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A FAST DETERMINISTIC METHOD FOR STOCHASTIC ELLIPTIC INTERFACE PROBLEMS BASED ON LOW-RANK APPROXIMATION

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Abstract. In this work, we propose a fast deterministic numerical method to solve stochastic elliptic interface problems with random interfaces. Shape calculus is first employed to derive the shape-type Taylor expansion in the framework of the asymptotic perturbation approach. Given a priori known mean field and two-point correlation function of random interface variations, we can quantify the mean field and variance of random solutions in terms of certain orders of the perturbation magnitude by solving a deterministic elliptic interface problem and its tensorized counterpart with respect to the reference interface. Error estimates are derived for interface-resolved finite element approximation in both physical and stochastic dimensions. In particular, a fast finite difference scheme is proposed to compute the two-point correlation function of random solutions using the low-rank approximation based on the pivoted Cholesky decomposition. Numerical experiments are presented to demonstrate the advantages of the proposed method.

1. Introduction

Assorted models in science and engineering give rise to partial differential equations (PDE), which can be solved with high accuracy by numerical methods if the data given are known exactly. Nevertheless, the input data are seldom, if not at all, known exactly. As a consequence, accurate numerical solutions are of limited use in the presence of randomness. Thus the research on numerical methods of stochastic PDE with random input data has recently attracted increasingly more interest.

Broadly speaking, there are two general categories of approaches to solve stochastic PDE.

(A) Monte Carlo methods (MC) (see [25, 31] and the references therein): This is the most general methodology to treat randomness by sampling numerous draws of the random input data according to some a priori known or empirical distribution, where each draw entails the computation of a deterministic PDE, and then forming the sample statistics like the mean and variance based on these sample solutions. By interpreting the realizations as draws of distinct random variables of independently identical distribution

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(i.i.d.) with respect to the original one, one may show the convergent rate of the MC methods is inversely proportionate to the square root of the number of samples. Dimension-independence allows the MC method well- suited for general purposes. Nevertheless, to guarantee a certain accuracy, a huge number of PDEs have to be solved to obtain the ensemble average, which could require formidable computing resources in the naive way. Recently, an efficient multilevel MC method is proposed to solve the elliptic PDE with stochastic coefficient with optimal computational complexity [5].

(B) Deterministic approaches: if statistical description of the random input data is specified, one can mathematically characterize the uncertainty in the input data and recast the original stochastic PDE into a deterministic one, thus obtaining the deterministic statistics of the unknown random field. There are generally two subclasses in this case.

(B.1) Perturbation methods ([23, 24]): The *pivotal idea of the perturbation approach* to stochastic PDEs involves expanding all the random fields at hand about the expectation of the random input data via Taylor series expansion with a given small perturbation magnitude ε and retaining terms up to high order, mostly second or third order. Then all such expansions are substituted into the original problem. Equating terms of equal orders in the asymptotic expansions of related fields, one can arrive at the corresponding zeroth-, first- and second-order subproblems, etc.

(B.2) Stochastic Galerkin methods ([2, 3, 4, 9, 10, 13, 14, 29, 32, 33, 36]): The rationale behind is to express, through decomposition of physical and stochastic variables (e.g. Karhunen-Loève expansion), the random field as the tensor product of functions in the physical domain and random variables in the stochastic one. Then one may adopt, respectively, finite element spaces in the physical approximation and wavelets or chaos polynomials in the stochastic approximation. Efficient solvers can be achieved by combining with sparse grid techniques to circumvent the curse of dimensionality.

In the past decade, more intensive research focuses on PDEs with stochastic loadings or coefficients as input data. Recently, uncertainty of computational domains arouses more interest in modeling of randomness of domains as stochastic input parameter, see, e.g., [7, 17, 20, 37] and the references therein. For instance, it is inevitable that the shape of objects in industrial production does not exactly comply with the engineering design. In this paper, we are *first* concerned with *modeling of the interface randomness* in the equilibrium state of the physical process with composite materials governed by elliptic PDEs, which can be termed as *stochastic elliptic interface problems* (SEIP).

Elliptic interface problems (EIP) arise frequently in scientific computing and industrial applications, e.g., when the concerned physical process involves two or more materials or media of different properties, such as the conductivity of steel and bronze in heat diffusion. It is well known that the solutions of elliptic interface problems have high regularity on each individual material region but low regularity globally due to the discontinuity of material

coefficients across the interface. Many numerical methods such as finite difference, finite element and finite volume have been developed in the past few decades for elliptic interface problems. We refer to the monograph [28] and the references therein for more details about the background and the state of the art.

In this work, we would like to further pursue in this direction, namely investigating elliptic boundary value problems with random interfaces. It is of immerse interest in the computational simulation in nano-physics, biology and chemistry, where one uses unsharp interfaces like rough cross sections, cell membranes and molecular surfaces for instance. Due to the uncertainty of interfaces, the solution of the elliptic system itself becomes a random field. Alternatively, the problem may well be reformulated as follows: *Given statistics of the random interface perturbation, how to compute deterministic statistics of interest for random solutions of SEIPs?*

It is common sense that knowledge of complete statistics of the input random field is rarely a priori known in practice. Therefore, we impose two additional assumptions for models in the current work, as in [20], *(i) that the perturbation magnitude of random interfaces around the mean interface is relatively small* and *(ii) that the mean field and two-point correlation of the random interface variations are known empirically or from elsewhere.* It is emphasized that the underlying stochastic process needs not to be known explicitly under small perturbation assumption.

The second goal in the present paper aims at efficient and fast computation of the approximate mean and two-point correlation function of random solutions of SEIPs. It is worth remarking that the Monte Carlo approach employs a great number of *sample interfaces* to solve deterministic EIPs with each sample interface, which is a demanding job, not to mention the work about remeshing for each sample interface to avoid the sub-optimal convergence [27].

The main techniques here are as follows: It is first revealed of the Fréchet differentiability of the solution of EIPs with respect to the interface variations. Then, we develop the shape-Taylor expansion of random solutions via shape calculus (see, e.g., [11, 30, 35] and the references therein). With the shape gradient developed here, we set up a deterministic EIP and its tensorized version for the mean and two-point correlation function of random solutions, respectively. Instead of using sparse tensor finite element spaces as in [16, 20], we make use of a low-rank approximation of the two-point correlation of random solutions based on that of random interfaces in light of the linearity of mapping from random interfaces to random solutions, which leads to a fast finite difference implementation combined with the pivoted Cholesky decomposition.

The main contribution of this work is three-folded: First we study a SEIP model and characterize the shape-Taylor expansion of its random solution via shape calculus. Second, a deterministic EIP and its tensorized counterpart are formulated for the mean and two-point correlation function of random solutions, respectively, with respect to a fixed reference interface. Rigorous error estimates are derived accordingly in terms of both the perturbation

magnitude and mesh size. Last, a finite difference implementation for the fast computation of the two-point correlation function of random solutions using the low-rank approximation based on the pivoted Cholesky decomposition.

The rest of the paper is organized as follows. In Section 2, we formulate the mathematical description of the randomness of stochastic interfaces. In Section 3, we derive the shape gradient of solutions to EIPs via shape calculus [11, 30, 35]. In Section 4, we derive a deterministic elliptic interface problem and its tensorized counterpart for the mean and two-point correlation of random solutions, respectively. In Section 5, error estimates for the fully discrete approximation of the mean field and two-point correlation functions are derived in both stochastic and physical dimensions. A fast algorithm based on the low-rank approximation via the pivoted Cholesky decomposition is proposed as an efficient alternative to compute the two-point correlation function of random solutions. In Section 6, numerical experiments are shown to compare our proposed deterministic implementation with the Monte Carlo method to demonstrate promising advantages.

2. Mathematical formulation

2.1. **Model Problem.** Consider the following EIP arising from the heat conduction model in physics:

$$-\nabla\cdot(\alpha(\mathbf{x},\omega)\nabla u(\mathbf{x},\omega)) = f(\mathbf{x}) \quad \text{in } D^-(\omega)\cup D^+(\omega), \tag{2.1}$$

$$[u(\mathbf{x},\omega)] = 0 \qquad \text{on } \Gamma(\omega), \tag{2.2}$$

$$\left[\alpha(\mathbf{x},\omega)\frac{\partial u}{\partial \mathbf{n}}(\mathbf{x},\omega)\right] = 0 \qquad \text{on } \Gamma(\omega), \tag{2.3}$$

$$u(\mathbf{x},\omega) = 0 \qquad \text{on } \partial D, \tag{2.4}$$

where the domain $D\subset\mathbb{R}^d$, $d=2,3$, is assumed to be a fixed simply-connected bounded convex one with Lipschitz boundary, which is occupied by two random subdomains of different materials, resp. $D^-(\omega)$ and $D^+(\omega)$, where $D^-(\omega)\Subset D$, $D^+(\omega):=D\setminus\overline{D^-(\omega)}$. These two subdomains are separated by the random interface $\Gamma(\omega):=\partial D^-(\omega)$ (see Fig. 1), which is assumed to be at least $C^{2,1}$-smooth. Here (2.2) and (2.3) are the jump conditions which the solution $u(\mathbf{x},\omega)$ has to meet on the random interface $\Gamma(\omega)$, $f(\mathbf{x})$ is

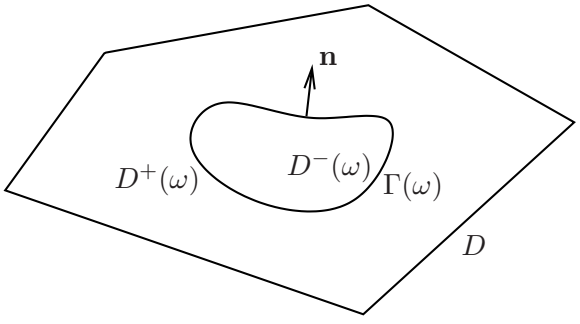

Figure 1. Domain sketch with stochastic interface.

a deterministic source term satisfying $f \in C^\infty(\overline{D})$, and $\mathbf{n}(\mathbf{x},\omega)$ denotes the unit normal vector to the interface $\Gamma(\omega)$ pointing to the interior of $D^+(\omega)$.

For any arbitrarily fixed realization ω of a continuous function $u(\cdot,\omega)$ we denote by $u^-(\cdot,\omega)$ (resp. $u^+(\cdot,\omega)$) its restriction onto $D^-(\omega)$ (resp. $D^+(\omega)$). Throughout the paper, the jump $[u(\cdot,\omega)]$ is always understood to be $u^-(\cdot,\omega) - u^+(\cdot,\omega)$ on $\Gamma(\omega)$ in the sense of trace for each sample ω. The random coefficient field $\alpha(\mathbf{x},\omega)$, due to the uncertainty of the interface $\Gamma(\omega)$, is assumed to be a piecewise smooth function, namely

$$\alpha(\mathbf{x},\omega) = \beta(\mathbf{x}) + \chi_{D^-(\omega)}\gamma(\mathbf{x}) \quad \text{in } D,$$

with smooth deterministic functions $\beta(\mathbf{x})$ and $\gamma(\mathbf{x})$. The function $\chi_{D^-(\omega)}$ is the characteristic function of the random subdomain $D^-(\omega)$, i.e., it is 1 if $\mathbf{x} \in D^-(\omega)$ and 0 otherwise. Moreover, we denote $\alpha^-(\mathbf{x},\omega)$ (resp. $\alpha^+(\mathbf{x},\omega)$) the restriction of $\alpha(\mathbf{x},\omega)$ onto $D^-(\omega)$ (resp. $D^+(\omega)$). Hence, the flux jump satisfies

$$\left[\alpha(\omega)\frac{\partial u}{\partial \mathbf{n}}(\omega)\right] := \alpha^-\frac{\partial u^-}{\partial \mathbf{n}}(\omega) - \alpha^+\frac{\partial u^+}{\partial \mathbf{n}}(\omega) \quad \text{on } \Gamma(\omega).$$

2.2. **Stochastic Interfaces.** To address the randomness of interfaces, it is of first priority to model the stochastic interfaces in a mathematical way.

Fix any fixed interface $\Gamma \in C^{3,1} \subset C^{2,1}$, which is a closed and orientable manifold of co-dimension one separating two fixed subdomains D^- and D^+. For a given smooth, nontangential interface variation $\mathbf{V} \in C^{2,1}(\Gamma,\mathbb{R}^d)$ with $\|\mathbf{V}\|_{C^{2,1}(\Gamma,\mathbb{R}^d)} \le 1$ there exists some sufficiently small constant $\varepsilon_0 > 0$ such that the perturbed interface can be defined for any $0 \le \varepsilon < \varepsilon_0$ by

$$\Gamma_\varepsilon := \{\mathbf{x} + \varepsilon\mathbf{V}(\mathbf{x}) \,:\, \mathbf{x} \in \Gamma\} \in C^{2,1}.$$

Moreover, Γ_ε uniquely defines the deterministic subdomains D_ε^- and thus $D_\varepsilon^+ := D \setminus \overline{D_\varepsilon^-}$. For ease of exposition, in the rest of the paper, we will restrict ourselves to normal variations [11, 30]. More precisely, letting $\mathbf{n}(\mathbf{x})$ be the unit normal vector along Γ pointing into D^+, we can fully characterize the interface variation by its normal component

$$\mathbf{V}(\mathbf{x}) := \kappa(\mathbf{x})\mathbf{n}(\mathbf{x}),$$

where

$$\kappa \in \mathscr{A} := \left\{\nu \in C^{2,1}(\Gamma,\mathbb{R}) : \|\nu\|_{C^{2,1}(\Gamma,\mathbb{R})} \le 1\right\},$$

and thus

$$\Gamma_\varepsilon := \{\mathbf{x} + \varepsilon\kappa(\mathbf{x})\mathbf{n}(\mathbf{x}) \,:\, \mathbf{x} \in \Gamma\}.$$

Note that normal variations require $\Gamma \in C^{3,1}$ in order to ensure that the normal satisfies $\mathbf{n} \in C^{2,1}(\Gamma,\mathbb{R}^d)$.

To account for the randomness of stochastic interfaces, it is equivalent to mathematically describe the random field

$$\kappa(\mathbf{x},\omega) \,:\, \Gamma \times \Omega \to \mathbb{R}. \tag{2.5}$$

The stochastic interfaces $\Gamma(\omega)$ can be rigorously characterized by a complete probability space (Ω,Σ,P) where Ω is the set of all admissible interfaces from sample draws, namely realizations $\omega \mapsto \kappa(\cdot,\omega) \in \mathscr{A}$, Σ is the Borel σ-algebra of $\mathscr{A}$, and $P : \Sigma \to [0,1]$ is a probability measure on the measurable space

(Ω, Σ). For probability space on Banach spaces see [6, 26] and references and therein.

Instead of grasping full knowledge of the random solutions, we are more interested in certain statistics of the random field $u : D \times \Omega \to \mathbb{R}$, which satisfies the PDE (2.1)–(2.4) P-a.s. in Ω.

2.3. **Mean and two-point correlation.** For a P-measureable mapping $\kappa(\mathbf{x}, \omega) : \Omega \to \mathscr{A}$ and the associated normal interface variation in the normal direction $\kappa(\mathbf{x}, \omega)\mathbf{n}(\mathbf{x})$, throughout the rest of the work, we assume that $\kappa(\mathbf{x}, \omega)$ has a finite second moment with respect to P, which belongs to the Bochner space $L^2(\Omega, C^{2,1}(\Gamma, \mathbb{R}))$.

Given a random interface field $\kappa \in L^2(\Omega, C^{2,1}(\Gamma, \mathbb{R}))$ and some perturbation magnitude ε with $0 \leq \varepsilon < \varepsilon_0$, the random interface can be parametrized by

$$\Phi_\varepsilon : \begin{cases} \Gamma \times \Omega \to \mathbb{R}^d, \\ (\mathbf{x}, \omega) \mapsto \mathbf{x} + \varepsilon \kappa(\mathbf{x}, \omega)\mathbf{n}(\mathbf{x}). \end{cases}$$

A realization of the subdomains $D^{\pm}(\omega)$ is thus separated by the interface

$$\Gamma_\varepsilon(\omega) := \{\Phi_\varepsilon(\mathbf{x}, \omega) \, : \, \mathbf{x} \in \Gamma\}, \quad \omega \in \Omega.$$

Due to $\kappa \in L^2(\Omega, C^{2,1}(\Gamma, \mathbb{R}))$, the first two statistical moments of the random interface variation $\kappa(\mathbf{x}, \omega)$ are pointwise finite. They are defined as follows: the *mean*

$$\mathbb{E}_\kappa(\mathbf{x}) := \int_\Omega \kappa(\mathbf{x}, \omega) \, \mathrm{d}P(\omega) = \mathbb{E}(\kappa(\mathbf{x}, \omega)), \quad \mathbf{x} \in \Gamma,$$

the *covariance*

$$\mathrm{Covar}_\kappa(\mathbf{x}, \mathbf{y}) := \int_\Omega (\kappa(\mathbf{x}, \omega) - \mathbb{E}_\kappa(\mathbf{x})) \, (\kappa(\mathbf{y}, \omega) - \mathbb{E}_\kappa(\mathbf{y})) \, \mathrm{d}P(\omega), \quad \mathbf{x}, \, \mathbf{y} \in \Gamma,$$

and the *two-point correlation function*

$$\mathrm{Cor}_\kappa(\mathbf{x}, \mathbf{y}) := \int_\Omega \kappa(\mathbf{x}, \omega)\kappa(\mathbf{y}, \omega) \, \mathrm{d}P(\omega) = \mathbb{E}(\kappa(\mathbf{x}, \omega)\kappa(\mathbf{y}, \omega)), \quad \mathbf{x}, \, \mathbf{y} \in \Gamma \, .$$

Here by $\mathbb{E}$ we denote the *expectation* or *ensemble average with respect to the probability measure P.*

In particular, we see that

$$\mathbb{E}(\Gamma_\varepsilon(\omega)) := \{\mathbb{E}(\Phi_\varepsilon(\mathbf{x}, \omega)), \, \mathbf{x} \in \Gamma\} = \{\mathbf{x} + \varepsilon \mathbb{E}_\kappa(\mathbf{x})\mathbf{n}(\mathbf{x}), \, \mathbf{x} \in \Gamma\}.$$

Without loss of generality, we may assume that the interface random field $\kappa(\mathbf{x}, \omega)$ is centered, namely

$$\mathbb{E}_\kappa(\mathbf{x}) = 0. \tag{2.6}$$

Otherwise, we may readjust the reference interface such that (2.6) holds. Therefore, $\mathbb{E}(\Gamma_\varepsilon(\omega)) = \Gamma$ and

$$\mathrm{Covar}_\kappa(\mathbf{x}, \mathbf{y}) = \mathrm{Cor}_\kappa(\mathbf{x}, \mathbf{y}).$$

Furthermore, once $\mathbb{E}_\kappa(\mathbf{x})$ and $\mathrm{Cor}_\kappa(\mathbf{x},\mathbf{y})$ are given, it holds

$$\begin{aligned}\mathrm{Cor}_{\Phi_\varepsilon}(\mathbf{x},\mathbf{y}) :&= \mathbb{E}(\Phi_\varepsilon(\mathbf{x},\omega)\Phi_\varepsilon(\mathbf{y},\omega))\\ &= \mathbf{x}\cdot\mathbf{y} + \varepsilon^2 \mathrm{Cor}_\kappa(\mathbf{x},\mathbf{y})\mathbf{n}(\mathbf{x})\cdot\mathbf{n}(\mathbf{y}),\end{aligned}$$

which means that the two-point correlation function of random interfaces can be modeled by that of the random normal variation $\kappa(\mathbf{x},\omega)$.

3. Shape calculus

In this section, we return to the deterministic world to develop the shape-Taylor expansion of solutions to EIPs with respect to the reference interface $\Gamma \in C^{3,1}$ via shape calculus. To that end, we derive the shape gradient based on the velocity method (cf. also [21, 22, 30, 35]).

Now consider a deterministic EIP with respect to the reference interface Γ:

$$-\nabla\cdot(\alpha\nabla u) = f \quad \text{in } D^-\cup D^+, \tag{3.1}$$

$$[u] = 0 \quad \text{on } \Gamma, \tag{3.2}$$

$$\left[\alpha\frac{\partial u}{\partial \mathbf{n}}\right] = 0 \quad \text{on } \Gamma, \tag{3.3}$$

$$u = 0 \quad \text{on } \partial D, \tag{3.4}$$

and a deterministic perturbed PDE with the perturbed interface Γ_ε

$$-\nabla\cdot(\alpha\nabla u_\varepsilon) = f \quad \text{in } D_\varepsilon^-\cup D_\varepsilon^+, \tag{3.5}$$

$$[u_\varepsilon] = 0 \quad \text{on } \Gamma_\varepsilon, \tag{3.6}$$

$$\left[\alpha\frac{\partial u_\varepsilon}{\partial \mathbf{n}}\right] = 0 \quad \text{on } \Gamma_\varepsilon, \tag{3.7}$$

$$u_\varepsilon = 0 \quad \text{on } \partial D, \tag{3.8}$$

where the perturbed interface $\Gamma_\varepsilon := \{\mathbf{x}+\varepsilon\kappa(\mathbf{x})\mathbf{n}(\mathbf{x}),\ \mathbf{x}\in\Gamma\}$, D_ε^- is the interior part of Γ_ε and $D_\varepsilon^+ := D\setminus\overline{D_\varepsilon^-}$, and the normal variation $\kappa(\mathbf{x})\in\mathscr{A}$. Moreover, we denote by u_ε^- (resp. u_ε^+) its restriction on D_ε^- (resp. D_ε^-).

The first order shape derivative for the elliptic interface problem is defined formally by the pointwise limit

$$\mathrm{d}u(\mathbf{x}) := \mathrm{d}u(\mathbf{x})[\kappa] = \lim_{\varepsilon\to 0}\frac{u_\varepsilon(\mathbf{x})-u(\mathbf{x})}{\varepsilon}, \quad \mathbf{x}\in\left(D^-\cap D_\varepsilon^-\right)\cup\left(D^+\cap D_\varepsilon^+\right),$$

and can be characterized by the following lemma.

Lemma 1. *Under the smoothness assumptions on the interface Γ, normal variation κ and small perturbation magnitude as before, the shape derivative $\mathrm{d}u := \mathrm{d}u[\kappa]$, which is written as $\mathrm{d}u^+$ and $\mathrm{d}u^-$ restricted onto D^- and D^+,*

respectively, satisfies the following EIP with nonhomogeneous jump conditions:

$$-\nabla\cdot(\alpha\nabla \mathrm{d}u) = 0 \qquad \text{in } D^-\cup D^+, \tag{3.9}$$

$$[\mathrm{d}u] = -\kappa\left[\frac{\partial u}{\partial \mathbf{n}}\right] \qquad \text{on } \Gamma, \tag{3.10}$$

$$\left[\alpha\frac{\partial \mathrm{d}u}{\partial \mathbf{n}}\right] = \nabla_\Gamma\cdot(\kappa[\alpha]\nabla_\Gamma u) \quad \text{on } \Gamma, \tag{3.11}$$

$$\mathrm{d}u = 0 \qquad \text{on } \partial D, \tag{3.12}$$

where ∇_Γ, $\nabla_\Gamma\cdot$ denote, respectively, the surface gradient and surface divergence operators which are defined by $\nabla_\Gamma v := \nabla v - (\nabla v\cdot\mathbf{n})\mathbf{n}$ for a scalar function v, and $\nabla_\Gamma\cdot\mathbf{v} := \nabla\cdot\mathbf{v} - (\nabla\mathbf{v}\mathbf{n})\cdot\mathbf{n}$ for a vector field $\mathbf{v}$.

Proof. The plan of the proof is as follows: We take the difference of the respective variational forms of the reference problem (3.1)–(3.4) and of the perturbed one (3.5)–(3.8), take the limit by letting $\varepsilon\to 0$ and deduce the PDE (3.9)–(3.12) of the shape gradient from this limiting variational form.

The variational formulations of the original PDE (3.1)–(3.4) and of the perturbed one (3.5)–(3.8) read as follows: Seek u, $u_\varepsilon\in H^1_0(D)$ such that

$$\int_{D^-}\alpha^-\nabla u^-\cdot\nabla v\,\mathrm{d}\mathbf{x} + \int_{D^+}\alpha^+\nabla u^+\cdot\nabla v\,\mathrm{d}x = \int_D fv\,\mathrm{d}\mathbf{x} \tag{3.13}$$

and

$$\int_{D_\varepsilon^-}\alpha^-\nabla {u^-}_\varepsilon\cdot\nabla v\,\mathrm{d}\mathbf{x} + \int_{D_\varepsilon^+}\alpha\nabla {u^+}_\varepsilon\cdot\nabla v\,\mathrm{d}\mathbf{x} = \int_D fv\,\mathrm{d}\mathbf{x} \tag{3.14}$$

for all $v\in H^1_0(D)$.

Subtracting (3.13) from (3.14), dividing by ε on both sides and taking the limit by letting ε tend to zero, we obtain, (see [35, Chap. 2] and [30, Chap. 4] for details), the variational form for the shape gradient $\mathrm{d}u$:

$$\begin{aligned}\int_{D^-}\alpha^-\nabla \mathrm{d}u^-\cdot\nabla v\,\mathrm{d}\mathbf{x} + \int_{D^+}\alpha^+\nabla \mathrm{d}u^+\cdot\nabla v\,\mathrm{d}\mathbf{x}\\ + \int_\Gamma \kappa(\alpha^-\nabla u^- - \alpha^+\nabla u^+)\cdot\nabla v\,\mathrm{d}\mathbf{x} = 0.\end{aligned} \tag{3.15}$$

Testing (3.15) by $\phi\in C_0^\infty(D^\pm)$, we arrive at the PDE in (3.9).

The flux jump condition (3.11) follows by first testing (3.15) with smooth functions $\psi\in C^\infty(\mathbb{R}^d)$ on Γ and employing the flux jump condition (3.3) on Γ. Then it yields

$$\alpha^-\frac{\partial \mathrm{d}u^-}{\partial\mathbf{n}} - \alpha^+\frac{\partial \mathrm{d}u^+}{\partial\mathbf{n}} = \nabla_\Gamma\cdot\left(\left(\alpha^- - \alpha^+\right)\kappa\nabla_\Gamma u\right)$$

by using the tangential Green formula (cf. [11]) on the surface of co-dimension one, namely

$$\int_\Gamma \nabla_\Gamma f\cdot\mathbf{v}\,\mathrm{d}s + \int_\Gamma f\nabla_\Gamma\cdot\mathbf{v}\,\mathrm{d}s = 0,$$

where f is a surface scalar function and $\mathbf{v}$ is a surface tangential vector field.

Let $\psi \in C^\infty(\mathbb{R}^d)$, then from the jump condition (3.6),

$$\int_{\Gamma_\varepsilon} \left(u_\varepsilon^- - u_\varepsilon^+\right) \psi \, \mathrm{d}s = 0.$$

Pulling back from Γ_ε to Γ and taking the derivative with respect to ε on both sides of this equality and evaluating it at $\varepsilon = 0$, we obtain, by the same argument [11, Eq. (4.16)], that

$$\begin{aligned}
&\int_\Gamma \left(\mathrm{d}u^- - \mathrm{d}u^+\right) \psi \, ds \\
&\quad = -\int_\Gamma \kappa \left[\frac{\partial \left(\left(u^- - u^+\right)\psi\right)}{\partial \mathbf{n}} + (d-1)\mathcal{H}\left(u^- - u^+\right)\psi\right] \mathrm{d}s \\
&\quad = -\int_\Gamma \kappa \left[\frac{\partial u}{\partial \mathbf{n}}\right] \psi \, \mathrm{d}s,
\end{aligned}$$

where $\mathcal{H}$ is the mean curvature of the interface Γ, and we have used the jump condition (3.2) in the second equality to simplify the formula. Then the first jump condition (3.10) follows from arbitrariness of ψ, which completes the proof. □

Remark. It is worth noting that the shape gradient $\mathrm{d}u$ is in general not in $H_0^1(D)$ since it may be discontinuous along the interface Γ.

With the shape gradient at hand, we can develop a deterministic shape-type Taylor expansion as follows:

$$u_\varepsilon(\mathbf{x}) = u(\mathbf{x}) + \varepsilon \mathrm{d}u[\kappa](\mathbf{x}) + \mathcal{O}(\varepsilon^2), \quad \mathbf{x} \in D \setminus U_{\varepsilon_0}(\Gamma), \tag{3.16}$$

where the constant hidden in the Landau symbol depends on the function u and the distance to the interface, and this expansion only holds away from the ε_0-tube region

$$U_{\varepsilon_0}(\Gamma) := \left\{\mathbf{y} = \mathbf{x} + t\varepsilon_0 \mathbf{n}(\mathbf{x}),\, t \in [0,1],\, \mathbf{x} \in \Gamma\right\}.$$

4. Statistics of Random Solutions

In this section, we study statistics of random solutions to SEIPs in terms of that of random interfaces through the perturbation method. The *main idea behind the perturbation approach* to the stochastic PDE is the *matched asymptotic principle*, which involves expanding all the random fields under concern about the expectation of the random interface via Taylor series expansion with a given small perturbation magnitude ε and retaining terms up to high order, mostly second or third order. For a sufficiently small $\varepsilon_0 > 0$, we can develop a random version shape-type Taylor expansion of random solutions to (2.1)–(2.4) with resort to the shape gradient, which is formulated in the following lemma.

Lemma 2. *Under the small perturbation assumption and smoothness conditions on admissible interface variations and given data, the random solution to* (2.1)–(2.4) *admits the following shape-type Taylor expansion:*

$$u(\mathbf{x}, \omega) = \overline{u}(\mathbf{x}) + \varepsilon \mathrm{d}u[\kappa(\mathbf{x}, \omega)](\mathbf{x}, \omega) + \mathcal{O}(\varepsilon^2), \tag{4.1}$$

for $\mathbf{x} \Subset K \in D \setminus U_{\varepsilon_0}(\Gamma)$*, P-a.s.* $\omega \in \Omega$*, where* $\overline{u}$ *is the deterministic solution to the elliptic problem with the fixed reference interface* Γ *and* $\mathrm{d}u(\mathbf{x},\omega)$ *is the associated shape gradient, namely the solution of the EIP* (3.9)–(3.12) *with* $\kappa(\mathbf{x})$ *being replaced by* $\kappa(\mathbf{x},\omega)$ *and* $D^{\pm}$ *by* $D^{\pm}(\omega)$*.*

Proof. Taylor expansion in (4.1) is the stochastic analog of (3.16). Thus, the assertion follows by repeating the argument in the proof of Lemma 1 in Section 3 for any fixed realization of the normal interface variation $\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x})$ associated with the sample ω. □

Now we can approximate the deterministic statistics of random solutions to (2.1)–(2.4) with the help of (4.1). More precisely, the mean field and variance of random solutions can be approximated by their deterministic surrogates with respect the reference interface in terms of certain approximation orders of the perturbation magnitude.

The following theorem addresses the semi-discrete approximation to the mean field in the stochastic dimension.

Theorem 3. *The expectation* $\mathbb{E}_u(\mathbf{x})$ *of random solutions to* (2.1)–(2.4) *can be approximated by solving the deterministic PDE* (3.1)–(3.4) *with respect to the reference interface* Γ*, up to the second order in terms of the perturbation magnitude. More precisely,*

$$\mathbb{E}_u(\mathbf{x}) = \overline{u}(\mathbf{x}) + \mathcal{O}(\varepsilon^2), \quad \mathbf{x} \in K \Subset D \setminus U_{\varepsilon_0}(\Gamma),$$

where $\overline{u}$ *is the deterministic solution to the EIP* (3.1)–(3.4) *with the reference interface* Γ*.*

Proof. Using the shape-Taylor expansion, we obtain

$$\mathbb{E}_u(\mathbf{x}) = \overline{u}(\mathbf{x}) + \varepsilon\mathbb{E}\left(\mathrm{d}u[\kappa(\mathbf{x},\omega)](\mathbf{x},\omega)\right) + \mathcal{O}(\varepsilon^2).$$

By the linearity of the expectation operator $\mathbb{E}$, taking the expectation on both sides of the stochastic version of the PDE (3.9)–(3.12) of the shape gradient $\mathrm{d}u(\mathbf{x},\omega)$, and taking account of the fact that $\mathbb{E}_\kappa(\mathbf{x}) = 0$, we have

$$\mathbb{E}\left(\mathrm{d}u[\kappa(\mathbf{x},\omega)](\mathbf{x},\omega)\right) = 0,$$

from which, the desired claim follows. Thus the proof is done. □

The second theorem studies the approximation of the variance of random solutions.

Theorem 4. *The variance* $\mathrm{Var}_u(\mathbf{x})$ *of random solutions to* (2.1)–(2.4) *can be approximated by solving the deterministic tensor product PDE* (4.5)–(4.14) *as follows with respect to the reference interface* Γ*, up to the third order in terms of the perturbation magnitude. More precisely,*

$$\mathrm{Var}_u(\mathbf{x}) = \varepsilon^2\mathrm{Var}_{\mathrm{d}u}(\mathbf{x}) + \mathcal{O}(\varepsilon^3), \quad \mathbf{x} \in K \Subset D \setminus U_{\varepsilon_0}(\Gamma), \tag{4.2}$$

where

$$\begin{aligned}\mathrm{Var}_{\mathrm{d}u}(\mathbf{x}) &= \mathrm{Var}(\mathrm{d}u[\kappa(\mathbf{x},\omega)](\mathbf{x},\omega)) = \mathrm{Cor}(\mathrm{d}u[\kappa](\mathbf{x}),\mathrm{d}u[\kappa](\mathbf{y}))\big|_{\mathbf{y}=\mathbf{x}}\\ &= \mathrm{Cor}_{\mathrm{d}u}(\mathbf{x},\mathbf{y})\big|_{\mathbf{y}=\mathbf{x}},\end{aligned}$$

and $\mathrm{Cor}_{\mathrm{d}u}(\mathbf{x},\mathbf{y})$ *is the solution to* (4.5)–(4.14)*.*

Proof. Observe the following variance identity

$$\mathrm{Var}(a+bX+cY) = b^2\mathrm{Var}(X) + 2bc\mathrm{Covar}(X,Y) + c^2\mathrm{Var}(Y), \tag{4.3}$$

where X and Y are two random variables with finite second moments.

As a result for random variables with finite variance, the following inequality holds via the Cauchy-Schwarz inequality:

$$\mathrm{Covar}(X,Y) \le \sqrt{\mathrm{Var}(X)\cdot\mathrm{Var}(Y)}\,. \tag{4.4}$$

Combining (4.3) and (4.4) with the shape-Taylor expansion (4.1), we have

$$\begin{aligned}\mathrm{Var}_u(\mathbf{x}) &= \varepsilon^2\mathrm{Var}(\mathrm{d}u[\kappa(\mathbf{x},\omega)](\mathbf{x},\omega)) + \mathcal{O}(\varepsilon^4) + \sqrt{\mathrm{Var}(\mathrm{d}u[\kappa(\mathbf{x},\omega)](\mathbf{x},\omega))}\mathcal{O}(\varepsilon^3)\\ &= \varepsilon^2\mathrm{Var}(\mathrm{d}u[\kappa(\mathbf{x},\omega)](\mathbf{x},\omega)) + \mathcal{O}(\varepsilon^3).\end{aligned}$$

Hence the proof is completed. □

We can approximate $\mathrm{Var}_u(\mathbf{x})$ by deterministically solving the tensor product PDE of $\mathrm{Cor}_{\mathrm{d}u}(\mathbf{x},\mathbf{y})$ on the tensor domain $D\times D\subset\mathbb{R}^{2d}$. Denote by $[\![\cdot]\!]$ the tensor-product of the jump operator which is given for any two-point correlation function $w(\mathbf{x},\mathbf{y})$ by

$$\begin{aligned}[\![w(\mathbf{x},\mathbf{y})]\!] = &\lim_{\substack{D^-\ni\mathbf{x}\to\Gamma\\ D^-\ni\mathbf{y}\to\Gamma}} w(\mathbf{x},\mathbf{y}) - \lim_{\substack{D^-\ni\mathbf{x}\to\Gamma\\ D^+\ni\mathbf{y}\to\Gamma}} w(\mathbf{x},\mathbf{y})\\ &- \lim_{\substack{D^+\ni\mathbf{x}\to\Gamma\\ D^-\ni\mathbf{y}\to\Gamma}} w(\mathbf{x},\mathbf{y}) + \lim_{\substack{D^+\ni\mathbf{x}\to\Gamma\\ D^+\ni\mathbf{y}\to\Gamma}} w(\mathbf{x},\mathbf{y}).\end{aligned}$$

Then the tensor product boundary value problem involving $\mathrm{Cor}_{\mathrm{d}u}(\mathbf{x},\mathbf{y})$ can be stated as follows:

– *Tensor-product-domain PDE*:

$$(\nabla_{\mathbf{x}}\otimes\nabla_{\mathbf{y}})\cdot(\kappa(\mathbf{x})\kappa(\mathbf{y})(\nabla_{\mathbf{x}}\otimes\nabla_{\mathbf{y}})\mathrm{Cor}_{\mathrm{d}u}(\mathbf{x},\mathbf{y})) = 0, \tag{4.5}$$

for all $(\mathbf{x},\mathbf{y})\in D^{\pm}\times D^{\pm}$,

– *Interface-domain PDE*:

$$-\nabla_{\mathbf{y}}\cdot(\alpha(\mathbf{y})\nabla_{\mathbf{y}}\left[\mathrm{Cor}_{\mathrm{d}u}(\mathbf{x},\mathbf{y})\right]_{\mathbf{x}}) = 0, \tag{4.6}$$

$$-\nabla_{\mathbf{y}}\cdot\left(\alpha(\mathbf{y})\nabla_{\mathbf{y}}\left[\alpha(\mathbf{x})\frac{\partial\mathrm{Cor}_{\mathrm{d}u}}{\partial\mathbf{n}_{\mathbf{x}}}(\mathbf{x},\mathbf{y})\right]_{\mathbf{x}}\right) = 0, \tag{4.7}$$

for all $(\mathbf{x},\mathbf{y})\in\Gamma\times D^{\pm}$;

– *Domain-interface PDE*:

$$-\nabla_{\mathbf{x}}\cdot\left(\alpha(\mathbf{x})\nabla_{\mathbf{x}}\left[\mathrm{Cor}_{\mathrm{d}u}(\mathbf{x},\mathbf{y})\right]_{\mathbf{y}}\right) = 0, \tag{4.8}$$

$$-\nabla_{\mathbf{x}}\cdot\left(\alpha(\mathbf{x})\nabla_{\mathbf{x}}\left[\alpha(\mathbf{y})\frac{\partial\mathrm{Cor}_{\mathrm{d}u}}{\partial\mathbf{n}_{\mathbf{y}}}(\mathbf{x},\mathbf{y})\right]_{\mathbf{y}}\right) = 0, \tag{4.9}$$

for all $(\mathbf{x},\mathbf{y})\in D^{\pm}\times\Gamma$;

– *DD tensor interface condition*:

$$[\![\mathrm{Cor}_{\mathrm{d}u}(\mathbf{x},\mathbf{y})]\!] = \mathrm{Cor}_{\kappa}(\mathbf{x},\mathbf{y})\left[\frac{\partial\overline{u}}{\partial\mathbf{n}}(\mathbf{x})\right]\left[\frac{\partial\overline{u}}{\partial\mathbf{n}}(\mathbf{y})\right], \tag{4.10}$$

for all $(\mathbf{x},\mathbf{y})\in\Gamma\times\Gamma$;

– *DN and ND tensor interface condition*:

$$\left[\!\left[\alpha(\mathbf{y})\frac{\partial \mathrm{Cor}_{\mathrm{d}u}}{\partial \mathbf{n}_{\mathbf{y}}}(\mathbf{x},\mathbf{y})\right]\!\right] = -\nabla_{\Gamma,\mathbf{y}}\cdot\left(\left[\frac{\partial \overline{u}}{\partial \mathbf{n}}(\mathbf{x})\right][\alpha(\mathbf{y})]\mathrm{Cor}_{\kappa}(\mathbf{x},\mathbf{y})\nabla_{\Gamma}\overline{u}(\mathbf{y})\right), \tag{4.11}$$

$$\left[\!\left[\alpha(\mathbf{x})\frac{\partial \mathrm{Cor}_{\mathrm{d}u}}{\partial \mathbf{n}_{\mathbf{x}}}(\mathbf{x},\mathbf{y})\right]\!\right] = -\nabla_{\Gamma,\mathbf{x}}\cdot\left(\left[\frac{\partial \overline{u}}{\partial \mathbf{n}}(\mathbf{y})\right][\alpha(\mathbf{x})]\mathrm{Cor}_{\kappa}(\mathbf{x},\mathbf{y})\nabla_{\Gamma}\overline{u}(\mathbf{x})\right), \tag{4.12}$$

for all $(\mathbf{x},\mathbf{y})\in\Gamma\times\Gamma$;

– *NN tensor interface condition*:

$$\begin{aligned}\left[\!\left[\alpha(\mathbf{x})\alpha(\mathbf{y})\frac{\partial^2 \mathrm{Cor}_{\mathrm{d}u}}{\partial \mathbf{n}_{\mathbf{x}}\partial \mathbf{n}_{\mathbf{y}}}(\mathbf{x},\mathbf{y})\right]\!\right]\\ = (\nabla_{\Gamma,\mathbf{x}}\otimes\nabla_{\Gamma,\mathbf{y}})\cdot([\alpha(\mathbf{x})][\alpha(\mathbf{y})]\mathrm{Cor}_{\kappa}(\mathbf{x},\mathbf{y})\nabla_{\Gamma}\overline{u}(\mathbf{x})\nabla_{\Gamma}\overline{u}(\mathbf{y}))\,,\end{aligned} \tag{4.13}$$

for all $(\mathbf{x},\mathbf{y})\in\Gamma\times\Gamma$;

– *Tensor-product boundary condition*:

$$\mathrm{Cor}_{\mathrm{d}u}(\mathbf{x},\mathbf{y}) = 0, \tag{4.14}$$

for all $(\mathbf{x},\mathbf{y})\in\partial\,(D\times D)$.

5. Error Estimates and Implementation

In this section, error estimates will be carried out for the full discrete approximations of the mean field and two-point correlation function of random solutions in terms of both the mesh size in the physical domain and the perturbation magnitude in the stochastic dimension. Algorithmic implementation of a fast finite difference method based on the low-rank approximation via the pivoted Cholesky decomposition is presented for the efficient computation of the two-point correlation function of random solutions.

In the sequel, interface-resolved triangulations are assumed for solving the EIP system (3.1)–(3.4) to achieve optimal convergence rates for the deterministic PDE, cf. [8, 27]. By the use of parametric mappings, we even are endowed with hierarchical finite element spaces amenable for the sparse tensor approximation of the two-point correlation function (see [16] for details).

5.1. **Computing the approximate expectation.** We have presented the discussion of the semi-discrete approximation in the stochastic dimension of the mean field and two-point correlation function in the continuous case by the asymptotic analysis in terms of the perturbation magnitude. Now we develop finite element discretization to yield fully discrete approximation and derive the convergence results in terms of both the finite element mesh size of the triangulation and the perturbation magnitude.

Assume that the triangulation $\{\mathscr{T}_h\}_{h>0}$ is a sequence of quasi-uniform and shape-regular triangulations with the mesh size h, which exactly resolve the interface via parametrization, and let $\{V_h\}_{h>0}$ be the corresponding finite element spaces over the given triangulations. We can obtain the discrete

finite element approximation $\overline{u}_h$ to $\overline{u}$ by solving the variational form of (3.1)–(3.4) with respect to the reference interface Γ in the finite dimensional space V_h.

The discretization error of the deterministic solution $\overline{u}$ can be quantified by the follow lemma adapted from [27, Thm. 4.1] with little modification.

Theorem 5. *Let $\{\mathscr{T}_h\}_{h>0}$, $\{V_h\}_{h>0}$ be a family of interface-resolved triangulations and the associated finite element spaces (cf.* [16, 27]*). Let $\overline{u}_h$ be the deterministic finite element solution corresponding to the deterministic solution $\overline{u}(\mathbf{x})$ of the elliptic problem* (3.1)–(3.4) *with respect to the reference interface Γ. Then there holds for $s = 0, 1$ that*

$$\|\overline{u} - \overline{u}_h\|_{H^s(D)} \leq Ch^{2-s} \|\overline{u}\|_{H^2(D^-)\cup H^2(D^+)}. \tag{5.1}$$

Let $\mathbb{E}_u$ be the expectation of random solutions to (2.1)–(2.4)*. Then, on $K \Subset D \setminus U_{\varepsilon_0}(\Gamma)$ there holds*

$$\|\mathbb{E}_u(\mathbf{x}) - \overline{u}_h(\mathbf{x})\|_{H^s(K)} \leq C\left(\varepsilon^2 + h^{2-s}\right) \|\overline{u}\|_{H^2(D^-)\cup H^2(D^+)}.$$

Proof. The estimate (5.1) follows easily from [27] for at least C^2-smooth interfaces. The estimates for expectation can be completed by combining Theorem 3, (5.1) and the following triangle inequality

$$\|\mathbb{E}_u - \overline{u}_h\|_{H^s(K)} \leq \|E_u - \overline{u}\|_{H^s(K)} + \|\overline{u} - \overline{u}_h\|_{H^s(K)}.$$

□

5.2. **Computing the two-point correlation function.**

5.2.1. *Computing local shape derivatives.* Notice that the PDE for the local shape derivative $\mathrm{d}u = \mathrm{d}u(\kappa)$ is not amenable for naive finite element discretization due to the non-homogeneous Dirichlet jump condition. Here we use the *offset function technique* to convert the original PDE (3.9)–(3.12) into two systems.

To this end, we assume that we have an offset function $\mathrm{d}u^-_{\mathrm{off}} = \mathrm{d}u^-_{\mathrm{off}}(\kappa) \in H^1(D^-)$ such that

$$-\nabla \cdot \left(\alpha \nabla \mathrm{d}u^-_{\mathrm{off}}\right) = 0 \qquad \text{in } D^-, \tag{5.2}$$

$$\mathrm{d}u^-_{\mathrm{off}} = -\kappa \left[\frac{\partial \overline{u}}{\partial \mathbf{n}}\right] \quad \text{on } \Gamma. \tag{5.3}$$

We extend this function trivially to D^+ by letting $\mathrm{d}u^+_{\mathrm{off}} = 0$. By subtracting $\mathrm{d}u_{\mathrm{off}}$ from $\mathrm{d}u$, we are led to seek $\mathrm{d}u_{\mathrm{hom}} = \mathrm{d}u_{\mathrm{hom}}(\kappa) \in H^1_0(D)$ such that

$$-\nabla \cdot (\alpha \nabla \mathrm{d}u_{\mathrm{hom}}) = 0 \qquad \text{in } D^- \cup D^+, \tag{5.4}$$

$$[\mathrm{d}u_{\mathrm{hom}}] = 0 \qquad \text{on } \Gamma, \tag{5.5}$$

$$\left[\alpha \frac{\partial \mathrm{d}u_{\mathrm{hom}}}{\partial \mathbf{n}}\right] = \nabla_\Gamma \cdot (\kappa[\alpha]\nabla_\Gamma \overline{u}) - \alpha^- \frac{\partial \mathrm{d}u^-_{\mathrm{off}}}{\partial \mathbf{n}} \quad \text{on } \Gamma, \tag{5.6}$$

$$\mathrm{d}u_{\mathrm{hom}} = 0 \qquad \text{on } \partial D. \tag{5.7}$$

The computation of $\mathrm{d}u_{\mathrm{off}}$ and $\mathrm{d}u_{\mathrm{hom}}$ from (5.2)–(5.3) and (5.4)–(5.7), respectively, by finite element methods is straightforward if we restrict the finite

element spaces V_j onto D^- and D, respectively. In particular, if we apply the Lagrange multiplier method [1] with λ_h being in the trace space $V_h|_\Gamma$, we get the optimal convergence rate.

Theorem 6. *Assume $\{\mathscr{T}_h\}_{h>0}$, $\{V_h\}_{h>0}$ to be specified as in Subsection 5.1. Let $\mathrm{d}u_h$ be the deterministic finite element approximation via combining the respective finite element solutions from (5.2)–(5.3) and (5.4)–(5.7) associated with the deterministic shape gradient $\mathrm{d}u[\kappa]$ to the elliptic problem (3.9)–(3.12) with respect to the reference interface Γ. Then there holds for $s=0,1$ that*

$$\begin{aligned}&\|\mathrm{d}u-\mathrm{d}u_h\|_{H^s(D^-)\cup H^s(D^+)}\\ &\quad\le Ch^{2-s}\left\{\left\|\kappa\left[\frac{\partial\overline{u}}{\partial\mathbf{n}}\right]\right\|_{H^{3/2}(\Gamma)}+\|\nabla_\Gamma\cdot(\kappa[\alpha]\nabla_\Gamma\overline{u})\|_{H^{1/2}(\Gamma)}\right\}\\ &\quad\le Ch^{2-s}\,\|\overline{u}\|_{H^2(D^-)\cup H^2(D^+)}\end{aligned}\tag{5.8}$$

where $\|\kappa\|_{C^{2,1}(\Gamma,\mathbb{R})}\le 1$, provided that the given data are sufficiently smooth.

Proof. Using the Lagrange multiplier approach we have for $s=0,1$

$$\|\mathrm{d}u_{\mathrm{off}}-\mathrm{d}u_{\mathrm{off},h}\|_{H^s(D^-)}+\left\|\lambda_h-\frac{\partial\mathrm{d}u_{\mathrm{off}}}{\partial\mathbf{n}}\right\|_{H^{s-3/2}(\Gamma)}\le Ch^{2-s}\left\|\kappa\left[\frac{\partial\overline{u}}{\partial\mathbf{n}}\right]\right\|_{H^{3/2}(\Gamma)}.$$

From [27], it follows

$$\begin{aligned}&\|\mathrm{d}u_{\mathrm{hom}}-\mathrm{d}u_{\mathrm{hom},h}\|_{H^s(D^-)\cup H^s(D^+)}\\ &\quad\le Ch^{2-s}\left\{\left\|\kappa\left[\frac{\partial\overline{u}}{\partial\mathbf{n}}\right]\right\|_{H^{3/2}(\Gamma)}+\|\nabla_\Gamma\cdot(\kappa[\alpha]\nabla_\Gamma\overline{u})\|_{H^{1/2}(\Gamma)}\right\}\end{aligned}$$

provided that the exact Neumann data of $\mathrm{d}u_{\mathrm{off}}$ are inserted. Since, however, only their approximation is available, then an additional consistency error appears in the right hand side. It is bounded by

$$\begin{aligned}\sup_{v\in H^{2-s}(D)}|\langle f-f_h,v\rangle|&=\left|\int_\Gamma\alpha^-\left(\lambda_h-\frac{\partial\mathrm{d}u_{\mathrm{off}}}{\partial\mathbf{n}}\right)v\mathrm{d}s\right|\\ &\le C\left\|\lambda_h-\frac{\partial\mathrm{d}u_{\mathrm{off}}}{\partial\mathbf{n}}\right\|_{H^{s-3/2}(\Gamma)}\|v\|_{H^{3/2-s}(\Gamma)}\\ &\le Ch^{2-s}\left\|\kappa\left[\frac{\partial\overline{u}}{\partial\mathbf{n}}\right]\right\|_{H^{3/2}(\Gamma)}\|v\|_{H^{2-s}(D)}.\end{aligned}$$

Putting these inequalities together proves our final assertion (5.8). □

5.2.2. *Low-rank approximation.* We can proceed in two different ways to compute the two-point correlation function $\mathrm{Cor}_{\mathrm{d}u}$ given by (4.5)–(4.14). The first way is a direct solution in the sparse tensor product space as considered in e.g. [16, 20]. The second way, which is simpler to implement, consists in computing a low-rank approximation

$$\mathrm{Cor}_\kappa\approx\sum_{i=1}^m\kappa_i\otimes\kappa_i\tag{5.9}$$

of the two-point correlation function of $\kappa(\omega)$ in the full tensor product space $V_h \otimes V_h$. With such a low-rank approximation at hand we have

$$\mathrm{Cor}_{\mathrm{d}u} \approx \sum_{i=1}^{m} \mathrm{d}u(\kappa_i) \otimes \mathrm{d}u(\kappa_i) \tag{5.10}$$

due to the linearity of the mapping $\kappa \mapsto \mathrm{d}u(\kappa)$. Hence, it suffices to solve (5.2)–(5.7) for all κ_i.

Assume that $\mathrm{Cor}_\kappa \in C(\Gamma \times \Gamma)$ is continuous, then the discrete version of the low-rank approximation (5.9) corresponds to the low-rank decomposition

$$\mathbf{C} \approx \mathbf{C}_m = \sum_{i=1}^{m} \boldsymbol{\ell}_i \boldsymbol{\ell}_i^T \tag{5.11}$$

of the matrix

$$\mathbf{C} = [\mathrm{Cor}_\kappa(\mathbf{x}_i, \mathbf{x}_j)]_{i,j} \in \mathbb{R}^{n \times n}$$

where $\{\mathbf{x}_i\}$ are the nodes of the finite element mesh.

The best low-rank approximation (5.9) with respect to $L^2(\Gamma \times \Gamma)$ is given by the spectral decomposition whose computation requires the knowledge of the eigenpairs (φ_i, λ_i) of the integral operator

$$(\mathcal{K}_\kappa u)(\mathbf{x}) := \int_\Gamma \mathrm{Cor}_\kappa(\mathbf{x}, \mathbf{y}) u(\mathbf{y}) \, \mathrm{d}\mathbf{y}, \quad \mathbf{x} \in \Gamma. \tag{5.12}$$

The decay of the eigenvalues $\{\lambda_i\}$ and thus the length m depends heavily on the smoothness of Cor_κ. Related decay rates have been proven in [15, 34].

Algorithm 1: Pivoted Cholesky decomposition

Data: matrix $\mathbf{C} = [\mathrm{Cor}_\kappa(\mathbf{x}_i, \mathbf{x}_j)]_{i,j} \in \mathbb{R}^{n \times n}$ and error tolerance $\varepsilon > 0$
Result: low-rank approximation $\mathbf{C}_m = \sum_{i=1}^{m} \boldsymbol{\ell}_i \boldsymbol{\ell}_i^T$ such that $\mathrm{trace}(\mathbf{C} - \mathbf{C}_m) \le \varepsilon$
begin
  set $m := 1$;
  set $\mathbf{d} := \mathrm{diag}(\mathbf{C})$ and $error := \|\mathbf{d}\|_1$;
  initialize $\boldsymbol{\pi} := (1, 2, \ldots, n)$;
  while $error > \varepsilon$ **do**
    set $i := \arg\max\{d_{\pi_j} : j = m, m+1, \ldots, n\}$;
    swap π_m and π_i;
    set $\ell_{m,\pi_m} := \sqrt{d_{\pi_m}}$;
    for $m + 1 \le i \le n$ **do**
      compute $\ell_{m,\pi_i} := \left(\mathrm{Cor}_\kappa(\mathbf{x}_{\pi_m}, \mathbf{x}_{\pi_i}) - \sum_{j=1}^{m-1} \ell_{j,\pi_m} \ell_{j,\pi_i} \right) \Big/ \ell_{m,\pi_m}$;
      update $d_{\pi_i} := d_{\pi_i} - \ell_{m,\pi_m} \ell_{m,\pi_i}$;
    compute $error := \sum_{i=m+1}^{n} d_{\pi_i}$;
    increase $m := m + 1$;
end

We use here the pivoted Cholesky decomposition to compute a low-rank approximation of Cor_κ as proposed in [18]. It is a purely algebraic approach which is quite simple to implement, see Algorithm 1. It produces a low-rank approximation to $\mathbf{C}$ for any given precision $\varepsilon > 0$. The approximation error is rigorously controlled in terms of the trace norm. Exponential convergence rates can be proven under the assumption that the eigenvalues of $\mathbf{C}$ exhibit a sufficiently fast exponential decay, see [18]. Numerical experiments show that the pivoted Cholesky decomposition in general converges optimally in the sense of the rank m being bounded by the number of terms required for the spectral decomposition of Cor_κ to get the error ε.

Having the low-rank decomposition (5.9) of the interface perturbation's two-point correlation function at hand, the complexity to compute the shape derivative's two-point correlation (5.10) is at least $m \times n$, if n denotes the number of finite elements. Therefore, log-linear complexity in n can only be achieved if $m \sim \log n$ which requires an exponential decay of the spectral decomposition of the two-point correlation Cor_κ. This, however, is only the case if Cor_κ is analytical (cf. [34]). In contrast to that, the sparse grid approach from [16, 20] produces approximations in log-linear complexity also for two-point correlation functions of finite smoothness. We refer the reader to [15] for a more extensive comparison of the spectral decomposition and the sparse grid approach.

5.2.3. *Non-intrusive approach.* Instead of computing the local shape derivative $\mathrm{d}u(\kappa_i)$, we can approximate it by a finite difference. This means that, for a small $h > 0$, we replace (5.10) by

$$\mathrm{Cor}_{\mathrm{d}u} \approx \frac{1}{h^2} \sum_{i=1}^{m} \big(u_{\Gamma(I+h\kappa_i)} - \overline{u}\big) \otimes \big(u_{\Gamma(I+h\kappa_i)} - \overline{u}\big), \tag{5.13}$$

where $u_{\Gamma(I+h\kappa_i)}$ denotes the solution of the interface problem (2.1)–(2.4) with respect to the perturbed interface

$$\Gamma(I + h\kappa_i) := \{\mathbf{x} + h\kappa_i(\mathbf{x})\mathbf{n}(\mathbf{x}) : \mathbf{x} \in \Gamma\}.$$

Thus, it is neither necessary to explicitly know the local shape derivative nor to implement it. In fact, besides the computation of the approximate expectation $\overline{u}$, we need then only the m "samples" $u_{\Gamma(I+h\kappa_i)}$ to calculate the approximate variance. This therefore constitutes an extremely fast non-intrusive algorithm in the quantification of domain uncertainties.

6. Numerical Experiments and Discussions

6.1. **Deterministic vs. Monte Carlo approach.** We present some numerical tests to demonstrate our theoretical predictions. Let $D := (-1, 1)^2$ be a square of edge length 2 and let

$$\Gamma := \{\mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\| = 1/2\}$$

be a circular interface which subdivides D into the interior domain D^- and the exterior domain D^+. In D^+ the diffusion coefficient is set as $\alpha^+ := 1$, in the interior domain D^- we consider $\alpha^- := 2$ in our first and $\alpha^- := 10$ in our second example.

We parametrize the interface Γ by polar coordinates

$$\overline{\gamma} : [0, 2\pi] \to \Gamma, \quad s \mapsto \overline{\gamma}(s) := \frac{1}{2} \begin{bmatrix} \cos(s) \\ \sin(s) \end{bmatrix}.$$

Correspondingly, the stochastic interface $\Gamma_\varepsilon(\omega)$ can be expressed via the perturbed parametrization

$$\gamma(s, \omega) := \overline{\gamma}(s) + \varepsilon\kappa(s, \omega) \begin{bmatrix} \cos(s) \\ \sin(s) \end{bmatrix}.$$

Herein, we assume that the stochastic interface perturbation is given by

$$\kappa(s, \omega) := \sum_{k=0}^{5} a_k(\omega) \cos(ks) + b_k(\omega) \sin(ks).$$

with stochastic coefficients $a_k(\omega)$ and $b_k(\omega)$ being equally distributed in $[-1, 1]$ and mutually stochastically independent. This leads to the two-point correlation function

$$\mathrm{Cor}_\kappa(s, t) = \frac{1}{3} \sum_{k=0}^{5} \cos(ks) \cos(kt) + \sin(ks) \sin(kt). \tag{6.1}$$

For our numerical experiments we choose $\varepsilon = 0.02$. Even though ε is small the perturbation is considerably large since the norm $\|\kappa(\omega)\|_{C^{2,1}([0,2\pi])}$ might be large.

We determine first the expectation and the variance of random solutions to this SEIP by a Monte Carlo method, using $M = 10000$ samples. The triangulation has to be reconstructed for each sample in order to resolve the interface exactly. In order to compute the sample mean and variance, we interpolate the solution to a fixed quadrangular grid with 65×65 nodes. The approximate expectation and variance are depicted in the first row of Figure 2 for $\alpha^- := 2$ and Figure 3 for $\alpha^- := 10$.

In the second row of Figures 2 and 3 the approximate expectation and variance of our deterministic algorithm is depicted. To ensure a fair comparison, we interpolated the finite element solutions on the same rectangular mesh as the Monte Carlo solutions. Notice that the pivoted Cholesky decomposition computes an exact rank-11 approximation of the two-point correlation (6.1) since it is of finite rank 11. This means that only 11 shape derivatives need to be determined to compute the approximate variance.

In the last row of Figures 2 and Figure 3, we plotted the differences of expectations and variances of both algorithms. We see that the deterministic approach produces quite accurate approximations except in the direct neighborhood of the reference interface, as predicted by our theory.

6.2. **Non-intrusive approach.** Our next example is concerned with the comparison of the shape derivative-based approach (5.10) and the non-intrusive approach (5.13). The domain D and the interface Γ are chosen as in the previous example while the associated coefficients are set as $\alpha^- := 2$ and $\alpha^+ = 1$. The stochastic perturbation of the interface is assumed to exhibit

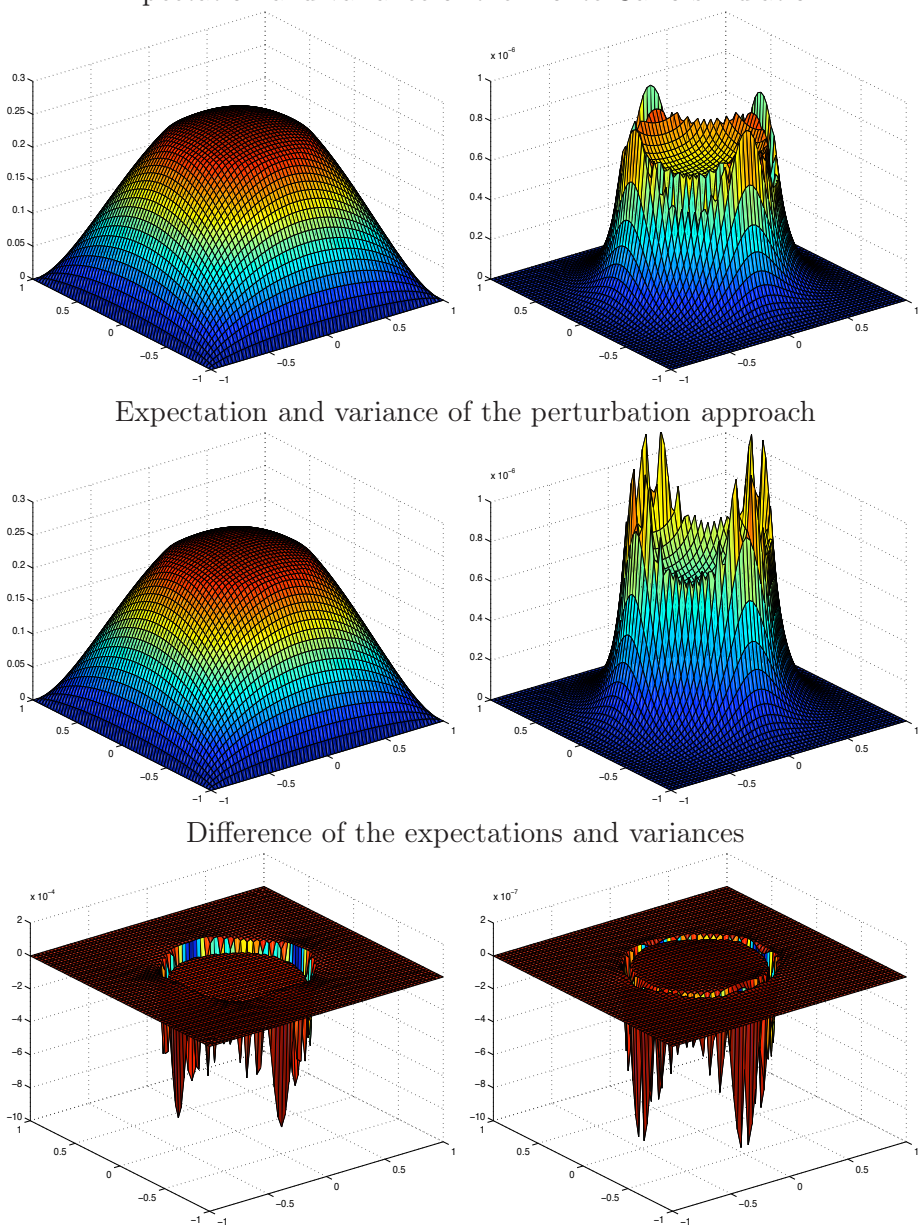

FIGURE 2. Approximate expectation and variation in case of $\alpha = 2$ and $\varepsilon = 0.02$.

the Gaussian two-point correlation

$$\mathrm{Cor}_\kappa = \exp\left(-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{\sigma}\right)$$

where we consider the choices $\sigma = 10, 100, 1000$.

We again use the pivoted Cholesky decomposition (Algorithm 1) to compute the discrete low-rank decomposition (5.11) with a trace error of $\varepsilon = 0.001$. It has the rank $m = 17$ if $\sigma = 10$, the rank $m = 54$ if $\sigma = 100$, and

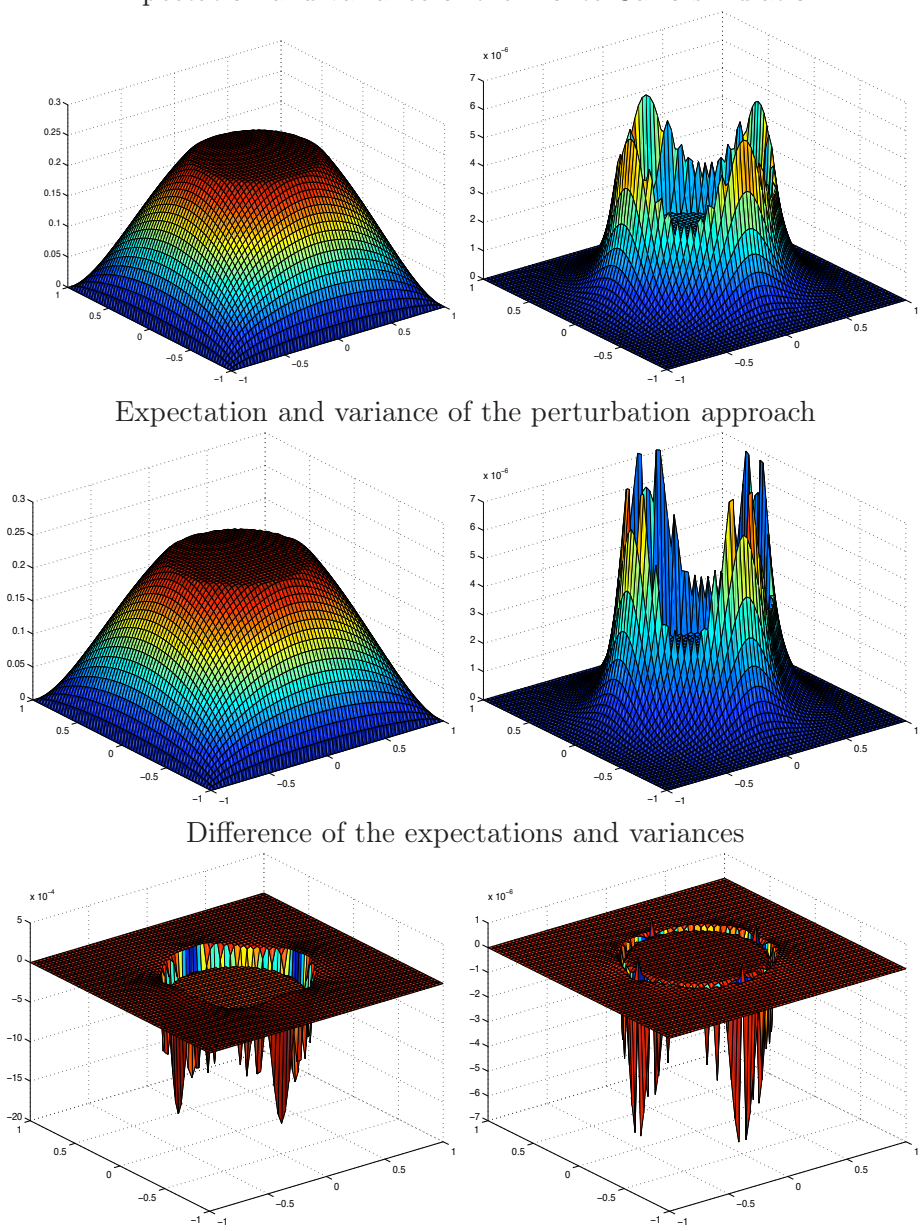

FIGURE 3. Approximate expectation and variation in case of $\alpha = 10$ and $\varepsilon = 0.02$.

the rank $m = 171$ if $\sigma = 1000$. The step size h in the finite differences of (5.13) are chosen as $h = 0.001$. The resulting approximate two-point correlations are plotted in Figures 4–6. As these plots demonstrate, the non-intrusive approach (5.13) produces reasonable approximations of the solution's variance while the implementation is extremely simple. Especially, we observe that influence of the stochastic interface becomes more localized as σ increases, i.e., if the correlation length of the interface perturbation decreases.

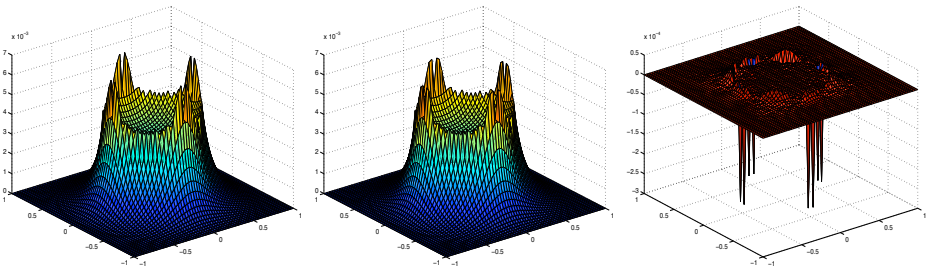

FIGURE 4. Approximate variations (left: via shape derivative / middle: via finite difference / right: difference between the approaches) in case of the Gaussian kernel with $\sigma = 10$.

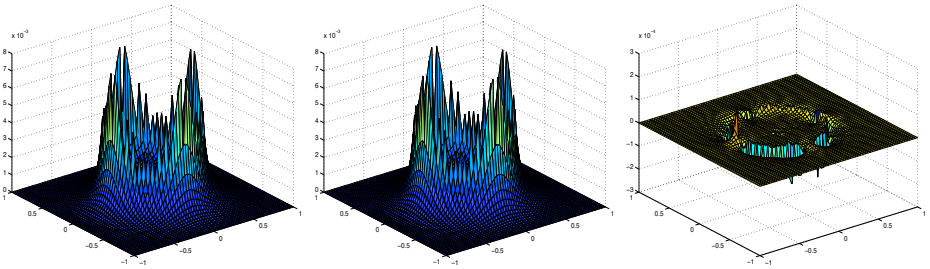

FIGURE 5. Approximate variations (left: via shape derivative / middle: via finite difference / right: difference between the approaches) in case of the Gaussian kernel with $\sigma = 100$.

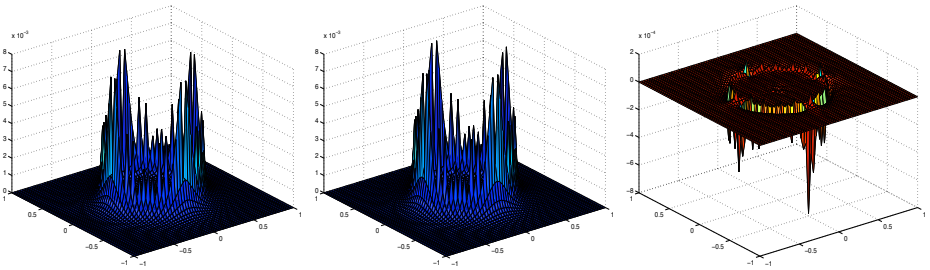

FIGURE 6. Approximate variations (left: via shape derivative / middle: via finite difference / right: difference between the approaches) in case of the Gaussian kernel with $\sigma = 1000$.

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