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Hemut Harbrecht, Michael Peters,
Markus Siebenmorgen

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Institute of Mathematics
University of Basel
Rheinsprung 21
CH - 4051 Basel
Switzerland

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NUMERICAL SOLUTION OF ELLIPTIC DIFFUSION PROBLEMS ON RANDOM DOMAINS

HELMUT HARBRECHT, MICHAEL PETERS, AND MARKUS SIEBENMORGEN

ABSTRACT. In this article, we provide regularity results for the solution to elliptic diffusion problems on random domains. Especially, based on the decay of the Karhunen-Loève expansion of the domain perturbation field, we establish decay rates for the derivatives of the random solution that are independent of the stochastic dimension. By taking into account only univariate derivatives, these regularity results can considerably be sharpened. For the implementation of a related approximation scheme, like quasi-Monte Carlo quadrature, stochastic collocation, etc., we propose parametric finite elements to compute the solution of the diffusion problem on each particular realization of the domain generated by the perturbation field. This simplifies the implementation and yields a non-intrusive approach. Having this machinery at hand, we can easily transfer it to stochastic interface problems. The theoretical findings are complemented by numerical examples for both, stochastic interface problems and boundary value problems on random domains.

1. INTRODUCTION

Many problems in science and engineering lead to boundary value problems for an unknown function. In general, the numerical simulation is well understood provided that the input parameters are given exactly. Often, however, the input parameters are not known exactly. Especially, the treatment of uncertainties in the computational domain has become of growing interest, see e.g. [6, 19, 34, 37]. Here, we consider the elliptic diffusion equation

$$-\operatorname{div}\big(\alpha\nabla u(\omega)\big) = f \text{ in } D(\omega), \quad u(\omega) = 0 \text{ on } \partial D(\omega), \tag{1}$$

as a model problem where the underlying domain $D \subset \mathbb{R}^d$ or respectively its boundary ∂D are random. For example, one might think of tolerances in the shape of products fabricated by line production or shapes which stem from inverse problems, like e.g. tomography. Besides the fictitious domain approach considered in [6], one might essentially distinguish two approaches: the *perturbation method* and the *domain mapping method*.

The perturbation method starts with a prescribed perturbation field

$$\mathbf{V}(\omega)\colon \partial D_{\text{ref}} \to \mathbb{R}^d$$

at the boundary ∂D_{ref} and uses a *shape Taylor expansion* with respect to this perturbation field to represent the solution to (1), cf. [15, 19]. Whereas, the domain mapping method requires that the perturbation field is also known in the interior of the domain D_{ref}, i.e.

$$\mathbf{V}(\omega)\colon \overline{D_{\text{ref}}} \to \mathbb{R}^d.$$

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Then, the problem may be transformed to the nominal, fixed domain D_{ref}. This yields a partial differential equation with correlated stochastic diffusion matrix and right hand side, cf. [7, 28, 34, 37].

The major drawback of the perturbation method is that it is only feasible for relatively small perturbations. Thus, in order to treat larger perturbations, the domain mapping method is the method of choice. Nevertheless, it might in practice be much easier to obtain measurements from the outside of a workpiece to estimate the perturbation field $\mathbf{V}(\omega)$ rather than from its interior. If no information of the vector field inside the domain is available, it has to be extended appropriately, e.g. by the Laplacian, as proposed in [28, 37].

We would like to point out that the two approaches are in fact not comparable at all. In the perturbation method, we use a problem description in terms of *Eulerian coordinates*, which means that we keep the points fixed and perturb just the domain's boundary. When considering the domain mapping method, we change to *Lagrangian coordinates*, which means that we keep track of the movement of each point. The correspondence between those two approaches can be expressed in terms of the *local shape derivative* $\delta u[\mathbf{V}(\omega)]$ and the *material derivative* $\dot{u}[\mathbf{V}(\omega)]$ of a given function u which differ by a transport term, cf. [33]:

$$\dot{u}[\mathbf{V}(\omega)] = \delta u[\mathbf{V}(\omega)] + \langle \nabla u, \mathbf{V}(\omega) \rangle.$$

In this article, we focus on the domain mapping method. In [7], it is shown for a specific class of variation fields that the solution to (1) provides analytic regularity with respect to the stochastic parameter. We will generalize the result from [7] to arbitrary domain perturbation fields which are described by their mean $\mathbb{E}[\mathbf{V}]\colon D_{\text{ref}} \to \mathbb{R}^d$, $\mathbb{E}[\mathbf{V}](\mathbf{x}) = \big[\mathbb{E}[v_1](\mathbf{x}), \ldots, \mathbb{E}[v_d](\mathbf{x})\big]^\intercal$ and their (matrix-valued) covariance function

$$\operatorname{Cov}[\mathbf{V}]\colon D_{\text{ref}} \times D_{\text{ref}} \to \mathbb{R}^{d\times d}, \quad \operatorname{Cov}[\mathbf{V}](\mathbf{x},\mathbf{x}') = \begin{bmatrix} \operatorname{Cov}_{1,1}(\mathbf{x},\mathbf{x}') & \cdots & \operatorname{Cov}_{1,d}(\mathbf{x},\mathbf{x}') \\ \vdots & & \vdots \\ \operatorname{Cov}_{d,1}(\mathbf{x},\mathbf{x}') & \cdots & \operatorname{Cov}_{d,d}(\mathbf{x},\mathbf{x}') \end{bmatrix}.$$

Taking the Karhunen-Loève expansion of $\mathbf{V}(\omega)$ as the starting point, we show decay rates for the derivatives of the solution to (1) with respect to the stochastic parameter. Given that the Karhunen-Loève expansion decays fast enough, our results imply the dimension independent convergence of the quasi-Monte Carlo method based on the Halton sequence, cf. [14, 17, 35]. Moreover, our results are convenient for the convergence theory of the anisotropic sparse collocation, cf. [29], and best N-term approximations, cf. [9]. The decay estimates can yet be sharpened in case of univariate derivatives, as they enter the error estimates in the stochastic collocation, cf. [3]. Although the presented results allow for a broad variety of methods for the stochastic approximation, we employ the quasi-Monte Carlo method in our numerical examples for the sake of simplicity.

For the spatial approximation, we propose to use parametric finite elements. Then, we are able to approximate the mean and the variance of the solution to (1) by computing each sample on the particular realization $D(\omega_i) = \mathbf{V}(D_{\text{ref}}, \omega_i)$ of the stochastic domain rather than on the reference domain D_{ref}. This yields a non-intrusive approach to solve the problem under consideration. In fact, any available finite element solver can be employed to compute the particular samples. Following this approach rather than mapping the diffusion problem always to the reference domain, we can easily treat also stochastic interface problems, cf. [15].

The rest of this article is organized as follows. In Section 2, we introduce some basic definitions and notation. Section 3 is dedicated to the vector-valued Karhunen-Loève decomposition. Although this is a straightforward adaption of the state of the art literature [30], we think that it is useful to explicitly introduce the related spaces, norms and operators. In Section 4, we present the essential contribution of this article: the regularity of the solution to the model problem defined in Section 2 with respect to the Karhunen-Loève expansion of the perturbation field. The results from Section 4 can considerably be sharpened if only univariate derivatives are taken into account. This topic is discussed separately in Section 5. Section 6 introduces parametric finite elements which are the basic ingredient for the numerical realization of our approach. In Section 7, we extend our approach to stochastic interface problems. Finally, Section 8 provides numerical examples to validate and quantify the theoretical findings.

In the following, in order to avoid the repeated use of generic but unspecified constants, by $C \lesssim D$ we mean that C can be bounded by a multiple of D, independently of parameters which C and D may depend on. Obviously, $C \gtrsim D$ is defined as $D \lesssim C$,and $C \approx D$ as $C \lesssim D$ and $C \gtrsim D$.

2. Problem formulation

Let $D_{\text{ref}} \subset \mathbb{R}^d$ for $d \in \mathbb{N}$ (of special interest are the cases $d = 2, 3$) denote a domain with Lipschitz continuous boundary ∂D_{ref} and let $(\Omega, \mathcal{F}, \mathbb{P})$ be a complete probability space with σ-field $\mathcal{F} \subset 2^\Omega$ and probability measure $\mathbb{P}$. In order to guarantee that $L^2_{\mathbb{P}}(\Omega)$ exhibits an orthonormal basis, we further assume that Ω is a separable set. Let $\mathbf{V}\colon \overline{D_{\text{ref}}} \times \Omega \to \mathbb{R}^d$ be an invertible vector field of class C^2, i.e. $\mathbf{V}$ is twice continuously differentiable with respect to $\mathbf{x}$ for almost every $\omega \in \Omega$. Moreover, we impose the uniformity condition $\|\mathbf{V}(\omega)\|_{C^2(\overline{D_{\text{ref}}};\mathbb{R}^d)}, \|\mathbf{V}^{-1}(\omega)\|_{C^2(\overline{D_{\text{ref}}};\mathbb{R}^d)} \leq C$ for some $C \in (0, \infty)$ and almost every $\omega \in \Omega$.[1] Thus, $\mathbf{V}$ defines a family of domains $D(\omega) := \mathbf{V}(D_{\text{ref}}, \omega)$.

For the subsequent analysis, we restrict ourselves to the case of the Poisson equation, i.e. $\alpha \equiv 1$,

$$-\Delta u(\mathbf{x}, \omega) = f(\mathbf{x}) \text{ in } D(\omega), \quad u(\mathbf{x}, \omega) = 0 \text{ on } \Gamma(\omega). \tag{2}$$

This considerably simplifies the analysis and the extension to non-constant diffusion coefficients is straightforward, cf. Remark 4.8. In order to guarantee solvability for almost every $\omega \in \Omega$, we consider the right hand side to be defined on the *hold-all* domain

$$\mathcal{D} := \bigcup_{\omega \in \Omega} D(\omega). \tag{3}$$

From the uniformity condition, we infer for almost every $\omega \in \Omega$ and every $\mathbf{x} \in D$ that the singular-values of the vector field $\mathbf{V}$'s Jacobian $\mathbf{J}(\omega, \mathbf{x})$ satisfy

$$0 < \underline{\sigma} \leq \min\big\{\sigma\big(\mathbf{J}(\mathbf{x}, \omega)\big)\big\} \leq \max\big\{\sigma\big(\mathbf{J}(\mathbf{x}, \omega)\big)\big\} \leq \overline{\sigma} < \infty. \tag{4}$$

In particular, we assume without loss of generality that $\underline{\sigma} \leq 1$ and $\overline{\sigma} \geq 1$.

[1] Regard that for the analysis it is sufficient to assume that $\mathbf{V}$ is a C^1-diffeomorphism and satisfies the uniformity in $C^1(\overline{D_{\text{ref}}}; \mathbb{R}^d)$. Nevertheless, in order to obtain H^2-regularity of the model problem, we make this stronger assumption.

2.1. **Reformulation on the reference domain.** In the sequel, we consider the spaces $H_0^1\big(D(\omega)\big)$ and $H_0^1(D_{\rm ref})$ to be equipped with the norms $\|\cdot\|_{H^1(D(\omega))} := \|\nabla\cdot\|_{L^2(D(\omega);\mathbb{R}^d)}$ and $\|\cdot\|_{H^1(D_{\rm ref})} := \|\nabla\cdot\|_{L^2(D_{\rm ref};\mathbb{R}^d)}$, respectively. Furthermore, we assume that the related dual spaces $H^{-1}\big(D(\omega)\big)$ and $H^{-1}(D_{\rm ref})$ are defined with respect to these norms. The main tool we use in the convergence analysis for the model problem (2) is the one-to-one correspondence between the problem which is pulled back to the reference domain $D_{\rm ref}$ and the problem on the actual realization $D(\omega)$. The equivalence between those two problems is described by the vector field $\mathbf{V}(\mathbf{x},\omega)$. For an arbitrary function v on $D(\omega)$, we denote the transported function by $\hat{v}(\mathbf{x},\omega) := (v\circ\mathbf{V})(\mathbf{x},\omega)$. According to the chain rule, we have for $v\in C^1\big(D(\omega)\big)$

$$(\nabla v)\big(\mathbf{V}(\mathbf{x},\omega)\big) = \mathbf{J}(\mathbf{x},\omega)^{-\intercal}\nabla\hat{v}(\mathbf{x},\omega). \tag{5}$$

For given $\omega\in\Omega$, the variational formulation for the model problem (2) is given as follows: Find $u(\omega)\in H_0^1\big(D(\omega)\big)$ such that

$$\int_{D(\omega)}\langle\nabla u,\nabla v\rangle\,\mathrm{d}\mathbf{x} = \int_{D(\omega)} fv\,\mathrm{d}\mathbf{x}\quad\text{for all } v\in H_0^1\big(D(\omega)\big). \tag{6}$$

Thus, with

$$\mathbf{A}(\mathbf{x},\omega) := \big(\mathbf{J}(\mathbf{x},\omega)^\intercal\mathbf{J}(\mathbf{x},\omega)\big)^{-1}\det\mathbf{J}(\mathbf{x},\omega) \tag{7}$$

and

$$f_{\rm ref}(\mathbf{x},\omega) := \hat{f}(\mathbf{x},\omega)\det\mathbf{J}(\mathbf{x},\omega), \tag{8}$$

we obtain the following variational formulation with respect to the reference domain: Find $\hat{u}(\omega)\in H_0^1(D_{\rm ref})$ such that

$$\int_{D_{\rm ref}}\langle\mathbf{A}(\omega)\nabla\hat{u}(\omega),\nabla\hat{v}(\omega)\rangle\,\mathrm{d}\mathbf{x} = \int_{D_{\rm ref}} f_{\rm ref}(\omega)\hat{v}(\omega)\,\mathrm{d}\mathbf{x}\quad\text{for all } \hat{v}(\omega)\in H_0^1(D_{\rm ref}). \tag{9}$$

Here and afterwards, $\langle\cdot,\cdot\rangle$ denotes the canonical inner product for $\mathbb{R}^d$.

Remark 2.1. *Since $\mathbf{V}$ is assumed to be a C^2-diffeomorphism, we have for almost every $\omega\in\Omega$ that*

$$\mathbf{V}^{-1}\circ\mathbf{V} = \mathrm{Id}\quad\Rightarrow\quad\mathbf{J}^{-1}\mathbf{J} = \mathbf{I}\quad\Rightarrow\quad\det\mathbf{J}^{-1}\det\mathbf{J} = 1\quad\textit{for all } \mathbf{x}.$$

Herein, $\mathbf{I}\in\mathbb{R}^{d\times d}$ denotes the identity matrix. Especially, we infer $\det\mathbf{J}^{-1},\det\mathbf{J}\neq 0$. The continuity of $\mathbf{J},\mathbf{J}^{-1}$ and of the determinant function imply now that either $\det\mathbf{J}^{-1},\det\mathbf{J}>0$ or $\det\mathbf{J}^{-1},\det\mathbf{J}<0$ for all $\mathbf{x}$. Therefore, without loss of generality, we will assume the positiveness of the determinants.

Notice that equation (9) contains for fixed $v\in H_0^1\big(D(\omega)\big)$ the related transported test function $\hat{v}(\omega)$.

The connection between the spaces $H_0^1(D_{\rm ref})$ and $H_0^1\big(D(\omega)\big)$ is given by the following

Lemma 2.2. *The spaces $H_0^1(D_{\rm ref})$ and $H_0^1\big(D(\omega)\big)$ are isomorphic by the isomorphism*

$$\mathcal{E}\colon H_0^1(D_{\rm ref})\to H_0^1\big(D(\omega)\big),\quad v\mapsto v\circ\mathbf{V}(\omega)^{-1}.$$

The inverse mapping is given by

$$\mathcal{E}^{-1}\colon H_0^1\big(D(\omega)\big)\to H_0^1(D_{\rm ref}),\quad v\mapsto v\circ\mathbf{V}(\omega).$$

Proof. The proof of this lemma is a consequence of the chain rule (5) and the ellipticity assumption (4). □ □

This lemma implies that the space of test functions is not dependent on $\omega \in \Omega$ at all: Obviously, we have $H_0^1\big(D(\omega)\big) = \{\mathcal{E}(v) : v \in H_0^1(D_{\text{ref}})\}$. Thus, for an arbitrary function $\mathcal{E}(v) \in H_0^1\big(D(\omega)\big)$ it holds $\widehat{\mathcal{E}(v)} = \mathcal{E}(v) \circ \mathbf{V} = v \circ \mathbf{V}^{-1} \circ \mathbf{V} = v \in H_0^1(D_{\text{ref}})$ independent of $\omega \in \Omega$. In particular, the solutions u to (6) and $\hat{u}$ to (9) satisfy

$$\hat{u}(\omega) = u \circ \mathbf{V}(\omega) \quad \text{and} \quad u(\omega) = \hat{u} \circ \mathbf{V}(\omega)^{-1}. \tag{10}$$

3. Karhunen-Loève expansion

In order to make the stochastic vector field $\mathbf{V}(\mathbf{x}, \omega)$ feasible for computations, we consider here its *Karhunen-Loève expansion*, cf. [27]. This section shall give a brief overview of the relevant facts concerning the Karhunen-Loève expansion of vector valued random fields. Especially, we introduce here the related function spaces which are used in the rest of this article. For further details on the Karhunen-Loève expansion in general and also on computational aspects, we refer to [11, 12, 18, 30].

Let $D \subset \mathbb{R}^d$ always denote a domain. Then, we define $L^2(D; \mathbb{R}^d)$ to be the Hilbert space which consists of all equivalence classes of square integrable functions $\mathbf{v}\colon D \to \mathbb{R}^d$ equipped with the inner product

$$(\mathbf{u}, \mathbf{v})_{L^2(D;\mathbb{R}^d)} := \int_D \langle \mathbf{u}, \mathbf{v} \rangle \, \mathrm{d}\mathbf{x} \quad \text{for all } \mathbf{u}, \mathbf{v} \in L^2(D; \mathbb{R}^d).$$

We assume that the vector field $\mathbf{V}$ satisfies

$$\mathbf{V}(\mathbf{x}, \omega) = [v_1(\mathbf{x}, \omega), \ldots, v_d(\mathbf{x}, \omega)]^\intercal \in L_{\mathbb{P}}^2\big(\Omega; L^2(D; \mathbb{R}^d)\big).$$

Here and in the sequel, given a Banach space B and $1 \le p \le \infty$, the *Lebesgue-Bochner* space $L_{\mathbb{P}}^p(\Omega; B)$ consists of all strongly measurable functions $v : \Omega \to B$ whose norm

$$\|v\|_{L_{\mathbb{P}}^p(\Omega;B)} := \begin{cases} \left(\displaystyle\int_\Omega \|v(\cdot, \omega)\|_B^p \, \mathrm{d}\mathbb{P}(\omega) \right)^{1/p}, & p < \infty \\ \operatorname*{ess\,sup}_{\omega \in \Omega} \|v(\cdot, \omega)\|_B, & p = \infty \end{cases}$$

is finite. If $B = H$ is a separable Hilbert space and $p = 2$, then the Lebesgue-Bochner space is isomorphic to the tensor product space $L_{\mathbb{P}}^2(\Omega) \otimes H$ equipped with the inner product

$$(u, v)_{L_{\mathbb{P}}^2(\Omega;H)} := \int_\Omega \big(u(\cdot, \omega), v(\cdot, \omega)\big)_H \, \mathrm{d}\mathbb{P}(\omega),$$

cf. [2, 26].

The *mean* of $\mathbf{V}$ is given by $\mathbb{E}[\mathbf{V}](\mathbf{x}) = \big[\mathbb{E}[v_1](\mathbf{x}), \ldots, \mathbb{E}[v_d](\mathbf{x})\big]^\intercal$ with

$$\mathbb{E}[v_i](\mathbf{x}) := \int_\Omega v_i(\mathbf{x}, \omega) \, \mathrm{d}\mathbb{P}(\omega), \quad i = 1, 2, \ldots, d.$$

From the theory of Bochner integrals, see e.g. [26], it follows that $\mathbb{E}[v_i](\mathbf{x}) \in L^2(D)$ and thus $\mathbb{E}[\mathbf{V}](\mathbf{x}) \in L^2(D; \mathbb{R}^d)$. Furthermore, the (matrix-valued) *covariance function* of $\mathbf{V}$ is given by $\operatorname{Cov}[\mathbf{V}](\mathbf{x}, \mathbf{y}) = [\operatorname{Cov}_{i,j}(\mathbf{x}, \mathbf{y})]_{i,j=1}^d$ with

$$\operatorname{Cov}_{i,j}(\mathbf{x}, \mathbf{y}) = \mathbb{E}\Big[\big(v_i(\mathbf{x}, \omega) - \mathbb{E}[v_i](\mathbf{x})\big)\big(v_j(\mathbf{y}, \omega) - \mathbb{E}[v_j](\mathbf{y})\big)\Big].$$

We have $\operatorname{Cov}_{i,j}(\mathbf{x},\mathbf{y}) \in L^2(D\times D)$ which also follows from the properties of the Bochner integral and the application of the Cauchy-Schwarz inequality. We therefore conclude $\operatorname{Cov}[\mathbf{V}](\mathbf{x},\mathbf{y}) \in L^2(D \times D;\mathbb{R}^{d\times d})$ where we endowed the space $\mathbb{R}^{d\times d}$ with the inner product

$$\mathbf{A} : \mathbf{B} := \sum_{i,j=1}^{d} a_{i,j} b_{i,j} \quad \text{for } \mathbf{A},\mathbf{B} \in \mathbb{R}^{d\times d} \quad \text{with } \mathbf{A} = [a_{i,j}]_{i,j=1}^d,\ \mathbf{B} = [b_{i,j}]_{i,j=1}^d.$$

This particularly induces the inner product on $L^2(D \times D;\mathbb{R}^{d\times d})$ given by

$$(\mathbf{A},\mathbf{B})_{L^2(D\times D;\mathbb{R}^{d\times d})} := \int_D \int_D \mathbf{A} : \mathbf{B} \,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y} \quad \text{for } \mathbf{A},\mathbf{B} \in L^2(D \times D;\mathbb{R}^{d\times d}).$$

Now, we shall introduce the operator

$$\mathcal{S}\colon L^2_{\mathbb{P}}(\Omega) \to L^2(D;\mathbb{R}^d), \quad (\mathcal{S}X)(\mathbf{x}) := \int_\Omega \big(\mathbf{V}(\mathbf{x},\omega) - \mathbb{E}[\mathbf{V}](\mathbf{x})\big) X(\omega)\,\mathrm{d}\mathbb{P}(\omega) \tag{11}$$

and its adjoint

$$\mathcal{S}^\star\colon L^2(D;\mathbb{R}^d) \to L^2_{\mathbb{P}}(\Omega), \quad (\mathcal{S}^\star\mathbf{u})(\omega) := \int_D \big(\mathbf{V}(\mathbf{x},\omega) - \mathbb{E}[\mathbf{V}](\mathbf{x})\big)^\intercal \mathbf{u}(\mathbf{x})\,\mathrm{d}\mathbf{x}. \tag{12}$$

Then, there holds the following

Lemma 3.1. *The operators $\mathcal{S}$ and $\mathcal{S}^\star$ given by* (11) *and* (12)*, respectively, are bounded with Hilbert-Schmidt norms $\|\mathcal{S}\|_{\mathrm{HS}} = \|\mathcal{S}^\star\|_{\mathrm{HS}} = \|\mathbf{V} - \mathbb{E}[\mathbf{V}]\|_{L^2_{\mathbb{P}}(\Omega;L^2(D;\mathbb{R}^d))}$. Moreover, the* covariance operator

$$\mathcal{C}\colon L^2(D;\mathbb{R}^d) \to L^2(D;\mathbb{R}^d), \quad (\mathcal{C}\mathbf{v})(\mathbf{x}) := \int_D \operatorname{Cov}[\mathbf{V}](\mathbf{x},\mathbf{y})\mathbf{v}(\mathbf{y})\,\mathrm{d}\mathbf{y} = (\mathcal{S}\mathcal{S}^\star\mathbf{v})(\mathbf{x})$$

is a non-negative, symmetric, trace class operator with trace $\|\mathbf{V} - \mathbb{E}[\mathbf{V}]\|^2_{L^2_{\mathbb{P}}(\Omega;L^2(D;\mathbb{R}^d))}$.

Proof. The statement on the norms of $\mathcal{S}$ and $\mathcal{S}^\star$ follows by the application of Parseval's identity, see last part of the proof. Moreover, we have for all $\mathbf{u} \in L^2(D;\mathbb{R}^d)$ that

$$\begin{aligned}
(\mathcal{S}\mathcal{S}^\star\mathbf{u})(\mathbf{x}) &= \int_\Omega \big(\mathbf{V}(\mathbf{x},\omega) - \mathbb{E}[\mathbf{V}](\mathbf{x})\big) \int_D \big(\mathbf{V}(\mathbf{y},\omega) - \mathbb{E}[\mathbf{V}](\mathbf{y})\big)^\intercal \mathbf{u}(\mathbf{y})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbb{P}(\omega)\\
&= \int_D \bigg(\int_\Omega \big(\mathbf{V}(\mathbf{x},\omega) - \mathbb{E}[\mathbf{V}](\mathbf{x})\big)\big(\mathbf{V}(\mathbf{y},\omega) - \mathbb{E}[\mathbf{V}](\mathbf{y})\big)^\intercal \,\mathrm{d}\mathbb{P}(\omega)\bigg)\mathbf{u}(\mathbf{y})\,\mathrm{d}\mathbf{y}\\
&= \int_D \operatorname{Cov}[\mathbf{V}](\mathbf{x},\mathbf{y})\mathbf{u}(\mathbf{y})\,\mathrm{d}\mathbf{y} = (\mathcal{C}\mathbf{u})(\mathbf{x}).
\end{aligned}$$

In particular, $\mathcal{C}$ is non-negative and symmetric according to

$$(\mathcal{C}\mathbf{u},\mathbf{u})_{L^2(D;\mathbb{R}^d)} = (\mathcal{S}^\star\mathbf{u},\mathcal{S}^\star\mathbf{u})_{L^2_{\mathbb{P}}(\Omega)} = \|\mathcal{S}^\star\mathbf{u}\|^2_{L^2_{\mathbb{P}}(\Omega)} \geq 0.$$

Finally, to show that $\mathcal{C}$ is of trace class, let $\{\boldsymbol{\varphi}_k\}_k$ be an arbitrary orthonormal basis in $L^2(D;\mathbb{R}^d)$. We thus have

$$\begin{aligned}
\sum_k (\mathcal{C}\boldsymbol{\varphi}_k,\boldsymbol{\varphi}_k)_{L^2(D;\mathbb{R}^d)} &= \sum_k \|\mathcal{S}^\star\boldsymbol{\varphi}_k\|^2_{L^2_{\mathbb{P}}(\Omega)} = \int_\Omega \sum_k (\mathcal{S}^\star\boldsymbol{\varphi}_k)^2\,\mathrm{d}\mathbb{P}(\omega)\\
&= \int_\Omega \sum_k \bigg(\int_D \big(\mathbf{V}(\mathbf{x},\omega) - \mathbb{E}[\mathbf{V}](\mathbf{x})\big)^\intercal \boldsymbol{\varphi}_k\,\mathrm{d}\mathbf{x}\bigg)^2 \mathrm{d}\mathbb{P}(\omega)\\
&= \int_\Omega \int_D \langle \mathbf{V}(\mathbf{x},\omega) - \mathbb{E}[\mathbf{V}](\mathbf{x}), \mathbf{V}(\mathbf{x},\omega) - \mathbb{E}[\mathbf{V}](\mathbf{x})\rangle \,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbb{P}(\omega)\\
&= \|\mathbf{V} - \mathbb{E}[\mathbf{V}]\|^2_{L^2_{\mathbb{P}}(\Omega;L^2(D;\mathbb{R}^d))},
\end{aligned}$$

where we employed Parseval's identity in the second last step. □ □

Trace class operators are especially compact, see e.g. [23, 31], and exhibit hence a spectral decomposition.

Theorem 3.2. *Let $\mathcal{C}\colon L^2(D;\mathbb{R}^d) \to L^2(D;\mathbb{R}^d)$ be the covariance operator related to $\mathbf{V}(\mathbf{x},\omega) \in L^2_{\mathbb{P}}\big(\Omega; L^2(D;\mathbb{R}^d)\big)$. Then, there exists an orthonormal set $\{\boldsymbol{\varphi}_k\}_k$ and a sequence $\lambda_1 \geq \lambda_2 \geq \ldots \geq 0$ such that $\mathcal{C}\boldsymbol{\varphi}_k = \lambda_k\boldsymbol{\varphi}_k$ for all $k = 1,2,\ldots$. Furthermore, it holds*

$$\mathcal{C}\mathbf{u} = \sum_k \lambda_k (\mathbf{u}, \boldsymbol{\varphi}_k)_{L^2(D;\mathbb{R}^d)}\boldsymbol{\varphi}_k \quad \text{for all } \mathbf{u} \in L^2(D;\mathbb{R}^d).$$

Proof. For a proof of this theorem, we refer to [2]. □ □

We have now all prerequisites at hand to define the Karhunen-Loève decomposition of the vector field $\mathbf{V}(\mathbf{x},\omega) \in L^2_{\mathbb{P}}\big(\Omega; L^2(D;\mathbb{R}^d)\big)$.

Definition 3.3. *Let $\mathbf{V}(\mathbf{x},\omega)$ be a vector field in $L^2_{\mathbb{P}}\big(\Omega; L^2(D;\mathbb{R}^d)\big)$. The expansion*

$$\mathbf{V}(\mathbf{x},\omega) = E[\mathbf{V}](\mathbf{x}) + \sum_k \sigma_k \boldsymbol{\varphi}_k(\mathbf{x}) X_k(\omega) \tag{13}$$

with $\sigma_k = \sqrt{\lambda_k}$ and $X_k = \mathcal{S}^\star\boldsymbol{\varphi}_k/\sigma_k$, where $\{(\lambda_k,\boldsymbol{\varphi}_k)\}_k$ is the sequence of eigenpairs of the underlying covariance operator $\mathcal{C} = \mathcal{S}\mathcal{S}^\star$, is called Karhunen-Loève expansion *of $\mathbf{V}(\mathbf{x},\omega)$.*

The space $L^2(D;\mathbb{R}^d)$ served as pivot space for our considerations in the preceding derivation of the Karhunen-Loève expansion. In order to control the error of truncating the expansion after $M \in \mathbb{N}$ terms, i.e.

$$\bigg\| \mathbf{V}(\mathbf{x},\omega) - E[\mathbf{V}](\mathbf{x}) - \sum_{k=1}^{M} \sigma_k \boldsymbol{\varphi}_k(\mathbf{x}) X_k(\omega) \bigg\|_{L^2(\Omega; L^2(D;\mathbb{R}^d))} = \bigg(\sum_{k=M+1}^{\infty} \lambda_k \bigg)^{\frac{1}{2}}, \tag{14}$$

one has to study the decay of the singular values σ_k in the representation (13). The particular rate of decay is known to depend on the spatial regularity of $\mathbf{V}(\mathbf{x},\omega)$. To that end, we consider the Sobolev space $H^p(D;\mathbb{R}^d)$ for $p > 0$. The related inner product is given by

$$(\mathbf{u},\mathbf{w})_{H^p(D;\mathbb{R}^d)} := \sum_{|\boldsymbol{\alpha}| \leq p} \int_D \langle \partial^{\boldsymbol{\alpha}}\mathbf{u}, \partial^{\boldsymbol{\alpha}}\mathbf{w} \rangle \,\mathrm{d}\mathbf{x}$$

for $p \in \mathbb{N}$ and

$$(\mathbf{u},\mathbf{w})_{H^p(D;\mathbb{R}^d)} := (\mathbf{u},\mathbf{w})_{H^{\lfloor p \rfloor}(D;\mathbb{R}^d)} + \sum_{|\boldsymbol{\alpha}| = \lfloor p \rfloor} \int_D \int_D \frac{\|\partial^{\boldsymbol{\alpha}}\mathbf{u}(\mathbf{x}) - \partial^{\boldsymbol{\alpha}}\mathbf{w}(\mathbf{y})\|_2^2}{\|\mathbf{x}-\mathbf{y}\|_2^{d+2s}} \,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}$$

for $p = \lfloor p \rfloor + s$ with $s \in (0,1)$. Its dual space with respect to the L^2-duality pairing ist denoted as $\tilde{H}^{-p}(D;\mathbb{R}^d)$.

For given $\mathbf{V}(\mathbf{x},\omega) \in L^2_{\mathbb{P}}\big(\Omega; H^p(D;\mathbb{R}^d)\big)$, it obviously holds

$$\mathrm{Cov}_{i,j}(\mathbf{x},\mathbf{y}) \in H^p(D) \otimes H^p(D) \quad \text{for } i,j = 1,\ldots,d,$$

cf. [12]. Therefore, the following theorem is a straightforward modification of [12, Theorem 3.3] for the vector valued case.

Theorem 3.4. *Let $\mathbf{V}(\mathbf{x},\omega) \in L^2_{\mathbb{P}}\big(\Omega; H^p(D;\mathbb{R}^d)\big)$. Then, the eigenvalues of the covariance operator $\mathcal{C}\colon \tilde{H}^{-p}(D;\mathbb{R}^d) \to H^p(D;\mathbb{R}^d)$ decay like $\lambda_k \lesssim (k/d)^{-2p/d}$ as $k \to \infty$.*

We may summarize the results of this section as follows. If the mean $\mathbb{E}[\mathbf{V}](\mathbf{x})$ and the covariance function $\operatorname{Cov}[\mathbf{V}](\mathbf{x},\mathbf{y})$ as well as the distribution of $\mathbf{V}(\mathbf{x},\omega)$ are known or appropriately estimated, cf. [30], we are able to reconstruct the vector field $\mathbf{V}(\mathbf{x},\omega)$ from its Karhunen-Loève expansion. In the following, in order to make the Karhunen-Loève expansion feasible for numerical computations, we make some common assumptions:

Assumption 3.5.

(1) *The random variables* $\{X_k\}_k$ *are centered and take values in* $[-1,1]$, *i.e.* $X_k(\omega)\in[-1,1]$ *for all* k *and almost every* $\omega\in\Omega$.
(2) *The random variables* $\{X_k\}_k$ *are independent and identically distributed.*
(3) *The sequence* $\{\gamma_k\}_k := \big\{\|\sigma_k\boldsymbol{\varphi}_k\|_{W^{1,\infty}(D;\mathbb{R}^d)}\big\}_k$ *is at least in* $\ell^1(\mathbb{N})$. *We denote its norm by* $c_{\boldsymbol{\gamma}} := \sum_{k=1}^{\infty}\gamma_k$.

Here and hereafter, we shall equip the space $W^{1,\infty}(D;\mathbb{R}^d)$ with the equivalent norm $\|\mathbf{v}\|_{W^{1,\infty}(D;\mathbb{R}^d)} = \max\big\{\|\mathbf{v}\|_{L^\infty(D;\mathbb{R}^d)}, \|\mathbf{v}'\|_{L^\infty(D;\mathbb{R}^{d\times d})}\big\}$, where $\mathbf{v}'$ denotes the Jacobian of $\mathbf{v}$ and $\|\mathbf{v}'\|_{L^\infty(D;\mathbb{R}^{d\times d})} := \operatorname{ess\,sup}_{\mathbf{x}\in D}\|\mathbf{v}'(\mathbf{x})\|_2$. Herein, $\|\cdot\|_2$ corresponds to the usual 2-norm of matrices, i.e. the largest singular value.

4. Regularity of the solution

In this section, we assume that the vector field $\mathbf{V}(\mathbf{x},\mathbf{y})$ is given by a finite rank Karhunen-Loève expansion, i.e.

$$\mathbf{V}(\mathbf{x},\mathbf{y}) = \mathbb{E}[\mathbf{V}](\mathbf{x}) + \sum_{k=1}^{M}\sigma_k\boldsymbol{\varphi}_k(\mathbf{x})y_k,$$

otherwise it has to be truncated appropriately. Nevertheless, we provide in this section estimates which are independent of $M\in\mathbb{N}$. Thus, we explicitly allow M to become arbitrarily large.

For the rest of this article, we will refer to the randomness only via the coordinates $\mathbf{y}\in\square := [-1,1]^M$, where $\mathbf{y}=[y_1,\ldots,y_M]$. Notice that due to the independence of the random variables, the related push-forward measure $\mathbb{P}_{\mathbf{X}} := \mathbb{P}\circ\mathbf{X}^{-1}$ where $\mathbf{X}(\omega) := [X_1(\omega),\ldots X_M(\omega)]$ is of product structure. Furthermore, we always think of the spaces $L^p(\square)$ for $p\in[1,\infty]$ to be equipped with the measure $\mathbb{P}_{\mathbf{X}}$. Moreover, we set $\boldsymbol{\gamma} = [\gamma_k]_{k=1}^M$.

Without loss of generality, we may assume that $\mathbb{E}[\mathbf{V}](\mathbf{x}) = \mathbf{x}$ is the identity mapping. Otherwise, we replace D_{ref} by

$$\widetilde{D}_{\text{ref}} := \mathbb{E}[\mathbf{V}](D_{\text{ref}}) \quad\text{and}\quad \widetilde{\boldsymbol{\varphi}}_k := \sqrt{\det(\mathbb{E}[\mathbf{V}]^{-1})'}\,\boldsymbol{\varphi}_k\circ\mathbb{E}[\mathbf{V}]^{-1}.$$

Therefore, we obtain

$$\mathbf{V}(\mathbf{x},\mathbf{y}) = \mathbf{x} + \sum_{k=1}^{M}\sigma_k\boldsymbol{\varphi}_k(\mathbf{x})y_k \quad\text{and}\quad \mathbf{J}(\mathbf{x},\mathbf{y}) = \mathbf{I} + \sum_{k=1}^{M}\sigma_k\boldsymbol{\varphi}_k'(\mathbf{x})y_k. \tag{15}$$

In the subsequent regularity results, we shall refer to the following Lebesgue-Bochner spaces. We define the space $L^\infty\big(\square;L^\infty(D_{\text{ref}};\mathbb{R}^d)\big)$ as the set of all strongly measurable functions $\mathbf{V}\colon\square\to L^\infty(D_{\text{ref}};\mathbb{R}^d)$ with finite norm

$$|||\mathbf{V}|||_d := \operatorname*{ess\,sup}_{\mathbf{y}\in\square}\|\mathbf{V}(\mathbf{y})\|_{L^\infty(D_{\text{ref}};\mathbb{R}^d)}.$$

Furthermore, the space $L^\infty\big(\square; L^\infty(D_{\text{ref}}; \mathbb{R}^{d\times d})\big)$ consists of all strongly measurable functions $\mathbf{M}\colon \square \to L^\infty(D_{\text{ref}}; \mathbb{R}^{d\times d})$ with finite norm

$$|||\mathbf{M}|||_{d\times d} := \operatorname*{ess\,sup}_{\mathbf{y}\in\square} \|\mathbf{M}(\mathbf{y})\|_{L^\infty(D_{\text{ref}};\mathbb{R}^{d\times d})}.$$

We start by providing bounds on the derivatives of $\big(\mathbf{J}(\mathbf{x},\mathbf{y})^\intercal \mathbf{J}(\mathbf{x},\mathbf{y})\big)^{-1}$.

Lemma 4.1. *Let $\mathbf{J}\colon D_{\text{ref}} \times \square \to \mathbb{R}^{d\times d}$ be defined as in* (15)*. Then, it holds for the derivatives of*

$$\big(\mathbf{J}(\mathbf{x},\mathbf{y})^\intercal \mathbf{J}(\mathbf{x},\mathbf{y})\big)^{-1}$$

under the conditions of Assumption 3.5.3 that

$$\big|\big|\big|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} (\mathbf{J}^\intercal\mathbf{J})^{-1}\big|\big|\big|_{d\times d} \le |\boldsymbol{\alpha}|! \frac{\boldsymbol{\gamma}^{\boldsymbol{\alpha}}}{\underline{\sigma}^2} \left(\frac{2(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^2 \log 2}\right)^{|\boldsymbol{\alpha}|}.$$

Proof. We define $\mathbf{B}(\mathbf{x},\mathbf{y}) := \mathbf{J}(\mathbf{x},\mathbf{y})^\intercal \mathbf{J}(\mathbf{x},\mathbf{y})$ and $\tilde{\mathbf{A}}(\mathbf{x},\mathbf{y}) := \big(\mathbf{B}(\mathbf{x},\mathbf{y})\big)^{-1}$. Expanding the expression for $\mathbf{B}(\mathbf{x},\mathbf{y})$ yields

$$\mathbf{B}(\mathbf{x},\mathbf{y}) = \mathbf{I} + \sum_{k=1}^{M} \sigma_k \big(\boldsymbol{\varphi}_k'(\mathbf{x}) + \boldsymbol{\varphi}_k'(\mathbf{x})^\intercal\big) y_k + \sum_{k,k'=1}^{M} \sigma_k \sigma_{k'} \boldsymbol{\varphi}_k'(\mathbf{x})^\intercal \boldsymbol{\varphi}_{k'}'(\mathbf{x}) y_k y_{k'}.$$

Thus, the first order derivatives of $\mathbf{B}(\mathbf{x},\mathbf{y})$ are given by

$$\partial_{y_i} \mathbf{B}(\mathbf{x},\mathbf{y}) = \sigma_i \big(\boldsymbol{\varphi}_i'(\mathbf{x}) + \boldsymbol{\varphi}_i'(\mathbf{x})^\intercal\big) + \sum_{k=1}^{M} \sigma_i \sigma_k \big(\boldsymbol{\varphi}_i'(\mathbf{x})^\intercal \boldsymbol{\varphi}_k'(\mathbf{x}) + \boldsymbol{\varphi}_k'(\mathbf{x})^\intercal \boldsymbol{\varphi}_i'(\mathbf{x})\big) y_k \tag{16}$$

and the second order derivatives according to

$$\partial_{y_j}\partial_{y_i} \mathbf{B}(\mathbf{x},\mathbf{y}) = \sigma_i \sigma_j \big(\boldsymbol{\varphi}_i'(\mathbf{x})^\intercal \boldsymbol{\varphi}_j'(\mathbf{x}) + \boldsymbol{\varphi}_j'(\mathbf{x})^\intercal \boldsymbol{\varphi}_i'(\mathbf{x})\big). \tag{17}$$

Obviously, all higher order derivatives with respect to $\mathbf{y}$ vanish.

The ellipticity assumption (4) now yields the following bounds:

$$\underline{\sigma}^2 \le |||\mathbf{B}|||_{d\times d} \le \overline{\sigma}^2 \quad \text{and} \quad \frac{1}{\overline{\sigma}^2} \le \big|\big|\big|\tilde{\mathbf{A}}\big|\big|\big|_{d\times d} \le \frac{1}{\underline{\sigma}^2},$$

respectively. Furthermore, we derive from (16) that

$$\big|\big|\big|\partial_{y_i}\mathbf{B}\big|\big|\big|_{d\times d} \le 2\gamma_i + 2\gamma_i \sum_{k=1}^{M} \gamma_k \le 2(1+c_{\boldsymbol{\gamma}})\gamma_i$$

and from (17) that $\big|\big|\big|\partial_{y_j}\partial_{y_i}\mathbf{B}\big|\big|\big|_{d\times d} \le 2\gamma_i\gamma_j$. Thus, we have

$$\big|\big|\big|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\mathbf{B}\big|\big|\big|_{d\times d} \le \begin{cases} 2(1+c_{\boldsymbol{\gamma}})\boldsymbol{\gamma}^{\boldsymbol{\alpha}}, & \text{if } |\boldsymbol{\alpha}| = 1,2 \\ 0, & \text{if } |\boldsymbol{\alpha}| > 2. \end{cases} \tag{18}$$

Since $\tilde{\mathbf{A}} = v \circ \mathbf{B}$ is a composite function with $v(x) = x^{-1}$, we may employ *Faà di Bruno's formula*, cf. [10], which is a generalization of the chain rule, to compute its derivatives. For $n = |\boldsymbol{\alpha}|$ Faà di

Bruno's formula formally yields[2]

$$\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\tilde{\mathbf{A}}(\mathbf{x},\mathbf{y})=\sum_{r=1}^{n}(-1)^r r!\tilde{\mathbf{A}}(\mathbf{x},\mathbf{y})^{r+1}\sum_{P(\boldsymbol{\alpha},r)}\boldsymbol{\alpha}!\prod_{j=1}^{n}\frac{\big(\partial_{\mathbf{y}}^{\boldsymbol{\beta}_j}\mathbf{B}(\mathbf{x},\mathbf{y})\big)^{k_j}}{k_j!(\boldsymbol{\beta}_j!)^{k_j}}. \tag{19}$$

Here, the set $P(\boldsymbol{\alpha},r)$ contains restricted integer partitions of a multiindex $\boldsymbol{\alpha}$ into r non-vanishing multiindices, i.e.

$$\begin{aligned}P(\boldsymbol{\alpha},r):=\bigg\{&\big((k_1,\boldsymbol{\beta}_1),\ldots,(k_n,\boldsymbol{\beta}_n)\big)\in(\mathbb{N}_0\times\mathbb{N}_0^M)^n:\sum_{i=1}^{n}k_i\boldsymbol{\beta}_i=\boldsymbol{\alpha},\ \sum_{i=1}^{n}k_i=r,\\ &\text{and }\exists\,1\le s\le n: k_i=0\text{ and }\boldsymbol{\beta}_i=\mathbf{0}\text{ for all }1\le i\le n-s,\\ &k_i>0\text{ for all }n-s+1\le i\le n\text{ and }\mathbf{0}\prec\boldsymbol{\beta}_{n-s+1}\prec\cdots\prec\boldsymbol{\beta}_n\bigg\}.\end{aligned}$$

Herein, for multiindices $\boldsymbol{\beta},\boldsymbol{\beta}'\in\mathbb{N}_0^M$, the relation $\boldsymbol{\beta}\prec\boldsymbol{\beta}'$ means either $|\boldsymbol{\beta}|<|\boldsymbol{\beta}'|$ or, if $|\boldsymbol{\beta}|=|\boldsymbol{\beta}'|$, it denotes the lexicographical order which means that it holds that $\beta_1=\beta_1',\ldots,\beta_k=\beta_k'$ and $\beta_{k+1}<\beta_{k+1}'$ for some $0\le k<m$.

Taking the norm in (19), we derive the estimate

$$\begin{aligned}\big|\!\big|\!\big|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\tilde{\mathbf{A}}\big|\!\big|\!\big|_{d\times d}&\le\sum_{r=1}^{n}r!\big|\!\big|\!\big|\tilde{\mathbf{A}}\big|\!\big|\!\big|_{d\times d}^{r+1}\sum_{P(\boldsymbol{\alpha},r)}\boldsymbol{\alpha}!\prod_{j=1}^{n}\frac{\big|\!\big|\!\big|\partial_{\mathbf{y}}^{\boldsymbol{\beta}_j}\mathbf{B}\big|\!\big|\!\big|_{d\times d}^{k_j}}{k_j!(\boldsymbol{\beta}_j!)^{k_j}}\\ &\le\sum_{r=1}^{n}r!\bigg(\frac{1}{\underline{\sigma}^2}\bigg)^{r+1}\sum_{P(\boldsymbol{\alpha},r)}\boldsymbol{\alpha}!\prod_{j=1}^{n}\frac{\big(2(1+c_{\boldsymbol{\gamma}})\boldsymbol{\gamma}^{\boldsymbol{\beta}_j}\big)^{k_j}}{k_j!(\boldsymbol{\beta}_j!)^{k_j}}\\ &=\boldsymbol{\gamma}^{\boldsymbol{\alpha}}\sum_{r=1}^{n}r!\bigg(\frac{1}{\underline{\sigma}^2}\bigg)^{r+1}\big(2(1+c_{\boldsymbol{\gamma}})\big)^r\sum_{P(\boldsymbol{\alpha},r)}\boldsymbol{\alpha}!\prod_{j=1}^{n}\frac{1}{k_j!(\boldsymbol{\beta}_j!)^{k_j}}.\end{aligned}$$

From [10] we know that

$$\sum_{P(\boldsymbol{\alpha},r)}\boldsymbol{\alpha}!\prod_{j=1}^{n}\frac{1}{k_j!(\boldsymbol{\beta}_j!)^{k_j}}=S_{n,r},$$

where $S_{n,r}$ are the Stirling numbers of the second kind, cf. [1]. Thus, we obtain

$$\big|\!\big|\!\big|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\tilde{\mathbf{A}}\big|\!\big|\!\big|_{d\times d}\le\frac{\boldsymbol{\gamma}^{\boldsymbol{\alpha}}}{\underline{\sigma}^2}\sum_{r=1}^{n}r!\bigg(\frac{2(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^2}\bigg)^{r}S_{n,r}\le\frac{\boldsymbol{\gamma}^{\boldsymbol{\alpha}}}{\underline{\sigma}^2}\bigg(\frac{2(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^2}\bigg)^{|\boldsymbol{\alpha}|}\sum_{r=1}^{n}r!S_{n,r}.$$

The term $\tilde{b}(n):=\sum_{r=0}^{n}r!S_{n,r}$ coincides with the *n-th ordered Bell number*. The ordered Bell numbers satisfy the recurrence relation

$$\tilde{b}(n)=\sum_{r=0}^{n-1}\binom{n}{k}\tilde{b}(r)\quad\text{with }\tilde{b}(0)=1, \tag{20}$$

[2]With "formally" we mean that we ignore here the fact that the product of matrices is in general not Abelian. Nevertheless, a differentiation yields exactly the appearing products in a permuted order. The formal representation is justified since we only consider the norm of the representation in the sequel.

see [13], and may be estimated as follows[3], cf. [4],

$$\tilde{b}(n) \leq \frac{n!}{(\log 2)^n}. \tag{21}$$

This finally proves the assertion. □ □

The next lemma bounds the derivatives of $\det \mathbf{J}(\mathbf{x}, \mathbf{y})$.

Lemma 4.2. *Let* $\mathbf{J} \colon \square \to L^\infty(D_{\text{ref}}; \mathbb{R}^{d\times d})$ *be defined as in* (15)*. Then, it holds for the derivatives of* $\det \mathbf{J}(\mathbf{x}, \mathbf{y})$ *under the conditions of Assumption 3.5.3 that*

$$\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \det \mathbf{J}\big\|_{L^\infty(\square; L^\infty(D_{\text{ref}}))} \leq C_{\det} |\boldsymbol{\alpha}|! \overline{\sigma}^d \left(\frac{4}{\underline{\sigma}}\right)^{|\boldsymbol{\alpha}|} \tilde{\boldsymbol{\gamma}}^{\boldsymbol{\alpha}}$$

with the modified sequence $\tilde{\gamma}_k = \gamma_k k^{1+\varepsilon}/c_\varepsilon$ *for arbitrary* $\varepsilon > 0$ *with a normalization constant* $c_\varepsilon > 0$ *and a constant* $C_{\det}$ *depending on the modified sequence and the dimension* d*.*

Proof. We start from the identity

$$\det \exp(\mathbf{M}) = \exp(\operatorname{tr} \mathbf{M}), \tag{22}$$

which holds for any matrix $\mathbf{M} \in \mathbb{R}^{d\times d}$, cf. [22]. From this, we derive

$$\det \mathbf{M} = \exp(\operatorname{tr} \log \mathbf{M}), \tag{23}$$

where the matrix logarithm exists, whenever $\mathbf{M}$ is non-singular, cf. [22]. Now, the derivatives of the Jacobian $\mathbf{J}(\mathbf{x}, \mathbf{y})$ with respect to y_i satisfy $\big|\!\big|\!\big|\partial_{y_i} \mathbf{J}\big|\!\big|\!\big|_{d\times d} \leq \gamma_i$.

Faà di Bruno's formula yields formally with $\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \operatorname{tr} \log \mathbf{J}(\mathbf{x}, \mathbf{y}) = \operatorname{tr} \partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \log \mathbf{J}(\mathbf{x}, \mathbf{y})$ that

$$\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \operatorname{tr} \log \mathbf{J}(\mathbf{x}, \mathbf{y}) = \operatorname{tr}\left(\sum_{r=1}^{n} (-1)^{r-1}(r-1)! \mathbf{J}(\mathbf{x}, \mathbf{y})^{-r} \sum_{P(\boldsymbol{\alpha}, r)} \boldsymbol{\alpha}! \prod_{j=1}^{n} \frac{\big(\partial_{\mathbf{y}}^{\boldsymbol{\beta}_j} \mathbf{J}(\mathbf{x}, \mathbf{y})\big)^{k_j}}{k_j!(\boldsymbol{\beta}_j!)^{k_j}}\right).$$

Taking into account that $|\operatorname{tr} \mathbf{M}| \leq d \max\{\sigma(\mathbf{M})\}$, we obtain

$$\begin{aligned}
&\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \operatorname{tr} \log \mathbf{J}\big\|_{L^\infty(\square; L^\infty(D_{\text{ref}}))} \\
&\qquad \leq d \left|\!\left|\!\left| \sum_{r=1}^{n} (-1)^{r-1}(r-1)! \mathbf{J}^{-r} \sum_{P(\boldsymbol{\alpha}, r)} \boldsymbol{\alpha}! \prod_{j=1}^{n} \frac{\big(\partial_{\mathbf{y}}^{\boldsymbol{\beta}_j} \mathbf{J}\big)^{k_j}}{k_j!(\boldsymbol{\beta}_j!)^{k_j}} \right|\!\right|\!\right|_{d\times d}.
\end{aligned}$$

Furthermore, we may estimate

$$\begin{aligned}
&\left|\!\left|\!\left| \sum_{r=1}^{n} (-1)^{r-1}(r-1)! \mathbf{J}^{-r} \sum_{P(\boldsymbol{\alpha}, r)} \boldsymbol{\alpha}! \prod_{j=1}^{n} \frac{\big(\partial_{\mathbf{y}}^{\boldsymbol{\beta}_j} \mathbf{J}\big)^{k_j}}{k_j!(\boldsymbol{\beta}_j!)^{k_j}} \right|\!\right|\!\right|_{d\times d} \\
&\qquad \leq \sum_{r=1}^{n} (r-1)! \big|\!\big|\!\big|\mathbf{J}^{-1}\big|\!\big|\!\big|_{d\times d}^{r} \sum_{P(\boldsymbol{\alpha}, r)} \boldsymbol{\alpha}! \prod_{j=1}^{n} \frac{\big|\!\big|\!\big|\partial_{\mathbf{y}}^{\boldsymbol{\beta}_j} \mathbf{J}\big|\!\big|\!\big|_{d\times d}^{k_j}}{k_j!(\boldsymbol{\beta}_j!)^{k_j}} \leq (|\boldsymbol{\alpha}|-1)! \left(\frac{1}{\underline{\sigma}}\right)^{|\boldsymbol{\alpha}|} \boldsymbol{\gamma}^{\boldsymbol{\alpha}}.
\end{aligned}$$

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[3] A more rigorous bound on the ordered Bell numbers is provided by [36]. There, it is shown that

$$\tilde{b}(n) = \frac{n!}{2(\log 2)^{n+1}} + \mathcal{O}\big((0.16)^n n!\big).$$

Nevertheless, for our purposes, the bound from [4] is sufficient.

The last inequality holds due to the fact that all derivatives of $\mathbf{J}$ vanish for $|\boldsymbol{\beta}_j| > 1$. Thus, only if $\boldsymbol{\beta}_j = \mathbf{0}$ or $\boldsymbol{\beta}_j = \mathbf{e}_i$, where $\mathbf{e}_i$ is the i-th unit vector, the related summand does not vanish. Due to the definition of $P(\boldsymbol{\alpha}, r)$, this choice of $\boldsymbol{\beta}_j$ is only possible if $r = |\boldsymbol{\alpha}|$. Thus, we arrive at

$$\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \operatorname{tr}\log\mathbf{J}\right\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))} \le d|\boldsymbol{\alpha}|!\left(\frac{1}{\underline{\sigma}}\right)^{|\boldsymbol{\alpha}|}\boldsymbol{\gamma}^{\boldsymbol{\alpha}}. \tag{24}$$

By spending a convergent series, i.e. $\{c_\varepsilon/k^{1+\varepsilon}\}_k$, with normalization constant c_ε, we have by Lemma .1 from the Appendix that

$$\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \operatorname{tr}\log\mathbf{J}\right\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))} \le d\tilde{c}\boldsymbol{\alpha}!\left(\frac{1}{\underline{\sigma}}\right)^{|\boldsymbol{\alpha}|}\tilde{\boldsymbol{\gamma}}^{\boldsymbol{\alpha}} \tag{25}$$

with $\tilde{c} = 1/(1-c_\varepsilon)$.

The combination of (23) and (25) provides

$$\begin{aligned}
&\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \det\mathbf{J}\right\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))} = \left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \exp\big(\operatorname{tr}\log\mathbf{J}\big)\right\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\\
&\quad= \left\|\sum_{r=1}^{n}\exp\big(\operatorname{tr}\log\mathbf{J}\big)\sum_{P(\boldsymbol{\alpha},r)}\boldsymbol{\alpha}!\prod_{j=1}^{n}\frac{\big(\partial_{\mathbf{y}}^{\boldsymbol{\beta}_j}\operatorname{tr}\log\mathbf{J}\big)^{k_j}}{k_j!(\boldsymbol{\beta}_j!)^{k_j}}\right\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\\
&\quad\le \|\det\mathbf{J}\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\sum_{r=1}^{n}\sum_{P(\boldsymbol{\alpha},r)}\boldsymbol{\alpha}!\prod_{j=1}^{n}\frac{\Big(d\tilde{c}\boldsymbol{\beta}_j!\big(\frac{1}{\underline{\sigma}}\big)^{|\boldsymbol{\beta}_j|}\tilde{\boldsymbol{\gamma}}^{\boldsymbol{\beta}_j}\Big)^{k_j}}{k_j!(\boldsymbol{\beta}_j!)^{k_j}}\\
&\quad= \|\det\mathbf{J}\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\left(\frac{1}{\underline{\sigma}}\right)^{|\boldsymbol{\alpha}|}\tilde{\boldsymbol{\gamma}}^{\boldsymbol{\alpha}}\sum_{r=1}^{n}(d\tilde{c})^r\sum_{P(\boldsymbol{\alpha},r)}\boldsymbol{\alpha}!\prod_{j=1}^{n}\frac{1}{k_j!}.
\end{aligned}$$

Now, the application of Lemma .3 from the Appendix gives us

$$\begin{aligned}
&\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \det\mathbf{J}\right\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\\
&\quad\le \|\det\mathbf{J}\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\left(\frac{1}{\underline{\sigma}}\right)^{|\boldsymbol{\alpha}|}\tilde{\boldsymbol{\gamma}}^{\boldsymbol{\alpha}}\sum_{r=1}^{n}(d\tilde{c})^r\frac{|\boldsymbol{\alpha}|!}{r!}\binom{|\boldsymbol{\alpha}|+r-1}{r-1}.
\end{aligned}$$

It holds by the ellipticity assumption (4) that

$$\underline{\sigma}^d \le \det\mathbf{J}(\mathbf{x},\mathbf{y}) \le \overline{\sigma}^d \tag{26}$$

for almost every $\mathbf{y}\in\square$. Noticing in addition that

$$\sum_{r=1}^{n}(d\tilde{c})^r\frac{1}{r!}\binom{|\boldsymbol{\alpha}|+r}{r} \le \sum_{r=1}^{n}\frac{(d\tilde{c})^r}{r!}\sum_{r=1}^{n}\binom{|\boldsymbol{\alpha}|+r}{r} \le e^{d\tilde{c}}2^{2|\boldsymbol{\alpha}|},$$

we end up with the assertion due to

$$\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \det\mathbf{J}\right\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))} \le |\boldsymbol{\alpha}|!\overline{\sigma}^d\left(\frac{4}{\underline{\sigma}}\right)^{|\boldsymbol{\alpha}|}e^{d\tilde{c}}\tilde{\boldsymbol{\gamma}}^{\boldsymbol{\alpha}}.$$

□ □

The application of the Leibniz rule now yields a regularity estimate for the diffusion matrix $\mathbf{A}(\mathbf{x},\mathbf{y})$.

Theorem 4.3. *The derivatives of the diffusion matrix $\mathbf{A}(\mathbf{x},\mathbf{y})$ defined in (7) satisfy*

$$\left|\!\left|\!\left|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\mathbf{A}\right|\!\right|\!\right|_{d\times d} \le C_{\det}(|\boldsymbol{\alpha}|+1)!\frac{\overline{\sigma}^d}{\underline{\sigma}^2}\left(\frac{4(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^2\log 2}\right)^{|\boldsymbol{\alpha}|}\tilde{\boldsymbol{\gamma}}^{\boldsymbol{\alpha}},$$

where $\tilde{\boldsymbol{\gamma}}$ is the modified sequence from the previous Lemma.

Proof. The Leibniz rule for $\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\mathbf{A}(\mathbf{x},\mathbf{y})$ reads as

$$\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\mathbf{A}(\mathbf{x},\mathbf{y}) = \sum_{\boldsymbol{\alpha}'\le\boldsymbol{\alpha}} \binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'} \partial_{\mathbf{y}}^{\boldsymbol{\alpha}'} \big(\mathbf{J}(\mathbf{x},\mathbf{y})^\intercal \mathbf{J}(\mathbf{x},\mathbf{y})\big)^{-1} \partial_{\mathbf{y}}^{\boldsymbol{\alpha}-\boldsymbol{\alpha}'} \det \mathbf{J}(\mathbf{x},\mathbf{y}).$$

Inserting the results of Lemma 4.1 and Lemma 4.2 yields

$$\begin{aligned}
&\big|\big|\big|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\mathbf{A}\big|\big|\big|_{d\times d} \\
&\le \sum_{\boldsymbol{\alpha}'\le\boldsymbol{\alpha}} \binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'} |\boldsymbol{\alpha}'|! \frac{\boldsymbol{\gamma}^{\boldsymbol{\alpha}'}}{\underline{\sigma}^2} \left(\frac{2(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^2\log 2}\right)^{|\boldsymbol{\alpha}'|} |\boldsymbol{\alpha}-\boldsymbol{\alpha}'|!\overline{\sigma}^d C_{\det} \left(\frac{4}{\underline{\sigma}}\right)^{|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|} \tilde{\boldsymbol{\gamma}}^{\boldsymbol{\alpha}-\boldsymbol{\alpha}'} \\
&\le \frac{\overline{\sigma}^d}{\underline{\sigma}^2} \left(\frac{4(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^2\log 2}\right)^{|\boldsymbol{\alpha}|} \tilde{\boldsymbol{\gamma}}^{\boldsymbol{\alpha}} \sum_{\boldsymbol{\alpha}'\le\boldsymbol{\alpha}} \binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'} |\boldsymbol{\alpha}'|!|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|!.
\end{aligned}$$

Now, we employ the combinatorial identity

$$\sum_{\substack{\boldsymbol{\alpha}'\le\boldsymbol{\alpha}\\ |\boldsymbol{\alpha}'|=j}} \binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'} = \binom{|\boldsymbol{\alpha}|}{j} \tag{27}$$

and obtain

$$\begin{aligned}
\sum_{\boldsymbol{\alpha}'\le\boldsymbol{\alpha}} \binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'} |\boldsymbol{\alpha}'|!|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|! &= \sum_{j=0}^{|\boldsymbol{\alpha}|} j!(|\boldsymbol{\alpha}|-j)! \sum_{\substack{\boldsymbol{\alpha}'\le\boldsymbol{\alpha}\\ |\boldsymbol{\alpha}'|=j}} \binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'} \\
&= \sum_{j=0}^{|\boldsymbol{\alpha}|} j!(|\boldsymbol{\alpha}|-j)! \binom{|\boldsymbol{\alpha}|}{j} = |\boldsymbol{\alpha}|! \sum_{j=0}^{|\boldsymbol{\alpha}|} 1 = (|\boldsymbol{\alpha}|+1)!.
\end{aligned}$$

□ □

In order to prove regularity results for the right hand side f_{ref} in (9), we have to assume that f is a smooth function.

Lemma 4.4. *Let $f \in C^\infty(\mathcal{D})$ be analytic, i.e. $\|\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} f\|_{L^\infty(\mathcal{D};\mathbb{R}^d)} \le \boldsymbol{\alpha}!\rho^{-|\boldsymbol{\alpha}|}c_f$ for all $\boldsymbol{\alpha} \in \mathbb{N}_0^d$ and some $\rho \in (0,1]$, and let Assumption 3.5.3 be satisfied. Then, the derivatives of $\hat{f} = f \circ \mathbf{V}$ are bounded by*

$$\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \hat{f}\big\|_{L^\infty(\square;L^\infty(D_{\text{ref}}))} \le |\boldsymbol{\alpha}|! c_f \left(\frac{d}{\rho\log 2}\right)^{|\boldsymbol{\alpha}|} \boldsymbol{\gamma}^{\boldsymbol{\alpha}}.$$

Proof. In view of (15), differentiation of $\mathbf{V}(\mathbf{x},\mathbf{y})$ yields $\partial_{y_i}\mathbf{V}(\mathbf{x},\mathbf{y}) = \sigma_i\boldsymbol{\varphi}_i(\mathbf{x})$. Thus, all higher order derivatives with respect to an arbitrary direction y_j vanish. The norm of the first order derivatives is bounded by $\big|\big|\big|\partial_{y_i}\mathbf{V}\big|\big|\big|_d \le \gamma_i$.

The rest of the proof is also based on the application of Faà di Bruno's formula. Nevertheless, we have this time to consider the multivariate case. To that end, we define the set $P(\boldsymbol{\alpha},\boldsymbol{\alpha}')$ given by

$$\begin{aligned}
P(\boldsymbol{\alpha},\boldsymbol{\alpha}') := \Bigg\{ \big((\mathbf{k}_1,\boldsymbol{\beta}_1),\ldots,(\mathbf{k}_n,\boldsymbol{\beta}_n)\big) \in (\mathbb{N}_0^d\times\mathbb{N}_0^M)^n : \sum_{i=1}^n |\mathbf{k}_i|\boldsymbol{\beta}_i = \boldsymbol{\alpha},\ \sum_{i=1}^n \mathbf{k}_i = \boldsymbol{\alpha}', \\
\text{and } \exists\, 1\le s\le n : |\mathbf{k}_j| = |\boldsymbol{\beta}_a| = 0 \text{ for all } 1\le i\le n-s, \\
|\mathbf{k}_i| \ne 0 \text{ for all } n-s+1\le i\le n \text{ and } \mathbf{0}\prec\boldsymbol{\beta}_{n-s+1}\prec\cdots\prec\boldsymbol{\beta}_n \Bigg\}
\end{aligned}$$

with $n = |\boldsymbol{\alpha}|$. The application of the multivariate Faà di Bruno formula yields now

$$\begin{aligned}
&\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \hat{f}\big\|_{L^\infty(\square;L^\infty(D_{\text{ref}}))} \\
&\le \sum_{1\le|\boldsymbol{\alpha}'|\le n} \big\|\partial_{\mathbf{x}}^{\boldsymbol{\alpha}'} f\big\|_{L^\infty(\square;L^\infty(\mathcal{D}))} \sum_{P(\boldsymbol{\alpha},\boldsymbol{\alpha}')} \boldsymbol{\alpha}! \prod_{j=1}^{n} \frac{\big\|(\partial_{\mathbf{y}}^{\boldsymbol{\beta}_j}\mathbf{V})^{\mathbf{k}_j}\big\|_{L^\infty(\square;L^\infty(D_{\text{ref}}))}}{\mathbf{k}_j!(\boldsymbol{\beta}_j!)^{|\mathbf{k}_j|}} \\
&\le \sum_{1\le|\boldsymbol{\alpha}'|\le n} \boldsymbol{\alpha}'!\rho^{-|\boldsymbol{\alpha}'|} c_f \sum_{P(\boldsymbol{\alpha},\boldsymbol{\alpha}')} \boldsymbol{\alpha}! \prod_{j=1}^{n} \frac{\big(\boldsymbol{\gamma}^{\boldsymbol{\beta}_j}\big)^{\mathbf{k}_j}}{\mathbf{k}_j!(\boldsymbol{\beta}_j!)^{|\mathbf{k}_j|}} \\
&= c_f \boldsymbol{\gamma}^{\boldsymbol{\alpha}} \sum_{1\le|\boldsymbol{\alpha}'|\le n} \boldsymbol{\alpha}'!\rho^{-|\boldsymbol{\alpha}'|} \sum_{P(\boldsymbol{\alpha},\boldsymbol{\alpha}')} \boldsymbol{\alpha}! \prod_{j=1}^{n} \frac{1}{\mathbf{k}_j!(\boldsymbol{\beta}_j!)^{|\mathbf{k}_j|}}.
\end{aligned}$$

From [10], we know that

$$\sum_{|\boldsymbol{\alpha}'|=r} \sum_{P(\boldsymbol{\alpha},\boldsymbol{\alpha}')} \boldsymbol{\alpha}! \prod_{j=1}^{n} \frac{1}{\mathbf{k}_j!(\boldsymbol{\beta}_j!)^{|\mathbf{k}_j|}} = d^r S_{n,r},$$

where again $S_{n,r}$ is the Stirling number of the second kind. Thus, we obtain

$$\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} \hat{f}\big\|_{L^\infty(\square;L^\infty(D_{\text{ref}}))} \le c_f \boldsymbol{\gamma}^{\boldsymbol{\alpha}} \sum_{r=1}^{n} \left(\frac{d}{\rho}\right)^r r! S_{n,r} \le c_f \boldsymbol{\gamma}^{\boldsymbol{\alpha}} \left(\frac{d}{\rho}\right)^{|\boldsymbol{\alpha}|} \sum_{r=0}^{n} r! S_{n,r}.$$

Analogously to the proof of Lemma 4.1, we finally arrive at the assertion. □ □

Now, in complete analogy to Theorem 4.3, we have the following regularity result for the right hand side f_{ref}.

Theorem 4.5. *The derivatives of the right hand side $f_{\text{ref}}(\mathbf{x},\mathbf{y})$ defined in (8) satisfy*

$$\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} f_{\text{ref}}\big\|_{L^\infty(\square;L^\infty(D_{\text{ref}}))} \le (|\boldsymbol{\alpha}|+1)! c_f C_{\det} \overline{\sigma}^d \left(\frac{4d}{\underline{\sigma}\rho\log 2}\right)^{|\boldsymbol{\alpha}|} \tilde{\boldsymbol{\gamma}}^{\boldsymbol{\alpha}},$$

where $\tilde{\boldsymbol{\gamma}}$ is the modified sequence from Lemma 4.2.

Finally, we establish the dependency between the solution $\hat{u}$ to (9) and the data f_{ref}.

Lemma 4.6. *Let $\hat{u}(\mathbf{y})$ be the solution to (9) and $f_{\text{ref}} \in L^\infty\big(\square; L^\infty(D_{\text{ref}})\big)$. Then, there holds*

$$\|\hat{u}(\mathbf{y})\|_{H^1(D_{\text{ref}})} \le \frac{\overline{\sigma}^2}{\underline{\sigma}^d} c_D \|f_{\text{ref}}\|_{L^\infty(\square;L^\infty(D_{\text{ref}}))} \tag{28}$$

with a constant c_D only dependent on D_{ref} for almost every $\mathbf{y} \in \square$.

Proof. The bilinear form

$$(\mathbf{A}\nabla\,\cdot\,,\nabla\,\cdot\,)_{L^2(D_{\text{ref}};\mathbb{R}^d)}\colon H_0^1(D_{\text{ref}}) \times H_0^1(D_{\text{ref}}) \to \mathbb{R}$$

is coercive and bounded according to (4) and (26). It holds

$$\frac{\underline{\sigma}^d}{\overline{\sigma}^2} \|\hat{u}\|_{H^1(D_{\text{ref}})}^2 \le (\mathbf{A}\nabla\hat{u},\nabla\hat{u})_{L^2(D_{\text{ref}};\mathbb{R}^d)}$$

and

$$(\mathbf{A}\nabla\hat{u},\nabla\hat{v})_{L^2(D_{\text{ref}};\mathbb{R}^d)} \le \frac{\overline{\sigma}^d}{\underline{\sigma}^2} \|\hat{u}\|_{H^1(D_{\text{ref}})} \|\hat{v}\|_{H^1(D_{\text{ref}})}$$

for all $\hat{u}, \hat{v} \in H^1(D_{\text{ref}})$ and almost every $\mathbf{y} \in \square$. The assertion follows now by the application of the Lax-Milgram Lemma and the observation that

$$\|f_{\text{ref}}\|_{L^\infty(\square;H^{-1}(D_{\text{ref}}))} \leq \sqrt{|D_{\text{ref}}|}c_P\|f_{\text{ref}}\|_{L^\infty(\square;L^\infty(D_{\text{ref}}))},$$

where c_P denotes the Poincaré constant of D_{ref}. □ □

Combining the constants provided by Theorem 4.3 and Theorem 4.5 leads to the modified sequence

$$\{\mu_k\}_k := \left\{2C_{\text{det}} \max\left(\frac{4d\overline{\sigma}^d}{\underline{\sigma}\rho\log 2}, \frac{4\overline{\sigma}^d(1+c_\gamma)}{\underline{\sigma}^4\log 2}\right)\tilde{\gamma}_k\right\}_k.$$

Notice that we ignore here the fact that the constant $C_{\text{det}}\overline{\sigma}^d/\underline{\sigma}^2$ in the estimate for the diffusion matrix and the constant $C_{\text{det}}\overline{\sigma}^d$ in the estimate for the right hand side do only occur with multiplicity 1. Moreover, we introduce the additional factor 2 in order to obtain the factor $|\boldsymbol{\alpha}|!$ in the derivatives instead of the factor $(|\boldsymbol{\alpha}|+1)!$. Nevertheless, for the sake of readability, we also insert them into the sequence $\{\mu_k\}_k$.

Theorem 4.7. *The derivatives of the solution u to* (9) *satisfy under the assumptions of Lemma 4.1 and 4.5 that*

$$\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\big\|_{H^1(D_{\text{ref}})} \leq |\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}}\left(\frac{4\overline{\sigma}^2}{\underline{\sigma}^d}\max\{1, c_f c_D\}\right)^{|\boldsymbol{\alpha}|+1},$$

where c_D denotes the constant from the previous theorem.

Proof. Differentiating the variational formulation (9) with respect to $\mathbf{y}$ leads to

$$\Big(\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\big(\mathbf{A}(\mathbf{y})\nabla_{\mathbf{x}}\hat{u}(\mathbf{y})\big), \nabla_{\mathbf{x}}\hat{v}\Big)_{L^2(D_{\text{ref}};\mathbb{R}^d)} = \big(\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} f_{\text{ref}}(\mathbf{y}), \hat{v}\big)_{L^2(D_{\text{ref}};\mathbb{R})}.$$

The isomorphism of the spaces $H_0^1(D_{\text{ref}})$ and $H_0^1\big(D(\mathbf{y})\big)$ from Lemma 2.2 allows us to consider the test functions v to be independent of $\mathbf{y}$. Furthermore, the application of the Leibniz rule for the expression $\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\big(\mathbf{A}(\mathbf{y})\nabla_{\mathbf{x}}\hat{u}(\mathbf{y})\big)$ results in

$$\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\big(\mathbf{A}(\mathbf{y})\nabla_{\mathbf{x}}\hat{u}(\mathbf{y})\big) = \sum_{\boldsymbol{\alpha}'\leq\boldsymbol{\alpha}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'}\partial_{\mathbf{y}}^{\boldsymbol{\alpha}'}\mathbf{A}(\mathbf{y})\partial_{\mathbf{y}}^{\boldsymbol{\alpha}-\boldsymbol{\alpha}'}\nabla_{\mathbf{x}}\hat{u}(\mathbf{y}).$$

Thus, rearranging the preceding expression and using the linearity of the gradient, we arrive at

$$\begin{aligned}&\int_{D_{\text{ref}}}\mathbf{A}(\mathbf{y})\nabla_{\mathbf{x}}\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\nabla_{\mathbf{x}}v\,\mathrm{d}\mathbf{x}\\&\quad=\int_{D_{\text{ref}}}\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} f_{\text{ref}}(\mathbf{y})v\,\mathrm{d}\mathbf{x} - \sum_{\boldsymbol{\alpha}\neq\boldsymbol{\alpha}'\leq\boldsymbol{\alpha}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'}\int_{D_{\text{ref}}}\partial_{\mathbf{y}}^{\boldsymbol{\alpha}-\boldsymbol{\alpha}'}\mathbf{A}(\mathbf{y})\nabla_{\mathbf{x}}\partial_{\mathbf{y}}^{\boldsymbol{\alpha}'}\hat{u}(\mathbf{y})\nabla_{\mathbf{x}}v\,\mathrm{d}\mathbf{x}.\end{aligned}$$

By choosing $v = \partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})$ and by employing the estimates from Theorem 4.3 and Theorem 4.5, it follows that

$$\begin{aligned}&\frac{\underline{\sigma}^d}{\overline{\sigma}^2}\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\big\|_{H^1(D_{\text{ref}})}^2\\&\leq\int_{D_{\text{ref}}}\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} f_{\text{ref}}(\mathbf{y})\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\,\mathrm{d}\mathbf{x} - \sum_{\boldsymbol{\alpha}\neq\boldsymbol{\alpha}'\leq\boldsymbol{\alpha}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'}\int_{D_{\text{ref}}}\partial_{\mathbf{y}}^{\boldsymbol{\alpha}-\boldsymbol{\alpha}'}\mathbf{A}(\mathbf{y})\nabla_{\mathbf{x}}\partial_{\mathbf{y}}^{\boldsymbol{\alpha}'}\hat{u}(\mathbf{y})\nabla_{\mathbf{x}}\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\,\mathrm{d}\mathbf{x}\\&\leq|\boldsymbol{\alpha}|!c_f c_D\boldsymbol{\mu}^{\boldsymbol{\alpha}}\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\big\|_{H^1(D_{\text{ref}})}\\&\quad+\sum_{\boldsymbol{\alpha}\neq\boldsymbol{\alpha}'\leq\boldsymbol{\alpha}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'}|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|!\boldsymbol{\mu}^{\boldsymbol{\alpha}-\boldsymbol{\alpha}'}\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}'}\hat{u}(\mathbf{y})\big\|_{H^1(D_{\text{ref}})}\big\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\big\|_{H^1(D_{\text{ref}})}.\end{aligned}$$

From this, we obtain

$$\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\right\|_{H^1(D_{\mathrm{ref}})} \leq \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}} + \frac{C}{4}\sum_{\boldsymbol{\alpha}\neq\boldsymbol{\alpha}'\leq\boldsymbol{\alpha}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'}|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|!\boldsymbol{\mu}^{\boldsymbol{\alpha}-\boldsymbol{\alpha}'}\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}'}\hat{u}(\mathbf{y})\right\|_{H^1(D_{\mathrm{ref}})}$$

by setting

$$C := \frac{4\overline{\sigma}^2}{\underline{\sigma}^d}\max\{1, c_f c_D\}.$$

The proof is now by induction on $|\boldsymbol{\alpha}|$. The induction hypothesis is given by

$$\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\right\|_{H^1(D_{\mathrm{ref}})} \leq |\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}}C^{|\boldsymbol{\alpha}|+1}.$$

For $|\boldsymbol{\alpha}| = 0$, we conclude just the stability estimate (28), where the right hand side of the inequality is scaled by the factor 4. Therefore, let the assertion hold for all $|\boldsymbol{\alpha}| \leq n-1$ for some $n \geq 1$. Then, we have

$$\begin{aligned}
&\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\right\|_{H^1(D_{\mathrm{ref}})} \\
&\quad\leq \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}} + \frac{C}{4}\sum_{\boldsymbol{\alpha}\neq\boldsymbol{\alpha}'\leq\boldsymbol{\alpha}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'}|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|!\boldsymbol{\mu}^{\boldsymbol{\alpha}-\boldsymbol{\alpha}'}|\boldsymbol{\alpha}'|!\boldsymbol{\mu}^{\boldsymbol{\alpha}'}C^{|\boldsymbol{\alpha}'|+1} \\
&\quad\leq \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}} + \frac{C}{4}\boldsymbol{\mu}^{\boldsymbol{\alpha}}\sum_{\boldsymbol{\alpha}\neq\boldsymbol{\alpha}'\leq\boldsymbol{\alpha}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'}|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|!C^{|\boldsymbol{\alpha}'|+1} \\
&\quad= \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}} + \frac{C}{4}\boldsymbol{\mu}^{\boldsymbol{\alpha}}\sum_{j=0}^{n-1}\sum_{\substack{\boldsymbol{\alpha}'\leq\boldsymbol{\alpha}\\|\boldsymbol{\alpha}'|=j}}\binom{\boldsymbol{\alpha}}{\boldsymbol{\alpha}'}|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|!|\boldsymbol{\alpha}'|!C^{|\boldsymbol{\alpha}'|+1}.
\end{aligned}$$

Again, we make use of the combinatorial identity (27) and obtain the estimate

$$\begin{aligned}
\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\right\|_{H^1(D_{\mathrm{ref}})} &\leq \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}} + \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}}\sum_{j=0}^{n-1}\binom{|\boldsymbol{\alpha}|}{j}(|\boldsymbol{\alpha}|-j)!j!C^{|\boldsymbol{\alpha}'|+1} \\
&= \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}} + \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}}C\sum_{j=0}^{n-1}C^{|\boldsymbol{\alpha}'|} \\
&= \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}} + \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}}C\frac{C^{|\boldsymbol{\alpha}|}}{C-1}.
\end{aligned}$$

Now, the application of Lemma .4 from the Appendix gives us

$$\frac{C}{2}\frac{C^{|\boldsymbol{\alpha}|}}{C-1} \leq C^{|\boldsymbol{\alpha}|}$$

Since $C > 1$, we conclude

$$\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\right\|_{H^1(D_{\mathrm{ref}})} \leq \frac{C}{4}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}} + C\frac{C^{|\boldsymbol{\alpha}|}}{2}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}} \leq C^{|\boldsymbol{\alpha}|+1}|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}}.$$

This completes the proof. □ □

Taking into account the additional factor provided by the theorem, we end up with the sequence

$$\{\mu_k\}_k := \left\{\frac{8\overline{\sigma}^2}{\underline{\sigma}^d}C_{\mathrm{det}}\max\{1, c_f c_D\}\max\left(\frac{4d\overline{\sigma}^d}{\underline{\sigma}\rho\log 2}, \frac{4\overline{\sigma}^d(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^4\log 2}\right)\tilde{\gamma}_k\right\}_k$$

which yields in view of Theorem 4.7 that

$$\left\|\partial_{\mathbf{y}}^{\boldsymbol{\alpha}}\hat{u}(\mathbf{y})\right\|_{H^1(D_{\mathrm{ref}})} \leq C|\boldsymbol{\alpha}|!\boldsymbol{\mu}^{\boldsymbol{\alpha}}$$

with a constant $C > 0$ independent of the dimension M. Moreover, we observe $\mu_k \approx \gamma_k k^{1+\varepsilon}$. Therefore, we obtain for $\gamma_k \lesssim k^{-2-\delta}$ the analyticity of $\hat{u}$ by Lemma .1 from the Appendix for any $\varepsilon < \delta$.

Remark 4.8. *The discussion in this section only refers to the case of the Poisson equation. Of course, the analysis presented here straightforwardly applies also to the more general diffusion problem*

$$-\operatorname{div}\big(\alpha(\mathbf{x})\nabla u(\mathbf{x},\mathbf{y})\big) = f(\mathbf{x}) \quad \textit{for } \mathbf{x} \in D(\mathbf{y}).$$

In this case, one has to impose the restriction that $\alpha(\mathbf{x})$ is an analytic function which is bounded from above and below away from 0. Then, an estimate analogous to Lemma 4.4 applies for $\hat{\alpha}(\mathbf{x},\mathbf{y})$. The proof of a related Theorem 4.3 for $\hat{\alpha}(\mathbf{x},\mathbf{y})\mathbf{A}(\mathbf{x},\mathbf{y})$ then involves an additional application of the Leibniz rule.

Remark 4.9. *We can obtain similar approximation results for the moments of $\hat{u}$, i.e. for $\hat{u}^p$ with $p \in \mathbb{N}$, possibly with worse constants. To that end, one has to bound the derivatives of $\hat{u}^p$ with respect to $\mathbf{y}$, too. This is also achieved by the application of Faà di Bruno's formula. For an idea of the related proofs, we refer to* [17] *where this topic is discussed in case of a stochastic diffusion coefficient.*

5. Decay of the univariate derivatives

The results from the preceding section can be considerably sharpened if we only consider univariate derivatives $\partial_{y_i}^{\alpha}\hat{u}$ of the solution $\hat{u}$ to (9). The major obstruction in deriving estimates without powers of the term $|\boldsymbol{\alpha}|!$ in the estimates is the knowledge of proper bounds on the term $|\boldsymbol{\alpha}|!/\boldsymbol{\alpha}!$. To that end, we have only Lemma .1 at hand which tells us, that we have to spend a convergent series in order to bound the term $|\boldsymbol{\alpha}|!/\boldsymbol{\alpha}!$. The situation changes if one only considers univariate derivatives since then $|\alpha|! = \alpha!$ holds. This gives rise to a separate discussion of this situation.

We begin by sharpening the result on the derivatives of the Jacobian's determinant.

Lemma 5.1. *For the univariate derivatives of* $\det \mathbf{J}(\mathbf{x},\mathbf{y})$ *it holds under the condition of Assumption 3.5.3 that*

$$\big\|\partial_{y_i}^{\alpha}\det\mathbf{J}\big\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))} \le \alpha!\overline{\sigma}^d\left(\frac{2d}{\underline{\sigma}}\right)^{\alpha}\gamma_i^{\alpha}.$$

Proof. The univariate Faà di Bruno formula, cf. [10], yields

$$\begin{aligned}&\big\|\partial_{y_i}^{\alpha}\det\mathbf{J}\big\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\\ &\qquad = \left\|\sum_{r=1}^{\alpha}\exp\big(\operatorname{tr}\log\mathbf{J}\big)\sum_{P(\alpha,r)}\alpha!\prod_{j=1}^{\alpha}\frac{\big(\partial_{y_i}^{j}\operatorname{tr}\log\mathbf{J}\big)^{k_j}}{k_j!(j!)^{k_j}}\right\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\end{aligned}$$

with

$$P(\alpha,r) := \left\{(k_1,\ldots,k_\alpha)\in\mathbb{N}_0^{\alpha} : \sum_{i=1}^{\alpha}k_i = r,\ \sum_{i=1}^{\alpha}ik_i = \alpha\right\}.$$

It holds by estimate (24) that

$$\begin{aligned}
&\Big\|\sum_{r=1}^{\alpha}\exp\big(\operatorname{tr}\log\mathbf{J}\big)\sum_{P(\alpha,r)}\alpha!\prod_{j=1}^{\alpha}\frac{\big(\partial_{y_i}^{j}\operatorname{tr}\log\mathbf{J}\big)^{k_j}}{k_j!(j!)^{k_j}}\Big\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\\
&\qquad\le\sum_{r=1}^{\alpha}\big\|\exp\big(\operatorname{tr}\log\mathbf{J}\big)\big\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\sum_{P(\alpha,r)}\alpha!\prod_{j=1}^{\alpha}\frac{\Big(dj!\big(\frac{1}{\underline{\sigma}}\big)^{j}\gamma_i^{j}\Big)^{k_j}}{k_j!(j!)^{k_j}}\\
&\qquad\le\overline{\sigma}^{d}\Big(\frac{d}{\underline{\sigma}}\Big)^{\alpha}\gamma_i^{\alpha}\sum_{r=1}^{\alpha}\sum_{P(\alpha,r)}\alpha!\prod_{j=1}^{\alpha}\frac{1}{k_j!}.
\end{aligned}$$

Now, the assertion is easily obtained from the identity, cf. [10],

$$r!\sum_{P(\alpha,r)}\prod_{j=1}^{\alpha}\frac{1}{k_j!}=\binom{\alpha-1}{r-1}$$

and the estimate

$$\sum_{r=1}^{\alpha}\frac{\alpha!}{r!}\binom{\alpha-1}{r-1}\le 2^{\alpha}\alpha!.$$

□ □

The sharpened estimate for the Jacobian's determinant yields together with Lemma 4.1 an improved estimate for the univariate derivatives of the diffusion matrix $\mathbf{A}(\mathbf{x},\mathbf{y})$.

Theorem 5.2. *It holds for the univariate derivatives of the diffusion matrix $\mathbf{A}(\mathbf{x},\mathbf{y})$ that*

$$\big|\!\big|\!\big|\partial_{y_i}^{\alpha}\mathbf{A}\big|\!\big|\!\big|_{d\times d}\le(\alpha+1)!\frac{\overline{\sigma}^{d}}{\underline{\sigma}^{2}}\Big(\frac{2d(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^{2}\log 2}\Big)^{\alpha}\gamma_i^{\alpha}.$$

Proof. The Leibniz rule for $\partial_{y_i}^{\alpha}\mathbf{A}(\mathbf{x},\mathbf{y})$ yields

$$\partial_{y_i}^{\alpha}\mathbf{A}(\mathbf{x},\mathbf{y})=\sum_{r=0}^{\alpha}\binom{\alpha}{r}\partial_{y_i}^{r}\big(\mathbf{J}(\mathbf{x},\mathbf{y})^{\intercal}\mathbf{J}(\mathbf{x},\mathbf{y})\big)^{-1}\partial_{y_i}^{\alpha-r}\det\mathbf{J}(\mathbf{x},\mathbf{y}).$$

Inserting the estimates from Lemmata 4.1 and 5.1 yields

$$\begin{aligned}
\big|\!\big|\!\big|\partial_{y_i}^{\alpha}\mathbf{A}\big|\!\big|\!\big|_{d\times d}&\le\sum_{r=0}^{\alpha}\binom{\alpha}{r}r!\frac{\gamma_i^{r}}{\underline{\sigma}^{2}}\Big(\frac{2(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^{2}\log 2}\Big)^{r}(\alpha-r)!\overline{\sigma}^{d}\Big(\frac{2d}{\underline{\sigma}}\Big)^{\alpha-r}\gamma_i^{\alpha-r}\\
&\le\frac{\overline{\sigma}^{d}}{\underline{\sigma}^{2}}\Big(\frac{2d(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^{2}\log 2}\Big)^{\alpha}\gamma_i^{\alpha}\sum_{r=0}^{\alpha}\binom{\alpha}{r}r!(\alpha-r)!=(\alpha+1)!\frac{\overline{\sigma}^{d}}{\overline{\sigma}^{2}}\Big(\frac{2d(1+c_{\boldsymbol{\gamma}})}{\underline{\sigma}^{2}\log 2}\Big)^{\alpha}\gamma_i^{\alpha}.
\end{aligned}$$

□ □

In complete analogy to the previous theorem, we obtain a bound for the univariate derivatives of the right hand side f_{ref}.

Theorem 5.3. *It holds for the univariate derivatives of the right hand side $f_{\mathrm{ref}}(\mathbf{x},\mathbf{y})$ that*

$$\big\|\partial_{y_i}^{\alpha}f_{\mathrm{ref}}\big\|_{L^\infty(\square;L^\infty(D_{\mathrm{ref}}))}\le(\alpha+1)!c_f\overline{\sigma}^{d}\Big(\frac{2d}{\underline{\sigma}\rho\log 2}\Big)^{\alpha}\gamma_i^{\alpha}.$$

The results provided by Theorem 5.2 and Theorem 5.3 are sufficient to show that the solution $\hat{u}$ to (9) exhibits an analytic expansion into the complex plane with respect to each particular direction y_k. For a proof of this statement, see [3, Lemma 3.2]. This shows the applicability of the stochastic collocation method, cf. [3].

6. Curved domains and parametric finite elements

For the analysis of the regularity in the preceding section, we have exploited that there exists a one-to-one correspondence between the deterministic problem on the random domain and the random problem on the reference domain. For the computations, in contrast to [7, 37], we do however not aim at mapping the equation to the reference domain D_{ref} but rather to solve the equation on each particular realization $D(\mathbf{y}_i) = \mathbf{V}(D_{\mathrm{ref}}, \mathbf{y}_i)$ for a suitable set of samples $\{\mathbf{y}_i\}_{i=1}^N \subset \square$. A first step towards this approach is made by [28], where a random boundary variation is assumed and a mesh on the realization $D(\mathbf{y}_i)$ is generated via the solution of the Laplacian. Here, under the assumption that the random domain is obtained by a sufficiently smooth mapping $\mathbf{V}(\mathbf{y}_i)$, we will employ *parametric finite elements* to map the mesh on D_{ref} onto a mesh on $D(\mathbf{y}_i)$.

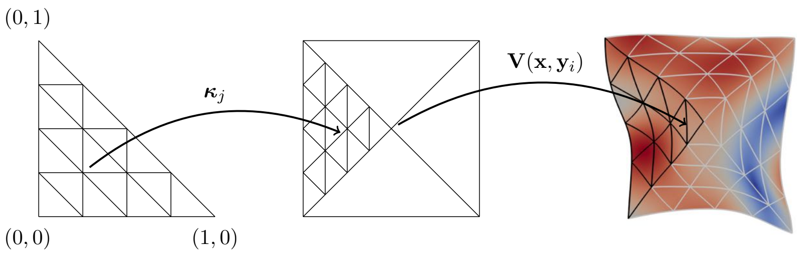

Figure 1. Construction of parametric finite elements.

We assume that the domain D_{ref} is given as a collection of simplicial smooth *patches*. More precisely, let $\triangle$ denote the reference simplex in $\mathbb{R}^d$. We assume that the domain D_{ref} is partitioned into K patches

$$\overline{D_{\mathrm{ref}}} = \bigcup_{j=1}^{K} \tau_{0,j}, \quad \tau_{0,j} = \boldsymbol{\kappa}_j(\triangle), \quad j = 1, 2, \ldots, K, \tag{29}$$

where each $\boldsymbol{\kappa}_j \colon \triangle \to \tau_{0,j}$ defines a diffeomorphism of $\triangle$ onto $\tau_{0,j}$. Thus, we have especially that

$$\frac{\sup\{\|\boldsymbol{\kappa}_j'(\mathbf{s})\mathbf{x}\|_2 : \mathbf{s} \in \triangle, \|\mathbf{x}\|_2 = 1\}}{\inf\{\|\boldsymbol{\kappa}_j'(\mathbf{s})\mathbf{x}\|_2 : \mathbf{s} \in \triangle, \|\mathbf{x}\|_2 = 1\}} \le \rho_j \quad \text{for all } j = 1, \ldots, K, \tag{30}$$

where $\boldsymbol{\kappa}_j'$ denotes as before the Jacobian of $\boldsymbol{\kappa}_j$. Since there are only finitely many patches, we may set $\rho := \max_{j=1}^K \rho_j$. The intersection $\tau_{0,j} \cap \tau_{0,j'}$, $j \neq j'$, of any two patches $\tau_{0,j}$ and $\tau_{0,j'}$ is supposed to be either $\emptyset$, or a common lower dimensional face.

A mesh on level ℓ on D_{ref} is now obtained by regular subdivisions of depth ℓ of the reference simplex into $2^{\ell d}$ sub-simplices. This generates the $2^{\ell d}$ elements $\{\tau_{\ell,j}\}_j$. In order to ensure that the triangulation $\mathcal{T}_\ell := \{\tau_{\ell,j}\}_j$ on the level ℓ forms a regular mesh on D_{ref}, the parametrizations $\{\boldsymbol{\kappa}_j\}_j$ are assumed to be C^0 compatible in the following sense: there exists a bijective, affine mapping $\boldsymbol{\Xi} : \triangle \to \triangle$ such that for all $\mathbf{x} = \boldsymbol{\kappa}_i(\mathbf{s})$ on a common interface of $\tau_{0,j}$ and $\tau_{0,j'}$ it holds that $\boldsymbol{\kappa}_j(\mathbf{s}) = (\boldsymbol{\kappa}_{j'} \circ \boldsymbol{\Xi})(\mathbf{s})$. In other words, the diffeomorphisms $\boldsymbol{\kappa}_j$ and $\boldsymbol{\kappa}_{j'}$ coincide at the common interface except for orientation. An illustration of such a triangulation is found in Figure 1. Notice that in our construction the local element mappings $\triangle \to \tau_{\ell,j}$ satisfy the same bound (30) by definition. Therefore, especially the uniformity condition for (iso-) parametric finite elements is fulfilled, cf. [5, 24].

Finally, we define the finite element ansatz functions via the parametrizations $\{\boldsymbol{\kappa}_j\}_j$ in the usual fashion, i.e. by lifting Lagrangian finite elements from $\triangle$ to the domain D_{ref} by using the mappings $\boldsymbol{\kappa}_j$. To that end, we define on the ℓ-th subdivision $\triangle_\ell$ of the reference domain the standard Lagrangian piecewise polynomial continuous finite elements $\Phi_\ell = \{\varphi_{\ell,i} : i \in \mathcal{I}_\ell\}$, where $\mathcal{I}_\ell$ denotes an appropriate index set. The corresponding finite element space is then given by

$$V_{\triangle,\ell} = \operatorname{span}\{\varphi_{\ell,j} : j \in \mathcal{I}_\ell\} = \{u \in C(\triangle) : u|_\tau \in \Pi_n \text{ for all } \tau \in \triangle_\ell\}$$

with $\dim V_{\triangle,\ell} \eqsim 2^{\ell d}$ and Π_n denoting the space of polynomials of degree at most n. Continuous basis functions whose support overlaps with several patches are obtained by gluing across patch boundaries, using the C^0 inter-patch compatibility. This yields a (nested) sequence of finite element spaces

$$V_{\text{ref},\ell} := \{v \in C(D_{\text{ref}}) : v|_{\boldsymbol{\kappa}_j(\triangle)} = \varphi \circ \boldsymbol{\kappa}_j^{-1}, \varphi \in V_{\triangle,\ell},\ j = 1, \ldots, K\} \subset H^1(D_{\text{ref}})$$

with $\dim V_{\text{ref},\ell} \eqsim 2^{\ell d}$. It is well known that the spaces $V_{\text{ref},\ell}$ satisfy the following Jackson and Bernstein type estimates for all $0 \le s \le t < 3/2$, $t \le q \le n+1$

$$\inf_{v_\ell \in V_{\text{ref},\ell}} \|u - v_\ell\|_{H^t(D_{\text{ref}})} \lesssim h_\ell^{q-t} \|u\|_{H^q(D_{\text{ref}})}, \quad u \in H^q(D_{\text{ref}}), \tag{31}$$

and

$$\|v_\ell\|_{H^t(D_{\text{ref}})} \lesssim h_\ell^{s-t} \|v_\ell\|_{H^s(D_{\text{ref}})}, \quad v_\ell \in V_{\text{ref},\ell}, \tag{32}$$

uniformly in ℓ, where we set $h_\ell := 2^{-\ell}$. Note that, by construction, h_ℓ scales like the mesh size $\max_k\{\operatorname{diam} \tau_{\ell,k}\}$, i.e. it holds $h_\ell \eqsim \max_k\{\operatorname{diam} \tau_{\ell,k}\}$ uniformly in $\ell \in \mathbb{N}$ due to (30).

We can employ the same argumentation to map the finite elements from the reference domain D_{ref} to the particular realization $D(\mathbf{y}) = \mathbf{V}(D_{\text{ref}}, \mathbf{y})$ for $\mathbf{y} \in \square$. The ellipticity condition (4) on the Jacobian $\mathbf{J}(\mathbf{x}, \omega)$ of the random vector field guarantees that (30) is satisfied with $\rho = \overline{\sigma}/\underline{\sigma}$. Also the Jackson and Bernstein type estimates (31) and (32) are still valid, where the only limitation is imposed by the smoothness of $\mathbf{V}(\mathbf{x}, \mathbf{y})$. If for example $\mathbf{V}(\mathbf{x}, \mathbf{y})$ is of class C^2, then we have the restriction $q \le 2$ such that

$$\inf_{v_\ell \in V_\ell(\mathbf{y})} \|u - v_\ell\|_{H^t(D(\mathbf{y}))} \lesssim h_\ell^{q-t} \|u\|_{H^q(D(\mathbf{y}))}$$

for all $0 \le t \le 3/2$, $t \le q \le 2$ where $V_\ell(\mathbf{y}) := \{\varphi \circ \mathbf{V}(\mathbf{y})^{-1} : \varphi \in V_{\text{ref},\ell}\} \subset H^1\big(D(\mathbf{y})\big)$.

The one-to-one correspondence between the solution $u_\ell(\mathbf{y}) \in V_\ell(\mathbf{y})$ to (6) and the solution $\hat{u}_\ell(\mathbf{y}) \in V_{\text{ref},\ell}$ to (9) is given by the following

Theorem 6.1. *Let $u_\ell(\mathbf{y}) \in V_\ell(\mathbf{y})$ be the Galerkin solution to* (6) *and $\hat{u}_\ell(\mathbf{y}) \in V_{\text{ref},\ell}$ the Galerkin solution to* (9), *respectively. Then, it holds*

$$\hat{u}_\ell(\mathbf{y}) = u_\ell \circ \mathbf{V}(\mathbf{y}) \quad \text{and} \quad u_\ell(\mathbf{y}) = \hat{u}_\ell \circ \mathbf{V}(\mathbf{y})^{-1}.$$

Proof. The proof is a straightforward consequence of the construction of the spaces $V_\ell(\mathbf{y})$ and the equivalence of the problems (6) and (9), see also (10). □ □

Remark 6.2. *The H^2-regularity of the mapped problem, i.e. on $D(\mathbf{y})$, follows from the H^2-regularity of the problem on the reference domain D_{ref} if the vector field $\mathbf{V}(\mathbf{x}, \mathbf{y})$ is at least a C^2-diffeomorphism. Especially, if $\mathbf{V}(\mathbf{x}, \mathbf{y}) = \mathbf{x} + \mathbf{V}_0(\mathbf{x}, \mathbf{y})$ is a perturbation of the identity as in* (15) *and $\mathbf{V}_0(\mathbf{x}, \mathbf{y})$ is of class C^2, then $\mathbf{V}(\mathbf{x}, \mathbf{y})^{-1}$ is also a C^2-diffeomorphism provided that $\|\mathbf{V}_0(\cdot, \mathbf{y})\|_{C^2(D_{\text{ref}})} < 1/2$, cf.* [32].

7. Stochastic interface problems

As a special case of a diffusion problem on a random domain, we shall focus on the stochastic interface problem as already discussed in e.g. [15].

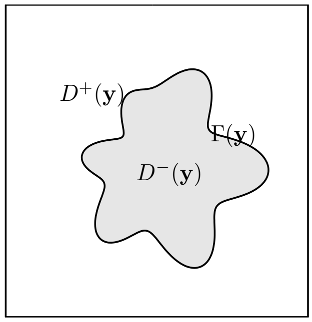

Figure 2. Visualization of the domain D and the random interface $\Gamma(\mathbf{y})$.

7.1. **Problem formulation.** Let the hold-all $\mathcal{D} \subset \mathbb{R}^d$, cf. (3), be a simply-connected and convex domain with Lipschitz continuous boundary $\partial\mathcal{D}$. Inscribed into $\mathcal{D}$, we have a randomly varying inclusion $D^-(\mathbf{y}) \subsetneq \mathcal{D}$ for $\mathbf{y} \in \square$ with a C^2-smooth boundary $\Gamma(\mathbf{y}) := \partial D^-(\mathbf{y})$. The complement of $\overline{D^-(\mathbf{y})}$ will be denoted by $D^+(\mathbf{y}) := \mathcal{D} \setminus \overline{D^-(\mathbf{y})}$. A visualization of this setup is found in Figure 2. For given $\mathbf{y} \in \square$, we can state the stochastic elliptic interface problem as follows:

$$-\operatorname{div}\big(\alpha(\mathbf{x},\mathbf{y})\nabla u(\mathbf{x},\mathbf{y})\big) = f(\mathbf{x}) \quad \text{in } \mathcal{D} \setminus \Gamma(\mathbf{y}), \tag{33}$$

$$[\![u(\mathbf{x},\mathbf{y})]\!] = 0 \quad \text{on } \Gamma(\mathbf{y}), \tag{34}$$

$$\left[\!\!\left[\alpha(\mathbf{x},\mathbf{y})\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x},\mathbf{y})\right]\!\!\right] = 0 \quad \text{on } \Gamma(\mathbf{y}), \tag{35}$$

$$u(\mathbf{x},\mathbf{y}) = 0 \quad \text{on } \partial\mathcal{D}. \tag{36}$$

Here, $\mathbf{n}$ denotes the outward normal vector on $\Gamma(\mathbf{y})$. Furthermore, the diffusion coefficient is given by

$$\alpha(\mathbf{x},\mathbf{y}) := \chi_{D^+(\mathbf{y})}(\mathbf{x})\alpha^+(\mathbf{x}) + \chi_{D^-(\mathbf{y})}(\mathbf{x})\alpha^-(\mathbf{x}) \quad \text{for } \mathbf{x} \in \mathcal{D},$$

where $\chi_{D^-(\mathbf{y})}$ is the characteristic function of $D^-(\mathbf{y})$ and α^+, α^- are smooth deterministic functions with

$$0 < \underline{\alpha} \leq \alpha^-(\mathbf{x}), \alpha^+(\mathbf{x}) \leq \overline{\alpha} < \infty \quad \text{for almost every } \mathbf{x} \in \mathcal{D}.$$

By $[\![u(\mathbf{x},\mathbf{y})]\!] := u^+(\mathbf{x},\mathbf{y}) - u^-(\mathbf{x},\mathbf{y})$, we denote the jump of the solution u across $\Gamma(\mathbf{y})$, where $u^-(\mathbf{x},\mathbf{y}) := u|_{D^-(\mathbf{y})}$ and $u^+(\mathbf{x},\mathbf{y}) := u|_{D^+(\mathbf{y})}$, respectively. Analogously, we define the jump of the co-normal derivative across $\Gamma(\mathbf{y})$ via

$$\left[\!\!\left[\alpha(\mathbf{x},\mathbf{y})\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x},\mathbf{y})\right]\!\!\right] := \alpha^+(\mathbf{x})\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x},\mathbf{y}) - \alpha^-(\mathbf{x})\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x},\mathbf{y}).$$

Remark 7.1. *This formulation of the stochastic interface problem also covers the case of elliptic equations on stochastic domains. For example, for $\alpha^+(\mathbf{x}) \equiv 0$ and $\alpha^-(\mathbf{x}) \equiv 1$ (perfect insulation), we have the Poisson equation on $D^-(\mathbf{y})$ with homogeneous Neumann data on $\Gamma(\mathbf{y})$ while, for $\alpha^+(\mathbf{x}) \equiv \infty$ and $\alpha^-(\mathbf{x}) \equiv 1$ (perfect conduction), we have the Poisson equation on $D^-(\mathbf{y})$ with homogeneous Dirichlet data on $\Gamma(\mathbf{y})$.*

7.2. **Modeling the stochastic interface.** Instead of solving the stochastic interface problem by a perturbation method by means of shape sensitivity analysis as in [15, 19], we propose here to apply the domain mapping approach. To that end, let $\Gamma_{\text{ref}} \subset \mathcal{D}$ denote a reference interface of class C^2 and co-dimension 1 which separates the interior domain D^-_{ref} and the outer domain D^+_{ref}. We assume that $\Gamma(\mathbf{y})$ is prescribed by the application of a vector field $\mathbf{V}\colon \mathcal{D} \times \square \to \mathcal{D}$, i.e. $\Gamma(\mathbf{y}) = \mathbf{V}(\Gamma_{\text{ref}}, \mathbf{y})$, which is a uniform C^2-diffeomorphism in the sense of Section 2. Furthermore, let the Jacobian of $\mathbf{V}$ satisfy the ellipticity condition (4).

As an example, we can consider here an extension of the vector field in [15], which only prescribes the perturbation at the boundary: If Γ_{ref} is of class C^3, then its outward normal $\mathbf{n}$ is of class C^2. Thus, given a stochastic field $\kappa\colon \Gamma_{\text{ref}} \times \square \to \mathbb{R}$ which satisfies $|\kappa(\mathbf{x}, \mathbf{y})| \le \overline{\kappa} < 1$ almost surely, we can define $\mathbf{V}(\mathbf{x}, \mathbf{y}) := \mathbf{x} + \kappa(\mathbf{x}, \mathbf{y})\mathbf{n}(\mathbf{x})$ for $\mathbf{x} \in \Gamma_{\text{ref}}$. A suitable extension of this vector field to the whole domain $\mathcal{D}$ is given by $\mathbf{V}(\mathbf{x}, \mathbf{y}) := \mathbf{x} + \kappa(P\mathbf{x}, \mathbf{y})\mathbf{n}(P\mathbf{x})B(\|\mathbf{x} - P\mathbf{x}\|_2)$, where $P\mathbf{x}$ is the orthogonal projection of $\mathbf{x}$ onto Γ_{ref} and $B\colon [0, \infty) \to [0, 1]$ is a smooth blending function with $B(0) = 1$ and $B(t) = 0$ for all $t \ge c$ for some constant $c \in (0, \infty)$. Notice that, if Γ_{ref} is of class C^3, the orthogonal projection P onto Γ_{ref} and thus $\mathbf{V}(\mathbf{x}, \mathbf{y})$ is at least of class C^2, cf. [21].

7.3. **Reformulation for the reference interface.** For $\mathbf{y} \in \square$, the variational formulation of the interface problem (33)–(36) is given as follows: Find $u \in H^1_0(\mathcal{D})$ such that

$$\int_{D^-(\mathbf{y}) \cup D^+(\mathbf{y})} \alpha \langle \nabla u, \nabla v \rangle \, \mathrm{d}\mathbf{x} = \int_{\mathcal{D}} f v \, \mathrm{d}\mathbf{x} \quad \text{for all } v \in H^1_0(\mathcal{D}).$$

As in Section 2, we can reformulate this variational formulation relative to the reference interface. As we have for the transported coefficient

$$\begin{aligned} \hat{\alpha}(\mathbf{x}, \mathbf{y}) &= \chi_{\mathbf{V}(D^+_{\text{ref}}, \mathbf{y})}\big(\mathbf{V}(\mathbf{x}, \mathbf{y})\big)\hat{\alpha}^+(\mathbf{x}, \mathbf{y}) + \chi_{\mathbf{V}(D^-_{\text{ref}}, \mathbf{y})}\big(\mathbf{V}(\mathbf{x}, \mathbf{y})\big)\hat{\alpha}^-(\mathbf{x}, \mathbf{y}) \\ &= \chi_{D^+_{\text{ref}}}(\mathbf{x})\hat{\alpha}^+(\mathbf{x}, \mathbf{y}) + \chi_{D^-_{\text{ref}}}(\mathbf{x})\hat{\alpha}^-(\mathbf{x}, \mathbf{y}), \end{aligned}$$

we obtain the following variational formulation with the definition (7) of the diffusion matrix $\mathbf{A}(\mathbf{x}, \mathbf{y})$: Find $\hat{u}(\mathbf{y}) \in H^1_0(\mathcal{D})$ such that

$$\int_{D^-_{\text{ref}} \cup D^+_{\text{ref}}} \hat{\alpha}(\mathbf{y}) \langle \mathbf{A}(\mathbf{y}) \nabla \hat{u}(\mathbf{y}), \nabla v \rangle \, \mathrm{d}\mathbf{x} = \int_{\mathcal{D}} \hat{f}(\mathbf{y}) v \det \mathbf{J}(\mathbf{y}) \, \mathrm{d}\mathbf{x} \tag{37}$$

for all $v \in H^1_0(\mathcal{D})$. Since $\hat{\alpha}(\mathbf{x}, \mathbf{y})$ is a smooth function with respect to $\mathbf{y}$, the regularity results from Section 4 remain valid here.

7.4. **Finite element approximation for the stochastic interface problem.** The application of parametric finite elements yields especially an interface-resolved triangulation for the discretization of the interface stochastic problem (33)–(36). By "interface-resolved" we mean that the vertices of elements around the interface lie exactly on the interface, cf. [8, 25]. Thus, the approximation error for a particular realization $u(\mathbf{y}_i)$ of the solution $u(\mathbf{y})$ to the stochastic interface problem (33)–(36) can be quantified by the following theorem adopted from [25, Theorem 4.1].

Theorem 7.2. *For $\mathbf{y} \in \square$, let $\{\mathcal{T}_\ell\}_{\ell > 0}$ be a family of interface resolved triangulations for $\mathbf{V}(\mathcal{D}, \mathbf{y})$ and $\{V_\ell(\mathbf{y})\}_{\ell > 0}$ the associated finite element spaces. Let $u_\ell(\mathbf{y})$ be the finite element solution corresponding to the realization $u(\mathbf{y})$ of the solution to the elliptic problem* (33)*–*(36)*. Then, for $s = 0, 1$, there holds that*

$$\|u(\mathbf{y}) - u_\ell(\mathbf{y})\|_{H^s(\mathcal{D})} \lesssim h_\ell^{2-s} \, \|u(\mathbf{y})\|_{H^2(D^-(\mathbf{y})) \cup H^2(D^+(\mathbf{y}))} \, , \tag{38}$$

where $H^2\big(D^-(\mathbf{y})\big) \cup H^2\big(D^+(\mathbf{y})\big)$ *is the broken Sobolev space equipped by the norm*

$$\|\cdot\|_{H^2(D^-(\mathbf{y}))\cup H^2(D^+(\mathbf{y}))} := \sqrt{\|\cdot\|^2_{H^2(D^-(\mathbf{y}))} + \|\cdot\|^2_{H^2(D^+(\mathbf{y}))}}.$$

In view of Theorem 6.1, the statement of the previous theorem is also valid for the realization of the solution which is pulled back to the domain $\mathcal{D}$ relative to the reference interface Γ_{ref}.

8. Numerical examples

In this section, we consider two examples for boundary value problems on random domains. On the one hand, we consider a stochastic interface problem, and on the other hand, we consider the Laplace equation on a random domain. In both examples, we employ the pivoted Cholesky decomposition, cf. [16, 18], in order to approximate the Karhunen-Loève expansion of $\mathbf{V}$. The spatial discretization is performed by using piecewise linear parametric finite elements on the mapped domain $\mathbf{V}(D_{\text{ref}}, \mathbf{y}_i)$ for each sample $\mathbf{y}_i$. It would of course be also possible to perform the computations on the reference domain. In this case, the diffusion matrix $\mathbf{A}$ has to be computed from Karhunen-Loève expansion of $\mathbf{V}$ for each particular sample.

For the stochastic approximation, we employ a quasi-Monte Carlo quadrature based on N Halton points $\{\boldsymbol{\xi}_i\}_{i=1}^N$, i.e.

$$\mathbb{E}[\hat{u}](\mathbf{x}) \approx (Q\hat{u})(\mathbf{x}) := \frac{1}{N}\sum_{i=1}^N u(\mathbf{x}, \boldsymbol{\xi}_i).$$

Following our results, this quadrature method converges independent of the dimension if $\gamma_k \lesssim k^{-4-\varepsilon}$, cf. [17, 35]. Then, for all $\delta > 0$, there exists a constant such that the quasi-Monte Carlo quadrature based on N points for approximating the mean of the solution $\hat{u}$ to (9) satisfies

$$\|\mathbb{E}[\hat{u}] - Q\hat{u}\|_{H^1(D_{\text{ref}})} \lesssim N^{\delta-1}$$

with a constant only dependent on δ which grows for $\delta \to 0$. Moreover, a similar result is valid for the variance of $\hat{u}$, cf. [17].

All computations have been carried out on a computing server consisting of four nodes[4] with up to 64 threads.

8.1. **The stochastic interface problem.**

We consider the stochastic interface problem from [15] where the hold-all is given as $\mathcal{D} = [-1,1]^2$ and the reference interface is given as $\Gamma_{\text{ref}} = \{\mathbf{x} \in \mathcal{D} : \|\mathbf{x}\|_2 = 0.5\}$. Thus, the outward normal is $\mathbf{n}(\mathbf{x}) = [\cos(\theta), \sin(\theta)]^\intercal$ where $\mathbf{x} = r[\cos(\theta), \sin(\theta)]^\intercal$ is the representation of $\mathbf{x}$ in polar coordinates. The random field under consideration reads

$$\kappa(\theta, \omega) = \frac{1}{30}\sum_{k=0}^5 \cos(k\theta)X_{2k}(\omega) + \sin(k\theta)X_{2k+1}(\omega).$$

Here, $X_1, \ldots, X_{11}$ are independent, uniformly distributed random variables with variance 1, i.e. their range is $[-\sqrt{3}, \sqrt{3}]$. We extend this random field onto $\mathcal{D}$ as described in Subsection 7.2 by using

[4]Each node consists of two quad-core Intel(R) Xeon(R) X5550 CPUs with a clock rate of 2.67GHz (hyperthreading enabled) and 48GB of main memory.

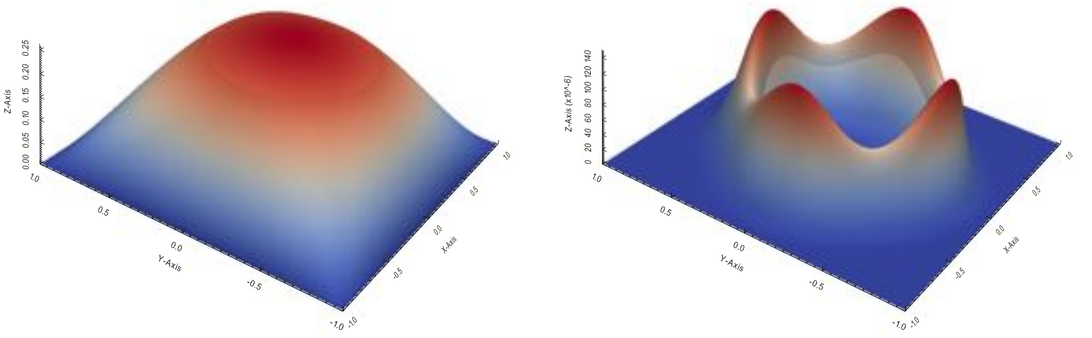

FIGURE 3. Mean (left) and variance (right) of the solution $\hat{u}$ to the stochastic interface problem.

the appropriately scaled quadratic B-spline as blending function, i.e. $B(\mathbf{x}) = \frac{4}{3}B_2(3\|\mathbf{x} - P\mathbf{x}\|_2)$. This yields the covariance

$$\operatorname{Cov}[\mathbf{V}](\mathbf{x},\mathbf{y}) = B(\mathbf{x})B(\mathbf{y})\operatorname{Cov}_\kappa(\theta_\mathbf{x},\theta_\mathbf{y})\begin{bmatrix}\cos(\theta_\mathbf{x})\cos(\theta_\mathbf{y}) & \cos(\theta_\mathbf{x})\sin(\theta_\mathbf{y})\\ \sin(\theta_\mathbf{x})\cos(\theta_\mathbf{y}) & \sin(\theta_\mathbf{x})\sin(\theta_\mathbf{y})\end{bmatrix}$$

with

$$\operatorname{Cov}_\kappa(\theta_\mathbf{x},\theta_\mathbf{y}) = \frac{1}{900}\sum_{k=0}^{5}\cos(k\theta_\mathbf{x})\cos(k\theta_\mathbf{y}) + \sin(k\theta_\mathbf{x})\sin(k\theta_\mathbf{y}).$$

Furthermore, we set $\mathbf{E}[\mathbf{V}](\mathbf{x}) := \mathbf{x}$. A visualization of the reference interface with a particular displacement field $\mathbf{V}(\mathbf{x},\mathbf{y}_i) - \mathbf{x}$ and the resulting perturbed interface is found in Figure 4. Finally, the diffusion coefficient is chosen as $\alpha^-(\mathbf{x}) \equiv 2$, $\alpha^+(\mathbf{x}) \equiv 1$ and the right hand side is chosen as $f(\mathbf{x}) \equiv 1$.

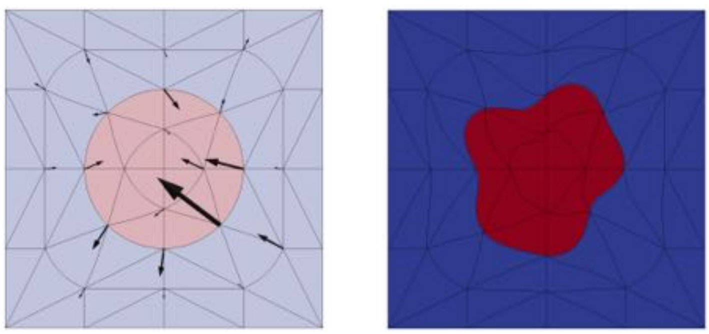

FIGURE 4. Realization of the displacement (left) and the related mapped interface (right).

A visualization of the mean and the variance computed by $N = 10^6$ quasi-Monte Carlo samples and 1048576 finite elements (level 8) is shown in Figure 3. This approximation serves as a reference solution in order to examine the convergence behavior of the quasi-Monte Carlo method. As a comparison and in order to validate the reference solution, we have also computed the approximate mean and variance on each level by the Monte Carlo method. According to [17, 35] and our regularity results, the Quasi-Monte Carlo method with N Halton points converges with the rate $N^{\delta-1}$ for any $\delta > 0$. In our experiments, we thus apply $N_\ell = 2^{\ell/(1-\delta)}$ Halton points on the finite element level $\ell = 1, \ldots, 7$ for the choices $\delta = 0.5, 0.4, 0.3, 0.2$. For the Monte Carlo method, we averaged five approximations each of which being computed with $N_\ell = 2^{2\ell}$ samples. Figure 5 depicts the error of the solution's mean measured in the H^1-norm on the right hand side and the error of the solutions variance measured in the $W^{1,1}$-norm on the left hand side. As can be seen, the error of the solution's mean provides the expected linear rate of convergence for each of the choices of δ. For the solution's variance, we observe a certain offset for the choices $\delta = 0.3$ and $\delta = 0.2$ until the asymptotic rate of convergence is achieved. The choices $\delta = 0.5$ and $\delta = 0.4$ as well as the Monte Carlo approximation yield even better rates of convergence than the expected linear rate. At least the error for the solution's mean seems to be dominated by the finite element discretization. Therefore, we found it instructive to present also the respective errors measured in the L^2-norm. They are plotted in Figure 6. Here, the error is dominated by the stochastic discretization and we can observe that the rate of convergence increases as δ increases even for the solution's mean.

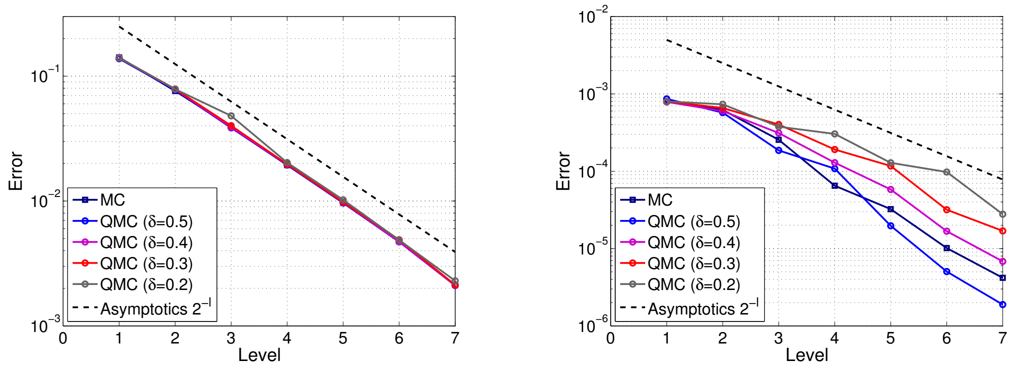

FIGURE 5. Error in the mean measured in H^1 (left) and in the variance measured in $W^{1,1}$ (right).

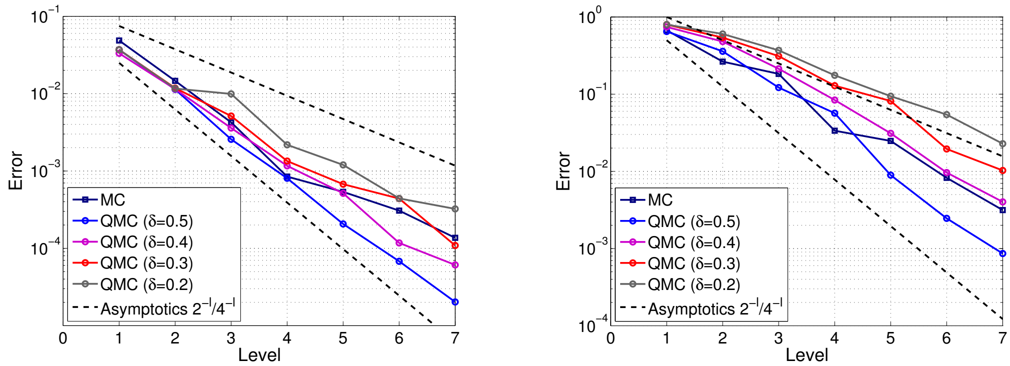

FIGURE 6. Error in the mean (left) and in the variance (right) measured in L^2.

8.2. **The Poisson equation on a random domain.** For our second example, we consider an infinite dimensional random field described by its mean $\mathbb{E}[\mathbf{V}](\mathbf{x}) = \mathbf{x}$ and its covariance function

$$\operatorname{Cov}[\mathbf{V}](\mathbf{x}, \mathbf{y}) = \frac{1}{100} \begin{bmatrix} 5\exp(-4\|\mathbf{x}-\mathbf{y}\|_2^2) & \exp(-0.1\|2\mathbf{x}-\mathbf{y}\|_2^2) \\ \exp(-0.1\|\mathbf{x}-2\mathbf{y}\|_2^2) & 5\exp(-\|\mathbf{x}-\mathbf{y}\|_2^2) \end{bmatrix}.$$

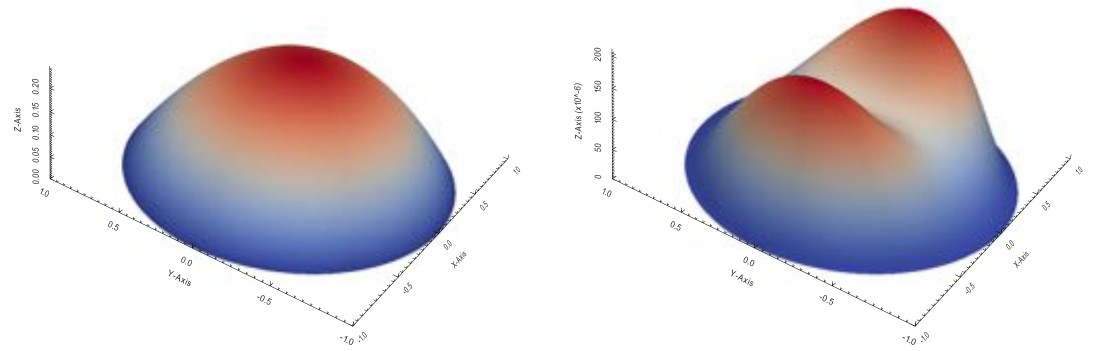

FIGURE 7. Mean (left) and variance (right) of the solution $\hat{u}$ to the Laplace equation on the randomly varying disc.

Furthermore, we consider the random variables in the Karhunen-Loève expansion to be uniformly distributed. The unit disc $D_{\text{ref}} = \{\mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\|_2 < 1\}$ serves as reference domain and the load is set to $f(\mathbf{x}) \equiv 1$. Figure 8 shows the reference domain with a particular displacement field and the resulting perturbed domain.

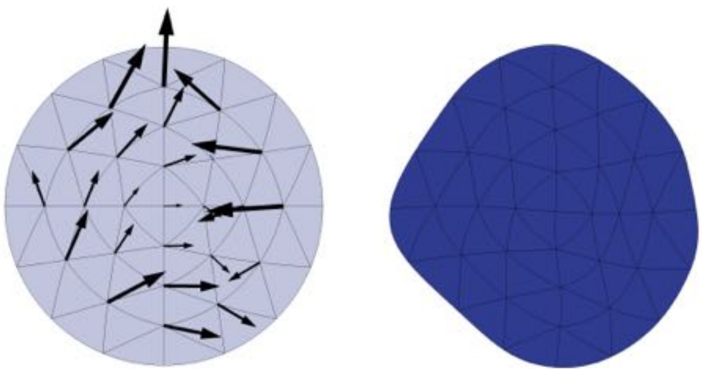

FIGURE 8. Realization of the displacement $\mathbf{V}(\mathbf{x}, \mathbf{y}_i) - \mathbf{x}$ (left) and the related mapped domain (right).

In Figure 7, a visualization of the mean and the variance computed by $N = 10^6$ quasi-Monte Carlo samples 1048576 finite elements (level 9) are found. Here, the Karhunen-Loève expansion has been truncated after $M = 303$ terms which yields a truncation error, cf. (14), smaller than 10^{-6}. For the convergence study, however, we have coupled the truncation error of the Karhunen-Loève expansion to the spatial discretization error of order $2^{-\ell}$ on the finite element level ℓ. It is observed that the truncation rank M linearly grows in the level ℓ, namely it holds $M = 10, 23, 37, 49, 64, 79, 91, 108$ for $\ell = 1, 2, 3, 4, 5, 6, 7, 8$.

The number of samples of the quadrature methods under consideration has been chosen in dependence on the finite element level ℓ as in the previous example. Figure 9 shows the error of the solution's mean and variance measured in the H^1-norm and the $W^{1,1}$-norm, respectively. For the mean, we observe again the expected linear rate of convergence with a slight deterioration for $\delta = 0.3$ and $\delta = 0.2$ on level 4. For the variance, we observe linear and even better rates of convergence except for $\delta = 0.2$. Again, we have also provided the respective errors with respect to the L^2-norm. The related plots are found in Figure 10. Here, the error is also dominated by the stochastic. For increasing values of δ, we again observe successively better rates of convergence.

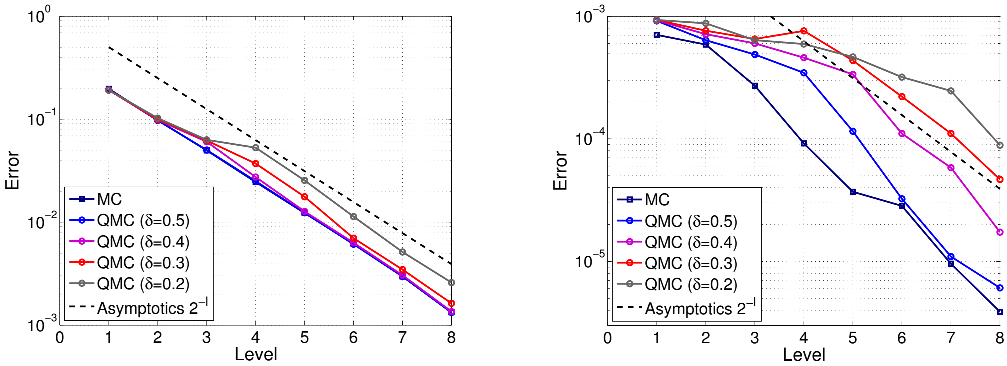

FIGURE 9. Error in the mean measured in H^1 (left) and in the variance measured in $W^{1,1}$ (right).

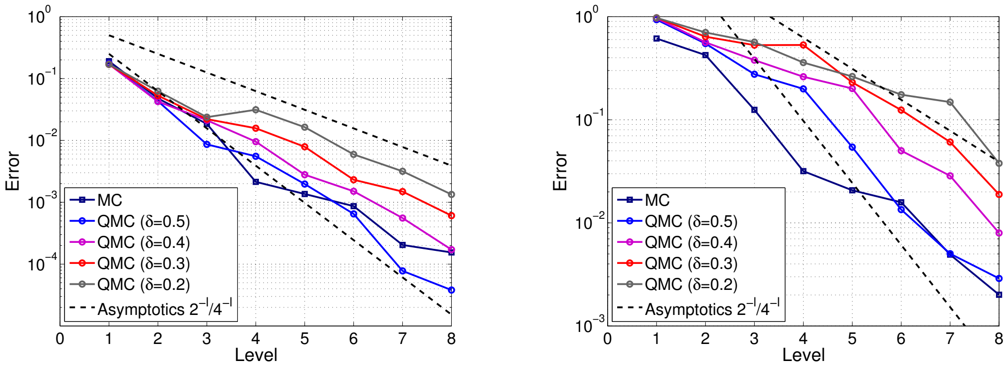

FIGURE 10. Error in the mean (left) and in the variance (right) measured in L^2.

APPENDIX

Lemma .1. *Let* $\boldsymbol{\gamma} = \{\gamma_k\}_k \in \ell^1(\mathbb{N})$ *with finite support* $\mathcal{I} \subset \mathbb{N}$ *and* $\gamma_k \geq 0$. *Moreover, assume that* $c_{\boldsymbol{\gamma}} := \sum_{k\in\mathcal{I}} \gamma_k < 1$. *Then, it holds*

$$\sum_{\boldsymbol{\alpha}} \frac{|\boldsymbol{\alpha}|!}{\boldsymbol{\alpha}!}\boldsymbol{\gamma}^{\boldsymbol{\alpha}} = \frac{1}{1-c_{\boldsymbol{\gamma}}}$$

and therefore there exists a constant with $|\boldsymbol{\alpha}|!/\boldsymbol{\alpha}!\boldsymbol{\gamma}^{\boldsymbol{\alpha}} \leq c$ *for all* $\boldsymbol{\alpha} \in \mathbb{N}_0^M$, *where we set* $M := |\mathcal{I}|$ *and* $0^0 = 1$.

Proof. It holds

$$\sum_{\boldsymbol{\alpha}} \frac{|\boldsymbol{\alpha}|!}{\boldsymbol{\alpha}!}\boldsymbol{\gamma}^{\boldsymbol{\alpha}} = \sum_{i=0}^{\infty} \sum_{|\boldsymbol{\alpha}|=i} \frac{i!}{\boldsymbol{\alpha}!}\boldsymbol{\gamma}^{\boldsymbol{\alpha}} = \sum_{i=0}^{\infty} \left(\sum_{k=1}^{M} \gamma_k\right)^i = \sum_{i=0}^{\infty} c_{\boldsymbol{\gamma}}^i = \frac{1}{1-c_{\boldsymbol{\gamma}}}$$

by the multinomial theorem and the limit of the geometric series. □

Lemma .2. *For all $\alpha, \beta, r \in \mathbb{N}_0$ with $r > 0$ it holds*

$$\binom{\alpha+r-1}{r-1}\binom{\beta+r-1}{r-1} \leq \frac{(\alpha+\beta)!}{\alpha!\beta!}\binom{\alpha+\beta+r-1}{r-1}.$$

Proof. It holds

$$\begin{aligned} & \binom{\alpha+r-1}{r-1}\binom{\beta+r-1}{r-1} \leq \frac{(\alpha+\beta)!}{\alpha!\beta!}\binom{\alpha+\beta+r-1}{r-1} \\ \iff & \binom{\alpha+r-1}{r-1}\frac{(\beta+r-1)!}{\beta!(r-1)!} \leq \frac{(\alpha+\beta)!}{\alpha!\beta!}\frac{(\alpha+\beta+r-1)!}{(\alpha+\beta)!(r-1)!} \\ \iff & \binom{\alpha+r-1}{r-1}(\beta+r-1)! \leq \frac{(\alpha+\beta+r-1)!}{\alpha!} \\ \iff & \binom{\alpha+r-1}{r-1} \leq \binom{\alpha+\beta+r-1}{\beta+r-1}. \end{aligned}$$

The last inequality is true due to the monotonically increasing diagonals in Pascal's triangle. This proves the assertion. □

Lemma .3. *It holds for $\boldsymbol{\alpha} \in \mathbb{N}_0^M$ and $r \in \mathbb{N}$ with $r \leq |\boldsymbol{\alpha}|$ that*

$$\boldsymbol{\alpha}! \sum_{P(\boldsymbol{\alpha},r)} \prod_{i=1}^{|\boldsymbol{\alpha}|} \frac{1}{k_i!} \leq \frac{|\boldsymbol{\alpha}|!}{r!}\binom{|\boldsymbol{\alpha}|+r-1}{r-1}.$$

Proof. From [10], we have the identity

$$r! \sum_{P(\boldsymbol{\alpha},r)} \prod_{i=1}^{|\boldsymbol{\alpha}|} \frac{1}{k_i!} = |s^+(\boldsymbol{\alpha}, r)|,$$

where

$$s^+(\boldsymbol{\alpha}, r) := \left\{ (\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_r) : |\boldsymbol{\beta}_i| \neq 0 \text{ and } \sum_{i=1}^{r} \boldsymbol{\beta}_i = \boldsymbol{\alpha} \right\}.$$

To bound the cardinality of the set $s^+(\boldsymbol{\alpha}, r)$ we use the identity for the number of weak integer compositions, see e.g. [20]: It holds

$$|\{(\beta_1, \ldots, \beta_r) : \beta_i \in \mathbb{N} \text{ and } \beta_1 + \ldots + \beta_r = \alpha\}| = \binom{\alpha+r-1}{r-1}.$$

Thus, we estimate $|s^+(\boldsymbol{\alpha}, r)|$, by the product of the number of weak compositions in each component. This yields

$$|s^+(\boldsymbol{\alpha}, r)| \leq \prod_{i=1}^{M} \binom{\alpha_i+r-1}{r-1}.$$

The proof is now by induction on M. The induction hypothesis is given by

$$\prod_{i=1}^{M} \binom{\alpha_i+r-1}{r-1} \leq \frac{|\boldsymbol{\alpha}|!}{\boldsymbol{\alpha}!}\binom{|\boldsymbol{\alpha}|+r-1}{r-1}.$$

For $M = 1$, we have

$$\binom{\alpha_1+r-1}{r-1} = \frac{\alpha_1!}{\alpha_1!}\binom{\alpha_1+r-1}{r-1},$$

which holds with equality. Let the induction hypothesis be valid for $M-1$ and set $\boldsymbol{\alpha}_{M-1} = [\alpha_1, \ldots, \alpha_{M-1}]$. Then, we derive with the previous lemma that

$$\begin{aligned}\prod_{i=1}^{M} \binom{\alpha_i + r - 1}{r-1} &\le \frac{|\boldsymbol{\alpha}_{M-1}|!}{\boldsymbol{\alpha}_{M-1}!} \binom{|\boldsymbol{\alpha}_{M-1}| + r - 1}{r-1} \binom{\alpha_M + r - 1}{r-1} \\ &\le \frac{|\boldsymbol{\alpha}_{M-1}|!}{\boldsymbol{\alpha}_{M-1}!} \frac{(|\boldsymbol{\alpha}_{M-1}| + \alpha_M)!}{|\boldsymbol{\alpha}_{M-1}|!\alpha_M!} \binom{|\boldsymbol{\alpha}_{M-1}| + \alpha_M + r - 1}{r-1} \\ &= \frac{|\boldsymbol{\alpha}|!}{\boldsymbol{\alpha}!} \binom{|\boldsymbol{\alpha}| + r - 1}{r-1}.\end{aligned}$$

We therefore arrive at

$$r! \sum_{P(\boldsymbol{\alpha},r)} \prod_{i=1}^{|\boldsymbol{\alpha}|} \frac{1}{k_i!} \le \frac{|\boldsymbol{\alpha}|!}{\boldsymbol{\alpha}!} \binom{|\boldsymbol{\alpha}| + r - 1}{r-1}.$$

Rearranging this expression yields the assertion. □

Lemma .4. *Let $c, m \in \mathbb{R}$ with $m \ge 2$ and $c \ge m/(m-1)$. It holds for $n \in \mathbb{N}$ that*

$$\frac{c}{m} \frac{c^n - 1}{c - 1} \le c^n.$$

Proof. It holds

$$\begin{aligned} & \frac{c}{m} \frac{c^n - 1}{c-1} \le c^n \\ \iff \quad & c^{n+1} - c \le m(c^{n+1} - c^n) \\ \iff \quad & mc^n \le (m-1)c^{n+1} + c \\ \iff \quad & \frac{m}{m-1} \le c + \frac{1}{(m-1)c^{n-1}} \end{aligned}$$

Omitting the second summand together with the condition $c \ge m/(m-1)$ yields the assertion. □

References

[1] M. Abramowitz and I. A. Stegun. *Handbook of Mathematical Functions: With Formulas, Graphs, and Mathematical Tables*. Applied mathematics series. Dover Publications, N. Chemsford, MA, 1964.

[2] H. W. Alt. *Lineare Funktionalanalysis*. Springer, London, 2007.

[3] I. Babuška, F. Nobile, and R. Tempone. A stochastic collocation method for elliptic partial differential equations with random input data. *SIAM Journal on Numerical Analysis*, 45(3):1005–1034, 2007.

[4] J. Beck, R. Tempone, F. Nobile, and L. Tamellini. On the optimal polynomial approximation of stochastic pdes by galerkin and collocation methods. *Mathematical Models and Methods in Applied Sciences*, 22(9):1250023, 2012.

[5] D. Braess. *Finite Elemente: Theorie, Schnelle Löser und Anwendungen in der Elastizitätstheorie*. Springer, London, 2007.

[6] C. Canuto and T. Kozubek. A fictitious domain approach to the numerical solution of PDEs in stochastic domains. *Numerische Mathematik*, 107(2):257–293, 2007.

[7] J. E. Castrillon-Candas, F. Nobile, and R. F. Tempone. Analytic regularity and collocation approximation for PDEs with random domain deformations. *ArXiv e-prints 1312.7845*, 2013.

[8] Z. Chen and J. Zou. Finite element methods and their convergence for elliptic and parabolic interface problems. *Numerische Mathematik*, 79(2):175–202, 1998.

[9] A. Cohen, R. DeVore, and C. Schwab. Convergence rates of best N-term Galerkin approximations for a class of elliptic sPDEs. *Foundations of Computational Mathematics*, 10:615–646, 2010.

[10] G. M. Constantine and T. H. Savits. A multivariate Faà di Bruno formula with applications. *Transactions of the American Mathematical Society*, 248:503–520, 1996.

[11] R. Ghanem and P. Spanos. *Stochastic finite elements: A spectral approach.* Springer, New York, 1991.

[12] Michael Griebel and Helmut Harbrecht. Approximation of bi-variate functions: singular value decomposition versus sparse grids. *IMA Journal of Numerical Analysis*, 34(1):28–54, 2014.

[13] Oliver A Gross. Preferential arrangements. *American Mathematical Monthly*, pages 4–8, 1962.

[14] J. H. Halton. On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals. *Numerische Mathematik*, 2(1):84–90, 1960.

[15] H. Harbrecht and J. Li. First order second moment analysis for stochastic interface problems based on low-rank approximation. *ESAIM: Mathematical Modelling and Numerical Analysis*, 47:1533–1552, 9 2013.

[16] H. Harbrecht, M. Peters, and R. Schneider. On the low-rank approximation by the pivoted Cholesky decomposition. *Applied numerical mathematics*, 62:28–440, 2012.

[17] H. Harbrecht, M. Peters, and M. Siebenmorgen. Tractability of the quasi-monte carlo quadrature with halton points for elliptic pdes with random diffusion. *Preprint 2013-28, Mathematisches Institut Universität Basel*, 2013.

[18] H. Harbrecht, M. Peters, and M. Siebenmorgen. Efficient approximation of random fields for numerical applications. *Preprint 2014-01, Mathematisches Institut Universität Basel (to appear in Numerical Linear Algebra with Applications)*, 2014.

[19] H. Harbrecht, R. Schneider, and C. Schwab. Sparse second moment analysis for elliptic problems in stochastic domains. *Numerische Mathematik*, 109(3):385–414, 2008.

[20] S. Heubach and T. Mansour. *Combinatorics of Compositions and Words.* CRC Press, Boca Raton, 2009.

[21] R. B. Holmes. Smoothness of certain metric projections on Hilbert space. *Transactions of the American Mathematical Society*, 184:87–100, 1973.

[22] R. A. Horn and C. R. Johnson. *Topics in Matrix Analysis.* Cambridge University Press, Cambridge, 1994.

[23] R. V. Kadison and J. R. Ringrose. *Fundamentals of the theory of operator algebras. V1: Elementary theory.* Academic Press, New York, 1986.

[24] M. Lenoir. Optimal isoparametric finite elements and error estimates for domains involving curved boundaries. *SIAM Journal on Numerical Analysis*, 23(3):562–580, 1986.

[25] J. Li, J. M. Melenk, B. Wohlmuth, and J. Zou. Optimal a priori estimates for higher order finite elements for elliptic interface problems. *Applied numerical mathematics*, 60(1):19–37, 2010.

[26] W. A. Light and E. W. Cheney. *Approximation theory in tensor product spaces.* Lecture notes in mathematics Volume 1169. Springer, New York, 1985.

[27] M. Loève. *Probability theory. I+II*, volume 45 of *Graduate Texts in Mathematics*. Springer, New York, 4th edition, 1977.

[28] P. S. Mohan, P. B. Nair, and A. J. Keane. Stochastic projection schemes for deterministic linear elliptic partial differential equations on random domains. *International Journal for Numerical Methods in Engineering*, 85(7):874–895, 2011.

[29] F. Nobile, R. Tempone, and C. G. Webster. An anisotropic sparse grid stochastic collocation method for partial differential equations with random input data. *SIAM Journal on Numerical Analysis*, 46(5):2411–2442, 2008.

[30] C. Schwab and R. Todor. Karhunen-Loève approximation of random fields by generalized fast multi-pole methods. *Journal of Computational Physics*, 217:100–122, 2006.

[31] B. Simon. *Methods of Modern Mathematical Physics: Functional Analysis*, volume 1. Academic Press, San Diego, 1980.

[32] J. Simon. Differentiation with respect to the domain in boundary value problems. *Numerical Functional Analysis and Optimization*, 2(7-8):649–687, 1980.

[33] J. Sokołowski and J. P. Zolésio. *Introduction to shape optimization. Shape sensitivity analysis.* Springer series in computational mathematics. Springer, Berlin Heidelberg, 1992.

[34] D. M. Tartakovsky and D. Xiu. Stochastic analysis of transport in tubes with rough walls. *Journal of Computational Physics*, 217(1):248–259, 2006.

[35] X. Wang. A constructive approach to strong tractability using quasi-Monte Carlo algorithms. *Journal of Complexity*, 18:683–701, 2002.

[36] H. S. Wilf. *Generatingfunctionology.* A. K. Peters, Ltd., Natick, MA, USA, 2006.

[37] D. Xiu and D. M. Tartakovsky. Numerical methods for differential equations in random domains. *SIAM Journal on Scientific Computing*, 28(3):1167–1185, 2006.

Mathematisches Institut, Universität Basel, Rheinsprung 21, 4051 Basel, Switzerland,

E-mail address: {helmut.harbrecht,michael.peters,markus.siebenmorgen}@unibas.ch