad \mathbf{t}^{(u_0)} = \left[t_i^{(u_0)} \right]_{i=1}^N,$$

where the coefficients $t_i^{(u_0)}$ are the coefficients of the basis expansion

$$t_h^{(u_0)} = \sum_{i=1}^N t_i^{(u_0)} \psi_i.$$

4.2. Computation of $\text{Cor}[\delta u]$

For determining $\text{Cor}[\delta u]$ via the representation formula (22), we have to compute $\rho^{(\text{Cor}[\delta u])}$, which is given as the solution of the tensor equation (21). We therefore introduce the Sobolev spaces $H_{\text{mix}}^{s,t}(\partial D_0 \times \partial D_0)$, $s, t \in \mathbb{R}$, of dominant mixed derivatives on $\partial D_0 \times \partial D_0$ defined by

$$H_{\text{mix}}^{s,t}(\partial D_0 \times \partial D_0) := H^s(\partial D_0) \otimes H^t(\partial D_0).$$

The variational formulation of (21) is then given as follows:

$$\begin{aligned} & \text{Find } \rho^{(\text{Cor}[\delta u])} \in H_{\text{mix}}^{-1/2, -1/2}(\partial D_0 \times \partial D_0) \text{ such that} \\ & \left((\mathcal{V} \otimes \mathcal{V}) \rho^{(\text{Cor}[\delta u])}, v \right)_{L^2(\partial D_0 \times \partial D_0)} = \left(g^{(\text{Cor}[\delta u])}, v \right)_{L^2(\partial D_0 \times \partial D_0)} \\ & \text{for all } v \in H_{\text{mix}}^{-1/2, -1/2}(\partial D_0 \times \partial D_0). \end{aligned}$$

Replacing the energy space $H_{\text{mix}}^{-1/2, -1/2}(\partial D_0 \times \partial D_0)$ by the finite dimensional ansatz space $S_h^d \otimes S_h^d \subset H_{\text{mix}}^{-1/2, -1/2}(\partial D_0 \times \partial D_0)$, choosing a basis $(\psi_i \otimes \psi_j)_{i,j=1}^n$ of $S_h^d \otimes S_h^d$, and replacing $g^{(\text{Cor}[\delta u])}$ by the approximation

$$g_h^{(\text{Cor}[\delta u])} := \left(\left(\frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right) \otimes \left(\frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right) \right) \left((\Pi_h \otimes \Pi_h) \text{Cor}[(\mathbf{V}, \mathbf{n})] \right),$$

we end up with the linear system of equations

$$(\mathbf{V} \otimes \mathbf{V}) \text{vec}(\mathbf{C}_{\rho, \text{Cor}[\delta u]}) = (\mathbf{N} \otimes \mathbf{N})(\mathbf{M} \otimes \mathbf{M})^{-1} \text{vec}(\mathbf{C}_{\text{Cor}[(\mathbf{V}, \mathbf{n})]}). \quad (24)$$

The corresponding system matrices are given by

$$\begin{aligned} \mathbf{N} &= \left[\left(\left(\frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right) \psi_j, \psi_i \right)_{L^2(\partial D_0)} \right]_{i,j=1}^n, \\ \mathbf{C}_{\text{Cor}[(\mathbf{V}, \mathbf{n})]} &= \left[(\text{Cor}[(\mathbf{V}, \mathbf{n})], \psi_i \otimes \psi_j)_{L^2(\partial D_0 \times \partial D_0)} \right]_{i,j=1}^n, \\ \mathbf{C}_{\rho, \text{Cor}[\delta u]} &= \left[c_{i,j}^{\rho, \text{Cor}[\delta u]} \right]_{i,j=1}^n, \end{aligned}$$

where the coefficients $c_{i,j}^{\rho, \text{Cor}[\delta u]}$ are the coefficients of the basis expansion

$$\rho_h^{(\text{Cor}[\delta u])} = \sum_{i,j=1}^n c_{i,j}^{\rho, \text{Cor}[\delta u]} (\psi_i \otimes \psi_j).$$

The tensor product in (24) has, as usual in connection with matrices, to be understood as the Kronecker product. Furthermore, for a matrix $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_n] \in \mathbb{R}^{m \times n}$, the operation $\text{vec}(\mathbf{A})$ is defined as

$$\text{vec}([\mathbf{a}_1, \dots, \mathbf{a}_n]) := \begin{bmatrix} \mathbf{a}_1 \\ \vdots \\ \mathbf{a}_n \end{bmatrix} \in \mathbb{R}^{mn}.$$

For matrices $\mathbf{A} \in \mathbb{R}^{k \times n}$, $\mathbf{B} \in \mathbb{R}^{\ell \times m}$ and $\mathbf{X} \in \mathbb{R}^{m \times n}$, there holds the relation

$$(\mathbf{A} \otimes \mathbf{B}) \text{vec}(\mathbf{X}) = \text{vec}(\mathbf{B}\mathbf{X}\mathbf{A}^\top),$$

which allows to rewrite (24) as

$$\mathbf{V}\mathbf{C}_{\rho, \text{Cor}[\delta u]}\mathbf{V}^\top = \mathbf{N}\mathbf{M}^{-1}\mathbf{C}_{\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]}\mathbf{M}^{-\top}\mathbf{N}^\top. \quad (25)$$

4.3. Computation of $\mathbb{E}[\delta^2 u]$

We shall now consider the numerical treatment of the computation of the correlation A as given by (18). Its variational formulation is

Find $A \in H_{\text{mix}}^{0, -1/2}(\partial D_0 \times \partial D_0)$ such that

$$\begin{aligned} \left((\text{Id} \otimes \mathcal{V})A, v \right)_{L^2(\partial D_0 \times \partial D_0)} = \\ \left(\left(\text{Id} \otimes \left(\frac{1}{2} + \mathcal{K} \right) \right) \left(\left(\mathbb{1} \otimes \left(\frac{\partial g}{\partial \mathbf{n}} - t^{(u_0)} \right) \right) \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle], v \right)_{L^2(\partial D_0 \times \partial D_0)} \end{aligned}$$

for all $v \in H_{\text{mix}}^{0, -1/2}(\partial D_0 \times \partial D_0)$.

Choosing a basis $(\psi_i \otimes \psi_j)_{i,j=1}^N$ of $S_h^d \otimes S_h^d \subset H_{\text{mix}}^{0, -1/2}(\partial D_0 \times \partial D_0)$ and employing L^2 -projections, as in the previous section, leads to a finite dimensional variational problem, and the linear system of equations

$$(\mathbf{M} \otimes \mathbf{V}) \text{vec}(\mathbf{A}) = \left(\mathbf{M} \otimes \left(\frac{1}{2} \mathbf{M} + \mathbf{K} \right) \right) (\mathbf{M} \otimes \mathbf{M})^{-1} (\mathbf{M} \otimes \mathbf{N}) (\mathbf{M} \otimes \mathbf{M})^{-1} \text{vec}(\mathbf{C}_{\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]}),$$

where \mathbf{A} contains the coefficients of the basis expansion of the Galerkin solution $A_h \in S_h^d \otimes S_h^d$. Rearranging as before yields the matrix equation

$$\mathbf{V}\mathbf{A}\mathbf{M}^\top = \left(\frac{1}{2} \mathbf{M} + \mathbf{K} \right) \mathbf{M}^{-1} \mathbf{N} \mathbf{M}^{-1} \mathbf{C}_{\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]}. \quad (26)$$

Having approximated the correlation A , the Dirichlet data of $\mathbb{E}[\delta^2 u]$ can now be computed. Following the considerations of the discretization of the Dirichlet-to-Neumann map from Section 4.1 and employing L^2 -projections, the Neumann data $t^{(\mathbb{E}[\delta^2 u])}$ of $\mathbb{E}[\delta^2 u]$ are given by

$$\mathbf{V}\mathbf{t}^{(\mathbb{E}[\delta^2 u])} = \left(\frac{1}{2} \mathbf{M} + \mathbf{K} \right) \mathbf{M}^{-1} \left((\mathbf{G} - \mathbf{L}\mathbf{M}^{-1}\mathbf{N}) \mathbf{M}^{-1} \mathbf{d} - 2\mathbf{b} \right) \quad (27)$$

with corresponding vectors and matrices

$$\begin{aligned} \mathbf{d} &= \left[(\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] |_{\mathbf{x}=\mathbf{y}}, \psi_i)_{L^2(\partial D_0)} \right]_{i=1}^n, & \mathbf{b} &= \left[(A_h |_{\mathbf{x}=\mathbf{y}}, \psi_i)_{L^2(\partial D_0)} \right]_{i=1}^n, \\ \mathbf{L} &= \left[(2\mathcal{H}\psi_j, \psi_i)_{L^2(\partial D_0)} \right]_{i,j=1}^n, & \mathbf{G} &= \left[(\Delta g \psi_j, \psi_i)_{L^2(\partial D_0)} \right]_{i,j=1}^n. \end{aligned}$$

The correction term $\mathbb{E}[\delta^2 u]$ itself is then given by the representation formula (20).

The error estimation of the approximate solutions is the topic of the next section.

5. Error Estimates

For the following error estimates, it is important to carefully distinguish between the regularity requirements of the involved shape calculus and the regularity assumptions for the Galerkin discretization. More specifically, let us remark that a regularity assumption on the boundary ∂D_0 of the reference domain does not necessarily imply the same regularity to the perturbations and the perturbed domains $D(\omega)$. Throughout our proofs, we require that domain D_0 is of class $C^{d,1}$.

5.1. Preliminaries

We start by restating a convergence result for the Dirichlet-to-Neumann map.

Lemma 5.1. *For the Neumann data $t^{(u_0)}$ of the solution u_0 of the unperturbed problem (2) and their approximation $t_h^{(u_0)}$, it holds for $-d \leq s \leq 0$ that*

$$\left\| t^{(u_0)} - t_h^{(u_0)} \right\|_{H^s(\partial D_0)} \lesssim h^{d-s}.$$

Proof. The proof for the case $-d \leq s \leq -1/2$ is standard, we refer to [25] and remark that $\mathcal{K}: H^s(\partial D_0) \rightarrow H^{s+1}(\partial D_0)$ is a continuous operator on $C^{d,1}$ -boundaries. To extend the result to the case $-1/2 < s \leq 0$, consider the inequality

$$\left\| t^{(u_0)} - t_h^{(u_0)} \right\|_{H^s(\partial D_0)} \leq \left\| t^{(u_0)} - \Pi_h t^{(u_0)} \right\|_{H^s(\partial D_0)} + \left\| \Pi_h t^{(u_0)} - t_h^{(u_0)} \right\|_{H^s(\partial D_0)}.$$

The first term on the right hand side can again be estimated by the standard approximation property of the L^2 -projection, whereas, for the second term on the right hand side, we employ the inverse estimate to obtain

$$\begin{aligned} \left\| \Pi_h t^{(u_0)} - t_h^{(u_0)} \right\|_{H^s(\partial D_0)} &\leq h^{s-1/2} \left\| \Pi_h t^{(u_0)} - t_h^{(u_0)} \right\|_{H^{-1/2}(\partial D_0)} \\ &\leq h^{s-1/2} \left(\left\| \Pi_h t^{(u_0)} - t^{(u_0)} \right\|_{H^{-1/2}(\partial D_0)} + \left\| t^{(u_0)} - t_h^{(u_0)} \right\|_{H^{-1/2}(\partial D_0)} \right). \end{aligned}$$

This yields the assertion. \square

The following technical lemma is needed for the error estimation and is inspired by part of the proof of [7, Theorem 7.3].

Lemma 5.2. *Assume that $\|a - a_h\|_{H^s(\partial D_0)} \lesssim h^{d-s}$, $\|a - a_h\|_{L^2(\partial D_0)} \lesssim h^d$, and $b \in H^d(\partial D_0)$ for $-d \leq s < -(n-1)/2$. Then, we have*

$$\|ab - a_h \Pi_h b\|_{H^s(\partial D_0)} \lesssim h^{d-s}.$$

Proof. We start by splitting the error into two parts

$$\|ab - a_h \Pi_h b\|_{H^s(\partial D_0)} \leq \|(a - a_h)b\|_{H^s(\partial D_0)} + \|a_h(\text{Id} - \Pi_h)b\|_{H^s(\partial D_0)}.$$

From the estimate $\|uv\|_{H^{-s}(\partial D_0)} \lesssim \|u\|_{H^{-s}(\partial D_0)} \|v\|_{H^{-s}(\partial D_0)}$, cf. [26, 27], we conclude by duality

$$\begin{aligned} \|uv\|_{H^s(\partial D_0)} &= \sup_{\|w\|_{H^{-s}(\partial D_0)}=1} (uv, w)_{L^2(\partial D_0)} \\ &= \sup_{\|w\|_{H^{-s}(\partial D_0)}=1} (u, vw)_{L^2(\partial D_0)} \\ &\leq \|u\|_{H^s(\partial D_0)} \sup_{\|w\|_{H^{-s}(\partial D_0)}=1} \|vw\|_{H^{-s}(\partial D_0)} \\ &\lesssim \|u\|_{H^s(\partial D_0)} \|v\|_{H^{-s}(\partial D_0)}. \end{aligned}$$

Thus, the first part of the error can easily be estimated by

$$\|(a - a_h)b\|_{H^s(\partial D_0)} \lesssim \|a - a_h\|_{H^s(\partial D_0)} \|b\|_{H^{-s}(\partial D_0)},$$

whereas the second part of the error is treated in accordance with

$$\begin{aligned} & \|a_h(\text{Id} - \Pi_h)b\|_{H^s(\partial D_0)} \\ &= \sup_{\|w\|_{H^{-s}(\partial D_0)}=1} (a_h(\text{Id} - \Pi_h)b, w)_{L^2(\partial D_0)} \\ &= \sup_{\|w\|_{H^{-s}(\partial D_0)}=1} \left(((a_h - a)(\text{Id} - \Pi_h)b, w)_{L^2(\partial D_0)} + (a(\text{Id} - \Pi_h)b, w)_{L^2(\partial D_0)} \right). \end{aligned}$$

Since $H^{-s}(\partial D_0)$ is continuously embedded into $L^\infty(\partial D_0)$ on $C^{d,1}$ -smooth boundaries for $-s > (n-1)/2$, one can estimate

$$\begin{aligned} \left((a_h - a)(\text{Id} - \Pi_h)b, w \right)_{L^2(\partial D_0)} &\leq \|(a_h - a)(\text{Id} - \Pi_h)b\|_{L^1(\partial D_0)} \|w\|_{L^\infty(\partial D_0)} \\ &\lesssim \|a - a_h\|_{L^2(\partial D_0)} \|(\text{Id} - \Pi_h)b\|_{L^2(\partial D_0)} \|w\|_{H^{-s}(\partial D_0)}, \end{aligned}$$

and, by employing Galerkin orthogonality,

$$\begin{aligned} (a(\text{Id} - \Pi_h)b, w)_{L^2(\partial D_0)} &= ((\text{Id} - \Pi_h)b, aw)_{L^2(\partial D_0)} \\ &= ((\text{Id} - \Pi_h)b, (\text{Id} - \Pi_h)(aw))_{L^2(\partial D_0)} \\ &\leq \|(\text{Id} - \Pi_h)b\|_{L^2(\partial D_0)} \|(\text{Id} - \Pi_h)(aw)\|_{L^2(\partial D_0)}. \end{aligned}$$

The assertion follows by applying the standard approximation estimates of the L^2 -projection, implying that the first part of product is bounded by $\lesssim h^d$ and the second part of product is bounded by $\lesssim h^{-s}$. \square

By a tensor product argument, we arrive at a similar statement on the tensor product domain.

Corollary 5.3. *Assume that $\|a - a_h\|_{H_{\text{mix}}^{s,s}(\partial D_0 \times \partial D_0)} \lesssim h^{d-s}$, $\|a - a_h\|_{L^2(\partial D_0 \times \partial D_0)} \lesssim h^d$ and $b \in H_{\text{mix}}^{d,d}(\partial D_0 \times \partial D_0)$ for $-d \leq s < -(n-1)/2$. Then, it holds that*

$$\|ab - a_h(\Pi_h \otimes \Pi_h)b\|_{H_{\text{mix}}^{s,s}(\partial D_0 \times \partial D_0)} \lesssim h^{d-s}.$$

Proof. The proof is very similar to the proof of the preceding lemma. We refer to the proof of [7, Theorem 7.3], where the details are given for the case $s = -d$, using the estimate $\|uv\|_{H^d(\partial D_0)} \leq \|u\|_{C^{d-1,1}(\partial D_0)} \|v\|_{H^d(\partial D_0)}$ instead of $\|uv\|_{H^d(\partial D_0)} \lesssim \|u\|_{H^d(\partial D_0)} \|v\|_{H^d(\partial D_0)}$. \square

Remark 5.4. *The focus of the present article is on the cases $n = 2, 3$ such that $(n-1)/2 < d$ implies $d \geq 1$ for $n = 2$ and $d \geq 2$ for $n = 3$, respectively. To simplify the presentation of the following results, we will therefore restrict ourselves to the case $d \geq 2$, i.e., we are considering discretizations with at least piecewise linear continuous ansatz functions.*

5.2. Approximation Error of $\text{Cor}[\delta u]$

In order to bound the approximation error of $\text{Cor}[\delta u]$ given by the representation formula (22), we first have to bound the approximation error of its boundary values. This is in parts due to the following

Lemma 5.5. *Let $\text{Cor}[(\mathbf{V}, \mathbf{n})] \in H_{\text{mix}}^{d,d}(\partial D_0 \times \partial D_0)$. Then, it holds*

$$\left\| g^{(\text{Cor}[\delta u])} - g_h^{(\text{Cor}[\delta u])} \right\|_{H_{\text{mix}}^{-d,-d}(\partial D_0 \times \partial D_0)} \lesssim h^{2d}.$$

Proof. The assertion is an immediate consequence of Corollary 5.3 with

$$a = \left(\frac{\partial g}{\partial \mathbf{n}} - t^{(u_0)} \right) \otimes \left(\frac{\partial g}{\partial \mathbf{n}} - t^{(u_0)} \right), \quad a_h = \left(\frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right) \otimes \left(\frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right),$$

and $b = \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]$. The required convergence in the $H^{-d}(\partial D_0)$ -norm and in the $L^2(\partial D_0)$ -norm is proven in Lemma 5.1 for the non-tensor product case. For the tensor product case, consider for $-d \leq s \leq 0$ that

$$\begin{aligned} & \|a - a_h\|_{H_{\text{mix}}^{s,s}(\partial D_0 \times \partial D_0)} \\ &= \left\| \left(\frac{\partial g}{\partial \mathbf{n}} - t^{(u_0)} \right) \otimes \left(t_h^{(u_0)} - t^{(u_0)} \right) + \left(t_h^{(u_0)} - t^{(u_0)} \right) \otimes \left(\frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right) \right\|_{H_{\text{mix}}^{s,s}(\partial D_0 \times \partial D_0)} \\ &\leq \left\| \frac{\partial g}{\partial \mathbf{n}} - t^{(u_0)} \right\|_{H^s(\partial D_0)} \left\| t^{(u_0)} - t_h^{(u_0)} \right\|_{H^s(\partial D_0)} + \left\| t^{(u_0)} - t_h^{(u_0)} \right\|_{H^s(\partial D_0)} \left\| \frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right\|_{H^s(\partial D_0)} \\ &\lesssim h^{d-s}, \end{aligned}$$

which completes the proof. \square

We are now finally in the position to estimate the error of $\text{Cor}[\delta u]_h$.

Lemma 5.6. *Let $\text{Cor}[\delta u]$ be given as in (22) and let $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \in H_{\text{mix}}^{d,d}(\partial D_0 \times \partial D_0)$. It then holds*

$$|\text{Cor}[\delta u](\mathbf{x}, \mathbf{y}) - \text{Cor}[\delta u]_h(\mathbf{x}, \mathbf{y})| \lesssim h^{2d} \quad \text{for all } \mathbf{x}, \mathbf{y} \in K \in D_{\cap \Omega}.$$

Proof. By employing the representation formula (22), we obtain

$$\begin{aligned} & |\text{Cor}[\delta u](\mathbf{x}, \mathbf{y}) - \text{Cor}[\delta u]_h(\mathbf{x}, \mathbf{y})| \\ &= \left| (\tilde{\mathcal{V}} \otimes \tilde{\mathcal{V}}) \left(\rho^{(\text{Cor}[\delta u])} - \rho_h^{(\text{Cor}[\delta u])} \right) (\mathbf{x}, \mathbf{y}) \right| \\ &\lesssim \left\| \frac{1}{16\pi^2 \|\mathbf{x} - \cdot\| \otimes \|\mathbf{y} - \cdot\|} \right\|_{H_{\text{mix}}^{d+1,d+1}(\partial D_0 \times \partial D_0)} \left\| \rho^{(\text{Cor}[\delta u])} - \rho_h^{(\text{Cor}[\delta u])} \right\|_{H_{\text{mix}}^{-d-1,-d-1}(\partial D_0 \times \partial D_0)}. \end{aligned}$$

Using Strang's first lemma and Lemma 5.5, we further derive

$$\left\| \rho^{(\text{Cor}[\delta u])} - \rho_h^{(\text{Cor}[\delta u])} \right\|_{H_{\text{mix}}^{-d-1,-d-1}(\partial D_0 \times \partial D_0)} \lesssim h^{2d},$$

which, in view of $K \in \partial D_0$ and thus $\text{dist}(K, \partial D_0) > 0$, implies the assertion. \square

Remark 5.7. *The assumptions of the presented result are slightly weaker than the related result from [7]. Whereas [7] requires $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]$ to be in $C_{\text{mix}}^{d-1,1}(\partial D_0 \times \partial D_0)$, we only require it to be in $H_{\text{mix}}^{d,d}(\partial D_0 \times \partial D_0)$. This means that we do not need any extra regularity of the boundary perturbation in addition to the regularity required for the first order shape derivative and the Galerkin approximation of $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]$.*

5.3. Approximation Error of $\mathbb{E}[\delta^2 u]$

In order estimate the discretization error of $\mathbb{E}[\delta^2 u]$ given by (12), we need to know the discretization error of its Dirichlet data. Especially, we need to estimate the error of the correlation A as given by (18).

Lemma 5.8. *Let $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \in H_{\text{mix}}^{d,d}(\partial D_0 \times \partial D_0)$. It then holds for*

$$A_h = (\text{Id} \otimes \mathcal{V}^{-1}) \left(\text{Id} \otimes \left(\frac{1}{2} + \mathcal{K} \Pi_h \right) \right) \left(\left(\mathbb{1} \otimes \left(\frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right) \right) (\Pi_h \otimes \Pi_h) \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \right)$$

that

$$\|A - A_h\|_{H_{\text{mix}}^{-d+1,-d+1}(\partial D_0 \times \partial D_0)} \lesssim h^{2(d-1)}.$$

Proof. For

$$a = \mathbb{1} \otimes \left(\frac{\partial g}{\partial \mathbf{n}} - t^{(u_0)} \right), \quad a_h = \mathbb{1} \otimes \left(\frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right), \quad b = \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle],$$

it holds

$$\begin{aligned} & \|A - A_h\|_{H_{\text{mix}}^{-d+1, -d+1}(\partial D_0 \times \partial D_0)} \\ & \leq \left\| \text{Id} \otimes \mathcal{V}^{-1} \right\|_{H_{\text{mix}}^{-d+1, -d+2}(\partial D_0 \times \partial D_0) \rightarrow H_{\text{mix}}^{-d+1, -d+1}(\partial D_0 \times \partial D_0)} \\ & \quad \left\| \left(\text{Id} \otimes \left(\frac{1}{2} + \mathcal{K} \right) \right) (ab) - \left(\text{Id} \otimes \left(\frac{1}{2} + \mathcal{K} \Pi_h \right) \right) (a_h (\Pi_h \otimes \Pi_h) b) \right\|_{H_{\text{mix}}^{-d+2, -d+2}(\partial D_0 \times \partial D_0)} \\ & \lesssim \left\| \text{Id} \otimes \mathcal{K} \right\|_{H_{\text{mix}}^{-d+2, -d+2}(\partial D_0 \times \partial D_0) \rightarrow H_{\text{mix}}^{-d+2, -d+2}(\partial D_0 \times \partial D_0)} \\ & \quad \left\| ab - (\text{Id} \otimes \Pi_h)(ab) \right\|_{H_{\text{mix}}^{-d+2, -d+2}(\partial D_0 \times \partial D_0)} \\ & \quad + \left\| \text{Id} \otimes \left(\frac{1}{2} + \mathcal{K} \Pi_h \right) \right\|_{H_{\text{mix}}^{-d+2, -d+2}(\partial D_0 \times \partial D_0) \rightarrow H_{\text{mix}}^{-d+2, -d+2}(\partial D_0 \times \partial D_0)} \\ & \quad \left\| ab - a_h (\Pi_h \otimes \Pi_h) b \right\|_{H_{\text{mix}}^{-d+2, -d+2}(\partial D_0 \times \partial D_0)}. \end{aligned}$$

The assertion now follows from the approximation property of the L^2 -projection, Lemma 5.1, and Corollary 5.3. \square

We are now in the position to bound the error of the Dirichlet data in the boundary value problem (12) for $\mathbb{E}[\delta^2 u]$.

Lemma 5.9. *Let $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]|_{\mathbf{x}=\mathbf{y}} \in H^d(\partial D_0)$ and $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \in H_{\text{mix}}^{d,d}(\partial D_0 \times \partial D_0)$. For the Dirichlet data of $\mathbb{E}[\delta^2 u]$ and their numerical approximation*

$$g_h^{(\mathbb{E}[\delta^2 u])} = \left(\Delta g - 2\mathcal{H} \Pi_h \left(\frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)} \right) \right) \Pi_h \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]|_{\mathbf{x}=\mathbf{y}} - 2A_h|_{\mathbf{x}=\mathbf{y}},$$

it holds

$$\left\| g^{(\mathbb{E}[\delta^2 u])} - g_h^{(\mathbb{E}[\delta^2 u])} \right\|_{H^{-d}(\partial D_0)} \lesssim h^{2(d-1)} \quad (28)$$

and

$$\left\| g^{(\mathbb{E}[\delta^2 u])} - \Pi_h g_h^{(\mathbb{E}[\delta^2 u])} \right\|_{H^{-d}(\partial D_0)} \lesssim h^{2(d-1)}. \quad (29)$$

Proof. By exploiting $\Pi_h t_h^{(u_0)} = t_h^{(u_0)}$ and setting

$$a = \frac{\partial g}{\partial \mathbf{n}} - t^{(u_0)}, \quad a_h = \Pi_h \frac{\partial g}{\partial \mathbf{n}} - t_h^{(u_0)}, \quad b = \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]|_{\mathbf{x}=\mathbf{y}},$$

we conclude

$$\begin{aligned} & \left\| g^{(\mathbb{E}[\delta^2 u])} - g_h^{(\mathbb{E}[\delta^2 u])} \right\|_{H^{-d}(\partial D_0)} \leq \left\| (\Delta g)(b - \Pi_h b) \right\|_{H^{-d}(\partial D_0)} \\ & \quad + \left\| 2\mathcal{H}(ab - a_h \Pi_h b) \right\|_{H^{-d}(\partial D_0)} + 2 \left\| A|_{\mathbf{x}=\mathbf{y}} - A_h|_{\mathbf{x}=\mathbf{y}} \right\|_{H^{-d}(\partial D_0)}. \end{aligned}$$

Herein, the first term on the right hand side can be bounded by a constant times h^{2d} by applying the L^2 -projection estimates. The second term on the right hand can be estimated by using the inequality $\|uv\|_{H^{-d+2}(\partial D_0)} \lesssim \|u\|_{H^{d-2}(\partial D_0)} \|v\|_{H^{-d+2}(\partial D_0)}$ as already used in Lemma 5.2:

$$\begin{aligned} \left\| 2\mathcal{H}(ab - a_h \Pi_h b) \right\|_{H^{-d}(\partial D_0)} & \leq \left\| 2\mathcal{H}(ab - a_h \Pi_h b) \right\|_{H^{-d+2}(\partial D_0)} \\ & \lesssim \left\| 2\mathcal{H} \right\|_{H^{d-2}(\partial D_0)} \left\| ab - a_h \Pi_h b \right\|_{H^{-d+2}(\partial D_0)}. \end{aligned}$$

To estimate the third term on the right hand side, we follow the arguments in [28, Chapter 3.3] and remark that the diagonal operator $H_{\text{mix}}^{s,s}(\partial D_0 \times \partial D_0) \rightarrow W^{s,1}(\partial D_0)$ is continuous. Exploiting that the embedding $W^{s,1}(\partial D_0) \hookrightarrow H^{s-1}(\partial D_0)$ is also continuous, we conclude by a density argument that

$$\left\| A|_{\mathbf{x}=\mathbf{y}} - A_h|_{\mathbf{x}=\mathbf{y}} \right\|_{H^{-d}(\partial D_0)} \lesssim \|A - A_h\|_{H_{\text{mix}}^{-d+1, -d+1}(\partial D_0 \times \partial D_0)}.$$

In view of Lemmata 5.2 and 5.8, this implies the estimate (28).

Estimate (29) follows finally from (28) and Strang's first lemma by considering the Galerkin projection as the solution of $Ix = g$ with a perturbed right-hand side. \square

We are now in the position to bound the error of the Neumann data $t^{(\mathbb{E}[\delta^2 u])}$ of $\mathbb{E}[\delta^2 u]$.

Lemma 5.10. *Let $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]|_{\mathbf{x}=\mathbf{y}} \in H^d(\partial D_0)$ and $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \in H_{\text{mix}}^{d,d}(\partial D_0 \times \partial D_0)$. Then, the Neumann data $t^{(\mathbb{E}[\delta^2 u])}$ are approximated with the rate*

$$\left\| t^{(\mathbb{E}[\delta^2 u])} - t_h^{(\mathbb{E}[\delta^2 u])} \right\|_{H^{-d-1}(\partial D_0)} \lesssim h^{2(d-1)}.$$

Proof. Since $\mathcal{V}: H^d(\partial D_0) \rightarrow H^{d+1}(\partial D_0)$ is self-adjoint, continuous, and boundedly invertible in case of a $C^{d,1}$ -boundary, it holds

$$\begin{aligned} \left\| t^{(u_0)} - t_h^{(u_0)} \right\|_{H^{-d-1}(\partial D_0)} &= \sup_{\|v\|_{H^{d+1}(\partial D_0)}=1} \left(t^{(u_0)} - t_h^{(u_0)}, v \right)_{L^2(\partial D_0)} \\ &= \sup_{\|w\|_{H^d(\partial D_0)}=1} \frac{\left(\mathcal{V} \left(t^{(u_0)} - t_h^{(u_0)} \right), w \right)_{L^2(\partial D_0)}}{\|\mathcal{V}w\|_{H^{d+1}(\partial D_0)}} \\ &\leq \sup_{\|w\|_{H^d(\partial D_0)}=1} \frac{\left(\mathcal{V} \left(t^{(u_0)} - t_h^{(u_0)} \right), w - \Pi_h w \right)_{L^2(\partial D_0)}}{\|\mathcal{V}w\|_{H^{d+1}(\partial D_0)}} \\ &\quad + \sup_{\|w\|_{H^d(\partial D_0)}=1} \frac{\left(\mathcal{V} \left(t^{(u_0)} - t_h^{(u_0)} \right), \Pi_h w \right)_{L^2(\partial D_0)}}{\|\mathcal{V}w\|_{H^{d+1}(\partial D_0)}}. \end{aligned}$$

Using the continuity and bounded invertibility of \mathcal{V} , we further estimate

$$\begin{aligned} &\sup_{\|w\|_{H^d(\partial D_0)}=1} \frac{\left(\mathcal{V} \left(t^{(u_0)} - t_h^{(u_0)} \right), w - \Pi_h w \right)_{L^2(\partial D_0)}}{\|\mathcal{V}w\|_{H^{d+1}(\partial D_0)}} \\ &\leq \left\| \mathcal{V} \left(t^{(u_0)} - t_h^{(u_0)} \right) \right\|_{H^{1/2}(\partial D_0)} \sup_{\|w\|_{H^d(\partial D_0)}=1} \frac{\|w - \Pi_h w\|_{H^{-1/2}(\partial D_0)}}{\|\mathcal{V}w\|_{H^{d+1}(\partial D_0)}} \\ &\lesssim \left\| t^{(u_0)} - t_h^{(u_0)} \right\|_{H^{-1/2}(\partial D_0)} \sup_{\|w\|_{H^d(\partial D_0)}=1} \frac{\|w - \Pi_h w\|_{H^{-1/2}(\partial D_0)}}{\|w\|_{H^d(\partial D_0)}}. \end{aligned}$$

Using standard error estimates for the Galerkin method, the error of the Neumann data in the $H^{-1/2}(\partial D_0)$ -norm is bounded by $\lesssim h^{d+1/2}$, whereas the second factor can be estimated by the standard error estimates for the L^2 -projection.

To estimate the second part of the sum, consider

$$\left(\mathcal{V} \left(t^{(u_0)} - t_h^{(u_0)} \right), v_h \right)_{L^2(\partial D_0)} = \left(\frac{1}{2}(g - g_h) + \mathcal{K}(g - \Pi_h g_h), v_h \right)_{L^2(\partial D_0)} \quad \text{for all } v_h \in S_h^d,$$

and conclude

$$\begin{aligned}
& \left(\mathcal{V}(t^{(u_0)} - t_h^{(u_0)}), \Pi_h w \right)_{L^2(\partial D_0)} \\
&= \left(\frac{1}{2}(g - g_h) + \mathcal{K}(g - \Pi_h g_h), \Pi_h w \right)_{L^2(\partial D_0)} \\
&= \left(\frac{1}{2}(g - g_h) + \mathcal{K}(g - \Pi_h g_h), w \right)_{L^2(\partial D_0)} \\
&\quad + \left(\mathcal{K}(g - \Pi_h g_h), \Pi_h w - w \right)_{L^2(\partial D_0)} + \frac{1}{2} \left(g - g_h, \Pi_h w - w \right)_{L^2(\partial D_0)} \\
&\lesssim \left(\|g - g_h\|_{H^{-d}(\partial D_0)} + \|\mathcal{K}(g - \Pi_h g_h)\|_{H^{-d}(\partial D_0)} \right) \|w\|_{H^d(\partial D_0)} \\
&\quad + \|\mathcal{K}(g - \Pi_h g_h)\|_{H^1(\partial D_0)} \|w - \Pi_h w\|_{H^{-1}(\partial D_0)} \\
&\quad + \|g - g_h\|_{L^2(\partial D_0)} \|w - \Pi_h w\|_{L^2(\partial D_0)}.
\end{aligned}$$

The assertion now follows by exploiting that $\mathcal{K}: H^s(\partial D_0) \rightarrow H^s(\partial D_0)$ is a continuous operator for $s = -d$ and $s = 1$ on $C^{d,1}$ -boundaries, the previous lemma, and inverse estimate in complete analogy to the proof of Lemma 5.1. \square

As an immediate consequence of the error estimates, we obtain finally an error estimate for the potential of the second order local shape derivative $\mathbb{E}[\delta^2 u]$. It holds the following approximation result by standard arguments, see [25] for instance.

Lemma 5.11. *Let $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]_{\mathbf{x}=\mathbf{y}} \in H^d(\partial D_0)$ and $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \in H_{\text{mix}}^{d,d}(\partial D_0 \times \partial D_0)$. Then, for the mean of the second order local shape derivative $\mathbb{E}[\delta^2 u]$ from (12), it holds that*

$$|\mathbb{E}[\delta^2 u](\mathbf{x}) - \mathbb{E}[\delta^2 u]_h(\mathbf{x})| \lesssim h^{2(d-1)} \quad \text{for all } \mathbf{x} \in K \Subset D_{\cap}.$$

Remark 5.12. *Although we can only prove a reduced convergence rate of $h^{2(d-1)}$, we will see in the numerical experiments that we reach the same convergence rate as for the correlation, i.e., h^{2d} .*

6. Hierarchical Matrix Compression of Dense Matrices

Depending on the properties of the underlying correlation kernel, correlation matrices are usually densely populated. Similarly, it is well known from the numerical treatment of boundary integral equations that the Dirichlet-to-Neumann map leads to dense system matrices of the single layer operator (15) and the double layer operator (16). Although both operators live on the boundary ∂D_0 , and have thus the spatial dimension reduced by one compared to D_0 , the memory requirements and assembly time still scale at least like $\mathcal{O}(N^2)$, if ansatz spaces with dimension N are used. To reduce the complexity to linear or almost linear (i.e. linear up to polylogarithmic terms) scaling in N , *fast boundary element methods* such as the fast multipole method [29], the panel clustering method [30], the wavelet Galerkin scheme [31, 32], and the adaptive cross approximation [33] exploit analytic properties of the kernel function to derive (data-)sparse approximations to the dense system matrices. Except for the wavelet Galerkin scheme, all these methods can be cast into the framework of hierarchical matrices, cf. [34, 35], which we are going to employ throughout the rest of the article.

6.1. Asymptotically Smooth Kernels

We discuss the compression of the boundary operator matrices of the Dirichlet-to-Neumann map in a terms of the more general asymptotic smooth *asymptotically smooth* kernels.

Definition 6.1. *The function $k: \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ is called asymptotically smooth if for some constants $c_1, c_2 > 0$ and $q \in \mathbb{R}$ there holds*

$$|\partial_{\mathbf{x}}^{\alpha} \partial_{\mathbf{y}}^{\beta} k(\mathbf{x}, \mathbf{y})| \leq c_1 \frac{(|\alpha| + |\beta|)!}{c_2^{|\alpha| + |\beta|}} \|\mathbf{x} - \mathbf{y}\|_2^{-n-2q-|\alpha|-|\beta|}, \quad \mathbf{x} \neq \mathbf{y}, \quad (30)$$

independently of α and β . It is called asymptotically smooth in one variable, if the above condition holds only for the derivatives in \mathbf{x} or \mathbf{y} .

We note especially that, besides the kernel functions of the single layer and the double layer operator, the widely used correlation kernels of the Matérn class, which include, in particular, the Gaussian kernel, cf. [36, 37] and the references therein, are asymptotically smooth or asymptotically smooth in one variable. We will therefore restrict ourselves to kernel functions of this type for the rest of this article and will exploit that they exhibit a data-sparse representation by means of hierarchical matrices (\mathcal{H} -matrices in short).

\mathcal{H} -matrices rely on local low-rank approximations of a given matrix $\mathbf{X} \in \mathbb{R}^{N \times N}$. For suitable nonempty 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 $\mathbf{X}|_{\nu \times \nu'} \approx \mathbf{Y}\mathbf{Z}^T$ 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*.

6.2. Cluster Tree

For a tree $\mathcal{T} = (V, E)$ with vertices V and edges E , we define its set of leaves by

$$\mathcal{L}(\mathcal{T}) := \{\sigma \in V : \sigma \text{ has no sons}\}.$$

Furthermore, we say that \mathcal{T} is a *cluster tree* for the set $\{1, \dots, N\}$ if the following conditions hold.

- $\{1, \dots, N\}$ is the *root* of \mathcal{T} .
- All $\sigma \in V \setminus \mathcal{L}(\mathcal{T})$ are the disjoint union of their sons.

The *level* of $\sigma \in \mathcal{T}$ is its distance to the root, i.e., the number of son relations that are required for traveling from $\{1, \dots, N\}$ to σ . We define the set of clusters on level j as

$$\mathcal{T}^{(j)} := \{\sigma \in \mathcal{T} : \sigma \text{ has level } j\}.$$

The construction of the cluster tree is based on the *support* of the clusters. The support Υ_{σ} of a cluster σ is defined as the union of the supports of the basis functions corresponding to their elements, that is

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

For computing complexity bounds, the cluster tree should match the following additional requirements, uniformly as $N \rightarrow \infty$:

- The cluster tree is a balanced tree in the sense that the maximal level satisfies $J \sim \log_2 N$.
- The diameter of the support Υ_{σ_j} , $\sigma_j \in \mathcal{T}^{(j)}$, is local with respect to the level j , i.e., $\text{diam } \Upsilon_{\sigma_j} \sim 2^{-j/d}$. Moreover, the number $\#\sigma_j$ of indices contained in a cluster $\sigma_j \in \mathcal{T}^{(j)}$ scales approximately like 2^{J-j} , i.e., $\#\sigma_j \sim 2^{J-j}$.

Until further notice, a binary 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, cf., e.g., [34, 35]. We begin by embedding the point set $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ in a top-level bounding-box. This bounding-box is subsequently subdivided into two cuboids of the same size where the corresponding clusters are described by the points in each bounding-box. This process is iterated until a bounding-box encloses less than a predetermined number of points. In accordance with [38], simplifications can be made by mapping an canonical cluster tree on the reference domain to the surface when a parametric surface representation is used for the boundary ∂D_0 . This situation appears especially in isogeometric analysis, see [39] and the references therein.

6.3. Hierarchical Matrix Approximation

For the discretization of kernel functions which are asymptotically smooth in at least one of the variables, we introduce a partition of its domain of definition which separates smooth and non-smooth areas of the kernel function.

Definition 6.2. *Two clusters σ and σ' are called admissible if*

$$\max\{\text{diam}(\Upsilon_\sigma), \text{diam}(\Upsilon_{\sigma'})\} \leq \eta \text{dist}(\Upsilon_\sigma, \Upsilon_{\sigma'}) \quad (31)$$

holds for some fixed $\eta > 0$.

We can obtain the set of admissible blocks by means of a recursive algorithm: Starting with the root $(\sigma_{0,0}, \sigma_{0,0})$, the bounding-boxes of the current cluster pair are checked for admissibility. If they are admissible, the cluster pair is added to the set \mathcal{F} , which corresponds to the correlation kernel's *farfield*. Otherwise, the admissibility check will be performed on all bounding-boxes of the possible pairs of son clusters of the two original clusters. When we arrive at a pair of leaf clusters with inadmissible bounding-boxes, the clusters are added to the set \mathcal{N} , which corresponds to the correlation kernel's *nearfield*. The set $\mathcal{B} = \mathcal{F} \cup \mathcal{N}$ obviously inherits a tree structure from the recursive construction of \mathcal{F} and \mathcal{N} and is called the *block cluster tree*, see [34, 35].

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

Definition 6.3. *The set $\mathcal{H}(\mathcal{B}, k)$ of \mathcal{H} -matrices of maximal block rank k is defined according to*

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

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

In accordance with [34, 35], the storage cost of an \mathcal{H} -matrix $\mathbf{X} \in \mathcal{H}(\mathcal{B}, k)$ is $\mathcal{O}(kN \log N)$. Here, for correlation kernels which are asymptotically smooth in at least one variable, the rank k depends poly-logarithmically on the desired approximation accuracy ε , which in turn usually depends on the degrees of freedom N . While the asymptotical smoothness of *explicitly* given kernel functions can easily be verified, other kernel functions are the topic of the next subsection.

6.4. Covariance Calculus

The compressibility of an *implicitly* given kernel function, such as $\rho^{(\text{Cor}[\delta u])}$ in (21), has been studied in [20] for the case of smooth domains and manifolds. We restate the main theorem for the setting of the present article which employs that the Hilbert-Schmidt operator

$$(\mathcal{C}_{\langle \mathbf{V}, \mathbf{n} \rangle} \psi)(\mathbf{x}) := \int_{\partial D_0} \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle](\mathbf{x}, \mathbf{y}) \psi(\mathbf{y}) \, d\sigma_{\mathbf{y}},$$

related with the correlation kernel $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]$, is in general a *pseudo-differential operator*, see, e.g., [40] and the references therein.

Theorem 6.4. *Let ∂D_0 be an analytic manifold and consider the correlation equation*

$$(\Psi \otimes \Psi) \text{Cor}[u] = \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]. \quad (32)$$

Assume that the correlation kernel $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]$ gives rise to an operator $\mathcal{C}_{\langle \mathbf{V}, \mathbf{n} \rangle} \in OPS_{cl,s}^\theta$, i.e., to a classical pseudo-differential operator with symbol $a_{\langle \mathbf{V}, \mathbf{n} \rangle}(\mathbf{x}, \boldsymbol{\xi})$ of order θ and of Gevrey class $s \geq 1$ in the sense of [41, Definition 1.1]. Then, if $\Psi \in OPS_{cl,s}^r$ is properly supported, the solution correlation kernel $\text{Cor}[u]$ is the Schwartz kernel of an operator $\mathcal{C}_u \in OPS_{cl,s}^{\theta-2r}$.

Moreover, the kernel $\text{Cor}[u]$ of the correlation operator \mathcal{C}_u is smooth in local coordinates away from the diagonal, and there holds the pointwise estimate

$$|\partial_{\mathbf{x}}^\alpha \partial_{\mathbf{y}}^\beta \text{Cor}[u](\mathbf{x}, \mathbf{y})| \leq c \mathcal{A}^{|\alpha+\beta|} (|\boldsymbol{\alpha}|!)^s |\boldsymbol{\beta}|! \|\mathbf{x} - \mathbf{y}\|_2^{-\theta-n-|\alpha|-|\beta|-2} \quad (33)$$

in local coordinates away from the diagonal for all $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_0^{n-1}$, with some constants c and \mathcal{A} which depend only on M , κ , and $a_{\langle \mathbf{V}, \mathbf{n} \rangle}$.

Obviously, for $s = 1$, estimate (33) directly implies condition (30) for the asymptotic smoothness of $\text{Cor}[u]$, whereas $s > 1$ implies the asymptotic smoothness in one variable. We can thus approximate $\text{Cor}[u]$ by means of \mathcal{H} -matrices. The assumption of an analytic manifold can be relaxed to a manifold of Gevrey class s in the case $s > 1$. In particular, [20] provides also some numerical evidence that the result could likely be extended to Lipschitz domains. An example of correlation kernels for $\text{Cor}_{(\mathbf{V}, \mathbf{n})}$, which satisfy the conditions of this theorem for $s \geq 1$, is again the Matérn class of kernels. We refer to [20] for more details on how to verify the assumptions of the theorem for other kernel functions.

Theorem 6.4 does not immediately show that the kernel functions A from (18) and $\rho^{(\text{Cor}[\delta u])}$ from (21) are asymptotically smooth, but it can be extended to the following slightly modified version.

Corollary 6.5. *Let ∂D_0 be a manifold of Gevrey class $s > 1$ or an analytic manifold (i.e. $s = 1$), and let $\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle]$ fulfil the same requirements as in Theorem 6.4 for $s \geq 1$. Let further g be analytic in the case $s = 1$ and of Gevrey class $s > 1$ otherwise. Then, the solutions of the equations (18) and (21) are asymptotically smooth functions for $s = 1$ and asymptotically smooth in one variable for $s > 1$.*

Proof. We first remark that the single layer operator belongs to $OPS_{cl,s}^{-1}$ and the double layer operator belongs to $OPS_{cl,s}^0$ for $s \geq 1$, cf. [40]. Let us further remark that the multiplication of two functions $g(\mathbf{x})f(\mathbf{x})$ can be written as an application of an integral operator

$$g(\mathbf{x})f(\mathbf{x}) = \int_{\partial D_0} k(\mathbf{x}, \mathbf{x} - \mathbf{y})f(\mathbf{y}) d\sigma_{\mathbf{y}} = (\Psi f)(\mathbf{x}).$$

with distributional Schwartz kernel $k(\mathbf{x}, \mathbf{x} - \mathbf{y}) = g(\mathbf{x})\delta(\mathbf{x} - \mathbf{y})$, with δ denoting the delta distribution. Since the Fourier transform of the delta distribution is a constant, the multiplication by a function gives thus rise to a pseudo differential operator $OPS_{cl,s}^0$. Rewriting finally (18) as

$$(\text{Id} \otimes \mathcal{V})A = \left(\text{Id} \otimes \left(\frac{1}{2} + \mathcal{K} \right) \right) \left(\left(\mathbb{1} \otimes \left(\frac{\partial g}{\partial \mathbf{n}} - t^{(u_0)} \right) \text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle] \right) \right),$$

the rest of the proof is in complete analogy to [20, Theorems 1,2, and 3]. \square

Since sparse matrices corresponding to local operators can easily be represented by \mathcal{H} -matrices, it is thus reasonable to compress all matrices in (25) and (26) as \mathcal{H} -matrices. However, it remains to explain how to actually compute the representations for $\mathbf{C}_{\rho, \text{Cor}[\delta u]}$ in (25) and \mathbf{A} in (26).

6.5. \mathcal{H} -Matrix Arithmetic and Iterative Solution

An important feature of \mathcal{H} -matrices is that efficient algorithms for approximate matrix arithmetic operations are available. For two \mathcal{H} -matrices $\mathbf{H}_1, \mathbf{H}_2 \in \mathcal{H}(\mathcal{B}, k)$, the approximate *matrix-matrix addition* $\mathbf{H}_1 + \mathbf{H}_2 \in \mathcal{H}(\mathcal{B}, k)$ can be performed in $\mathcal{O}(k^2 N \log N)$ operations, while the approximate *matrix-matrix multiplication* $\mathbf{H}_1 * \mathbf{H}_2 \in \mathcal{H}(\mathcal{B}, k)$ can be performed in $\mathcal{O}(k^2 N \log^2 N)$ operations. Both of these operations are essentially block matrix algorithms with successive recompression schemes. 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 $\mathcal{O}(k^2 N \log^2 N)$ operations. We refer the reader to [22, 34, 35, 42] for further results and implementation details.

In the context of correlation equations, this approximate \mathcal{H} -matrix arithmetic has successfully been used in [18, 19] to solve correlation equations as (32), where the operator Ψ has been a differential operator in a domain or a boundary integral operator on a domain's boundary. The resulting matrix equation has been solved by using an iterative solver based on *iterative refinement*, cf. [43, 44, 45], which we are also going to employ here and has originally been introduced in [45] for the improvement of solutions to linear systems of equations based on the LU-factorization.

More general, having all matrices in the general matrix equation $\Psi \mathbf{X} \Phi^\top = \mathbf{R}$ represented by \mathcal{H} -matrices, the solution is derived as follows. Let $\Xi \approx \hat{\mathbf{L}}_\Xi \hat{\mathbf{U}}_\Xi$, where $\hat{\mathbf{L}}_\Xi, \hat{\mathbf{U}}_\Xi \in \mathcal{H}(\mathcal{B}, k)$,

$\Xi \in \{\Psi, \Phi\}$, be approximate LU-decompositions to Ψ and Φ , e.g., computed by the \mathcal{H} -matrix arithmetic. Starting with the initial guess $\mathbf{X}_0 = \hat{\mathbf{U}}_{\Psi}^{-1} \hat{\mathbf{L}}_{\Psi}^{-1} \mathbf{R} \hat{\mathbf{L}}_{\Phi}^{-\top} \hat{\mathbf{U}}_{\Phi}^{-\top}$, we iterate

$$\Theta_i = \mathbf{R} - \Psi \mathbf{X}_i \Phi^{\top}, \quad \mathbf{X}_{i+1} = \mathbf{X}_i + \hat{\mathbf{U}}_{\Psi}^{-1} \hat{\mathbf{L}}_{\Psi}^{-1} \Theta_i \hat{\mathbf{L}}_{\Phi}^{-\top} \hat{\mathbf{U}}_{\Phi}^{-\top}, \quad i = 0, 1, \dots \quad (34)$$

The idea of iterative refinement is that the residual Θ_i is computed with a higher precision than the correction $\hat{\mathbf{U}}_{\Psi}^{-1} \hat{\mathbf{L}}_{\Psi}^{-1} \Theta_i \hat{\mathbf{L}}_{\Phi}^{-\top} \hat{\mathbf{U}}_{\Phi}^{-\top}$. This yields an improvement of the iterate in each step. Note that this algorithm also algebraically coincides with an undamped preconditioned Richardson iteration.

Before we conclude this section, we want to remark that the approximate LU-decomposition can be replaced by an approximate Cholesky decomposition if the corresponding matrix is symmetric and positive definite, such as the system matrix of the single layer operator.

7. Numerical Examples

The following numerical experiments are divided into three parts. The first part is concerned with the convergence of the Galerkin scheme for the correction terms $\text{Cor}[\delta u]_h$ and $\mathbb{E}[\delta^2 u]_h$ with respect to the mesh size h . The second part is concerned with the asymptotics of the perturbation approach in ε , whereas the third part deals with an example on non-smooth domains.

All of the computations in the following experiments have been carried out on a computing server with two Intel(R) Xeon(R) CPU E5-2643 v3 with a clock rate of 3.40GHz and a main memory of 256GB. Each of the CPUs provides 12 physical cores, thus, with Hyper-Threading enabled, we may access up to 24 cores in total. For the discretization and the assembly of the \mathcal{H} -matrices, we employ the black-box higher order fast \mathcal{H}^2 -multipole method proposed in [38]. The computations in the tensor product domain $\partial D_0 \times \partial D_0$ are based on discontinuous (elementwise) polynomial ansatz functions and for the computations in the non-tensor product domain globally continuous B-splines of the same order. For the arithmetic \mathcal{H} -matrix operations, we apply the \mathcal{H} -matrix arithmetic tailored to parametric surfaces as described in [18], where the almost linear scaling with respect to N has been verified. We employ a simple OpenMP parallelization to accelerate the computations and refer to [46], where a more sophisticated parallelization has been discussed.

7.1. Convergence in h

To construct an example, where the solution is analytically known, we consider the unit sphere whose boundary is perturbed in normal direction in accordance with

$$\langle \mathbf{V}(\omega, \mathbf{x}), \mathbf{n}_{\mathbf{x}} \rangle = Y_m^n(\mathbf{x}) X(\omega),$$

where Y_m^n is a spherical harmonic and $X(\omega)$ is a uniformly distributed random variable on $[-\varepsilon, \varepsilon]$. The correlation of this boundary perturbation thus implies

$$\text{Cor}[\langle \mathbf{V}, \mathbf{n} \rangle](\mathbf{x}, \mathbf{y}) = \frac{\varepsilon^2}{3} Y_m^n(\mathbf{x}) Y_m^n(\mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in \partial D_0.$$

Several possible shapes are depicted in Figure 2, while the used compactum K has been visualized in Figure 1.

As boundary values on the hold-all domain, we choose

$$g(\mathbf{x}) = \|\mathbf{x}\|^2, \quad \mathbf{x} \in D_{\varepsilon}^{\cup \Omega}.$$

Since $\|\mathbf{x}\|_2^n Y_m^n(\mathbf{x}/\|\mathbf{x}\|_2)$ is harmonic in \mathbb{R}^3 , it is then a short computation to show that it holds

$$\text{Cor}[\delta u](\mathbf{x}, \mathbf{y}) = \frac{4\varepsilon^2}{3} \left(\|\mathbf{x}\|_2^n Y_m^n \left(\frac{\mathbf{x}}{\|\mathbf{x}\|_2} \right) \right) \otimes \left(\|\mathbf{y}\|_2^n Y_m^n \left(\frac{\mathbf{y}}{\|\mathbf{y}\|_2} \right) \right) \quad \text{on } D_0 \times D_0.$$

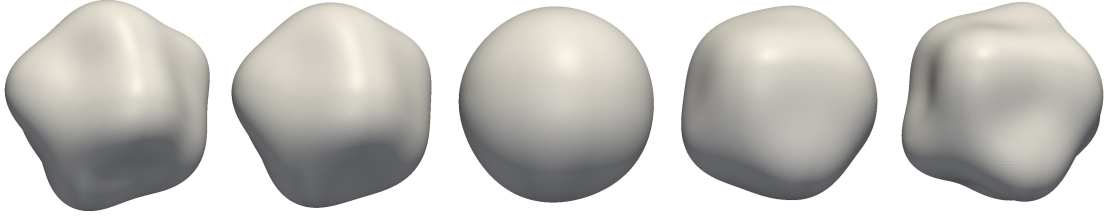


Figure 2: Different realizations of the jiggled unit sphere for the spherical harmonic Y_3^5 and $\varepsilon = 0.3$.

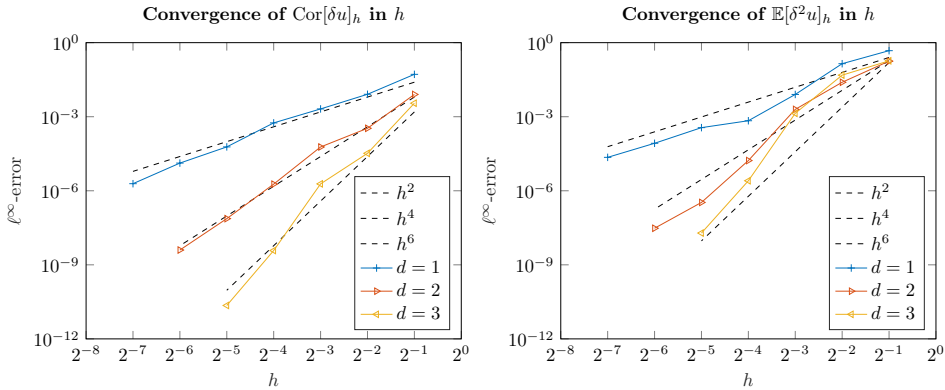


Figure 3: Convergence rates for $\text{Cor}[\delta u]$ and $\mathbb{E}[\delta^2 u]$ on the jiggled sphere for different orders d of the ansatz functions.

Since the spherical harmonic Y_m^n is an eigenfunction of the Dirichlet-to-Neumann map with eigenvalue n on the sphere, cf. [47], and since the unit sphere has the constant mean curvature of $\mathcal{H} = -1$, cf. [48], one verifies that there holds

$$g^{(\mathbb{E}[\delta^2 u])} = \frac{(2 - 4n)\varepsilon^2}{3} (Y_m^n)^2 \quad \text{on } \partial D_0,$$

for the Dirichlet data of the mean's second order correction term $\mathbb{E}[\delta^2 u]$ from (12). Having thus access to the exact Dirichlet data, we can easily compute an overkill solution of $\mathbb{E}[\delta^2 u]$ as a reference solution by an additional refinement in h .

Figure 3 validates that we achieve the convergence rates predicted by Lemma 5.6 and Lemma 5.11 for both, $\text{Cor}[\delta u]$ and $\mathbb{E}[\delta^2 u]$. In fact, $\mathbb{E}[\delta^2 u]$ has even a higher convergence rate than predicted. Although not covered by our theory, the case $d = 1$, i.e. the case of piecewise constant boundary elements, seems to converge as well at a rate of h^2 . Notice that the computed quantities are independent of the amplitude of the jiggling ε , as long as $K \in D_\varepsilon^{\cap \Omega}$ does not depend on ε .

7.2. Asymptotics in ε

As the mean, the correlation, and the covariance for the example on the sphere are not analytically known, we have to use quadrature methods to compute a reference solution in order to demonstrate the asymptotic in ε . Choosing $\varepsilon = 0.05, 0.1, 0.15, 0.2, 0.25, 0.3$, we use a one-dimensional 15 point Gauss-Legendre quadrature rule to compute the stochastic integral of the mean, the correlation, and the covariance on a spatial discretization with continuous piecewise linear ansatz functions on a mesh with 24'576 elements. The PDE solves are accelerated by an OpenMP parallelization.

Since the law of $\langle \mathbf{V}, \mathbf{n} \rangle$ is symmetric, we can expect fourth order accurate approximations to the mean, the correlation, and the covariance in ε . Thus, for the numerical solutions $\mathbb{E}[u_\varepsilon]_h$,

$\text{Cor}[u_\varepsilon]_h$, and $\text{Cov}[u_\varepsilon]_h$ computed by our expansions, the error should behave like

$$\begin{aligned} |\mathbb{E}[u_\varepsilon] - \mathbb{E}[u_\varepsilon]_h| &= \mathcal{O}(h^{2d} + \varepsilon^2 h^{2(d-1)} + \varepsilon^4) && \text{in } K, \\ |\text{Cor}[u_\varepsilon] - \text{Cor } E[u_\varepsilon]_h| &= \mathcal{O}(h^{2d} + \varepsilon^2 h^{2d} + \varepsilon^4) && \text{in } K \times K, \\ |\text{Cov}[u_\varepsilon] - \text{Cov } E[u_\varepsilon]_h| &= \mathcal{O}(\varepsilon^2 h^{2d} + \varepsilon^4) && \text{in } K \times K, \end{aligned}$$

as h and ε tend to zero. The fourth order asymptotic is then reached as soon as the mesh size is small enough.

Figure 4 shows the errors for the former second order (see [7] for the details) and the new fourth order accurate approximations. We indeed reach the fourth order accuracy already for relatively coarse mesh sizes. A comparison with the second order accurate approximation shows that the consideration of the correction terms for the fourth order approximation can improve the error by several orders of magnitude.

7.3. Non-smooth Boundaries

In order to demonstrate that the perturbation approach is not necessarily limited to smooth surfaces, we consider the unit cube $D_0 = [0, 1]^3$ as the reference domain. We assume the perturbing vector field to jiggle the upper side of the cube. More precisely, given uniformly distributed random variables $X_{i,j} \sim U[-1, 1]$, $i, j = 1, \dots, 4$, the perturbation field is given as

$$\mathbf{V}(\omega, \mathbf{x}) = \begin{cases} \sum_{i,j=1}^4 B_i(\mathbf{x}_1) B_j(\mathbf{x}_2) X_{i,j}(\omega), & \mathbf{x}_3 = 1, \\ 0, & \text{otherwise,} \end{cases}$$

where B_i , $i = 1, \dots, 4$ are fifth order B-splines on $[0, 1]$, which, as well as their derivatives, are zero at the interval boundaries. As a result, the shape derivatives are well defined and no singularities occur in the boundary values of the PDEs for the correction terms, which means that the expansions for the mean, the correlation, and the covariance are well defined.

A visualization of different realizations for $\varepsilon = 0.05$ for the Dirichlet boundary values

$$g(\mathbf{x}) = (\mathbf{x}_1 - 0.5)^2 + (\mathbf{x}_2 - 0.5)^2$$

and the used compactum K with the corresponding solution of (3) is found in Figure 5.

Since the stochastic domain is truly 16-dimensional, we use a Monte-Carlo simulation with 10'000 samples for a visual comparison with the asymptotic expansions for the choice $\varepsilon = 0.05$. All computations are performed using continuous piecewise linear ansatz functions on a mesh with 24'576 elements, while we accelerate the Monte-Carlo simulation by computing only the changed matrix entries for each sample. The computation time on all 24 cores takes for all quantities 67'241 seconds using the perturbation approach and 496'582 seconds using the Monte-Carlo simulation. Still, due to the slow convergence rate of the Monte-Carlo simulation and the high-dimensionality of the problem, we only aim at a qualitative comparison of the mean and the correlation, which is presented in Figure 6.

8. Conclusion

In this article, we considered the approximate computation of the mean, the correlation, and the covariance of the solution of PDE on random domains by the perturbation approach. Additionally to existing third order accurate expansions of the covariance discussed in [7], we derived third order accurate expansions of the mean and the correlation and discussed their numerical computation. The discussed expansions become even fourth order accurate for specific types of boundary variations. While the solution on the unperturbed domain yields a second order accurate solution, the correction terms for the more accurate expansions are given by correlation equations.

Omitting the meshing of the computational domain, we employ the boundary element method to discretize the correlation equations with ansatz spaces of piecewise polynomials of at least second

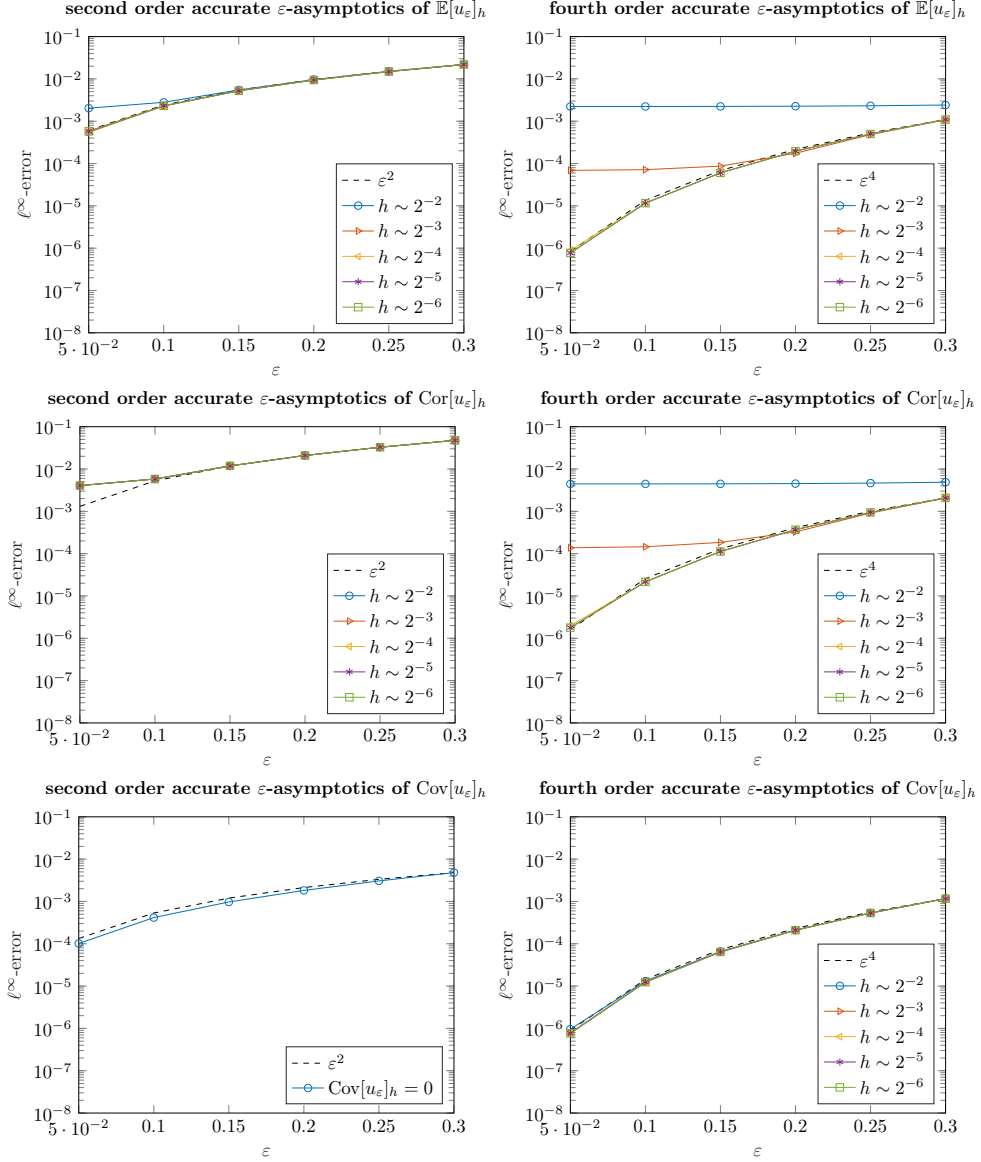


Figure 4: Asymptotics in ϵ for the numerical approximation of the second order and fourth order accurate expansions for the mean, the correlation, and the covariance by different mesh sizes h .

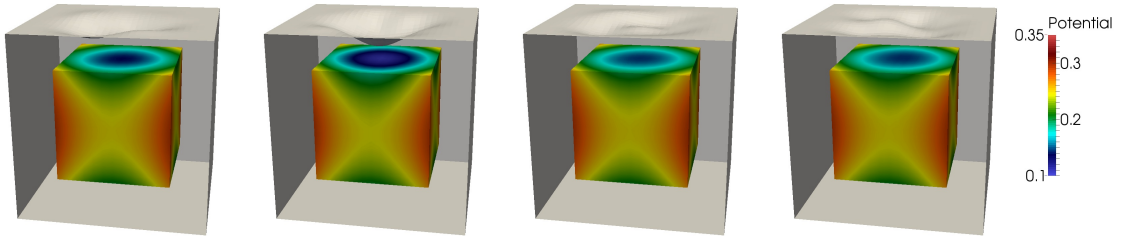


Figure 5: Realizations of the perturbed cube with its solution visualized on the inscribed compactum K for $\epsilon = 0.05$.

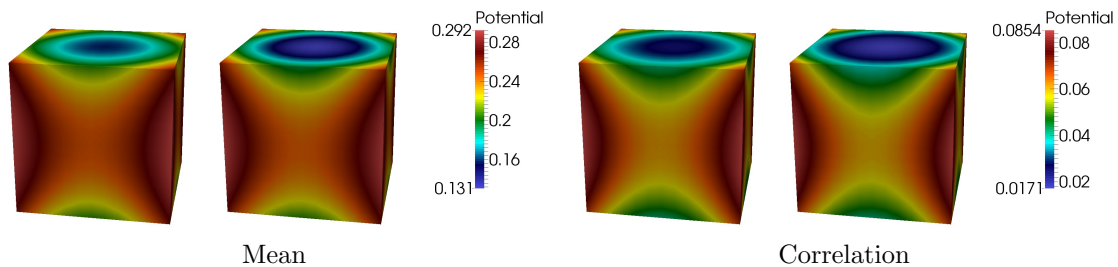


Figure 6: Comparison between the perturbation approach (left) and a Monte-Carlo simulation (right) with 10^4 samples for $\varepsilon = 0.05$.

order. To obtain computational efficiency, we solve the corresponding matrix equations in almost linear complexity by the \mathcal{H} -matrix approach. The numerical experiments in three dimensions verify the asymptotic expansions and show the convergence of the proposed method for piecewise linear and piecewise quadratic boundary elements. Piecewise constant boundary elements, although not covered by the theory, seem to work as well. Finally, we provided numerical experiments which indicate how the perturbation approach could be applied on nonsmooth domains.

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