SPARSE SECOND MOMENT ANALYSIS FOR ELLIPTIC PROBLEMS IN STOCHASTIC DOMAINS

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Abstract. We consider the numerical solution of elliptic boundary value problems in domains with random boundary perturbations. Assuming normal perturbations with small amplitude and known mean field and two-point correlation function, we derive, using a second order shape calculus, deterministic equations for the mean field and the two-point correlation function of the random solution for a model Dirichlet problem which are 3rd order accurate in the boundary perturbation size.

Using a variational boundary integral equation formulation on the unperturbed, nominal boundary and a wavelet discretization, we present and analyze an algorithm to approximate the random solution's two-point correlation function at essentially optimal order in essentially $\mathcal{O}(N)$ work and memory, where N denotes the number of unknowns required for consistent discretization of the boundary of the domain.

1. Introduction

The rapid development of scientific computing and numerical analysis in recent years allows the efficient numerical solution of large classes of partial differential equation models with high accuracy, *provided* the problem's input data are known exactly.

Often, however, exact input data for numerical simulation in engineering is not known. The practical significance of highly accurate numerical solution of differential equation models in engineering must thus address how to account for uncertain input data.

If a statistical description of the input data is available, one can mathematically describe data and solutions as random fields and aim at computation of corresponding deterministic statistics of the unknown random solution.

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In the present paper we consider elliptic boundary value problems on a class of uncertain domains. For example, one may think of tolerances in the shape of products fabricated by line production. Since the computational domain and its boundary are stochastic, the solution of the boundary value problem becomes itself a random field. Identifying the random domain with its boundary, the problem under consideration can be formulated as follows: *given complete statistical information of the random boundary perturbation, compute statistics of engineering interest for the random solution of the boundary value problem.*

Knowledge of complete statistical information on the input random fields (e.g. the joint probability densities of the random boundary perturbation) is hardly available in practice. Therefore, additional modeling assumptions must be imposed. In the present paper, we assume *small boundary perturbation amplitude* and that *mean field* and *two-point correlation of the boundary perturbation field are known.* This would determine, for example, a Gaussian probability measure on admissible boundary perturbations (see, e.g., [3] and the references there for more on measures on function spaces).

Our goal of computation is thus as follows: for given mean and two-point correlation of the boundary perturbation field, compute the mean and the two-point correlation of the random solution of the boundary value problem.

Since the Monte Carlo Approach to generate a large number M of 'sample' domains and to solve a deterministic boundary value problem on each sample is very expensive, we aim here at a direct, deterministic computation of the solution statistics in terms of statistics of boundary variation.

Since the solution's nonlinear dependence on the shape of the domain is Fréchet differentiable [14, 11, 19, 25, 26], we achieve this goal by linearizing around an unperturbed, so-called "nominal" domain D. We use the shape gradient and the shape Hessian derived in [7, 8] to derive deterministic problems for the random solution's statistics with respect to random perturbations of the domain.

While sensitivity analysis underlies also the so-called "worst case scenario" analysis in uncertainty quantification (e.g. [1] and the references there for uncertainty in coefficients and loadings), we derive deterministic problems which yield, to third order in the boundary perturbation amplitude, for given, nominal boundary and given two-point correlation function of the boundary perturbation field, approximate means and variances of the random solution at any interior point $\mathbf{x} \in D$.

Naturally, this approach requires smallness assumptions on the boundary perturbation size which must hold with probability 1. Since the second moments of spatially inhomogeneous random fields, their two-point correlations, are functions on

$\partial D \times \partial D$, the key to computational efficiency of our approach is the efficient, deterministic second moment analysis of the random solution.

We propose the numerical solution of these deterministic problems using a variational boundary integral equation approach combined with a wavelet discretization. We provide a numerical analysis which shows that variances of the random solution at any interior point can be computed in work and memory essentially proportional to N, the number of degrees of freedom needed to parametrize the unperturbed, nominal boundary ∂D. Here and throughout the paper, "essentially" means up to powers of $\log N$ resp., in the context of convergence rates, up to powers of $|\log h|$.

While our second moment analysis is asymptotic in the perturbation amplitude, it has the advantage of being *distribution free*, i.e. it does not depend on complete knowledge of all joint probability densities of the boundary perturbation field.

Essential ingredients in our analysis are shape calculus, boundary reduction of the problem characterizing the shape derivative leading to weakly singular boundary integral equations and a 'sparse' four dimensional representation of the two-point correlation function of the second moments of the unknown boundary flux developed in [23, 17].

We consider exemplarily a model Poisson equation with Dirichlet boundary conditions. Employing a Taylor expansion in terms of local shape derivatives, we show that the mean of the stochastic potential coincides to second order with the solution of the Poisson equation on the unperturbed domain. Moreover, the two-point correlation of the stochastic potential can be approximated to third order in the boundary perturbation amplitude by solving a boundary value problem defined on the cartesian product of the nominal domain D with itself. That way, we derive a *deterministic* problem for the first and second moment of the potential at any interior point of the unperturbed nominal domain D.

We choose a wavelet Galerkin discretization of the boundary integral equations (BIEs) to solve these boundary value problems in an efficient way. The proposed wavelet Galerkin discretization of the BIEs serves three purposes: a) to obtain a numerically sparse representation of the boundary integral operator reducing the N^2 matrix entries to $\mathcal{O}(N)$ many without reducing the convergence rate of the scheme (e.g. [21, 5]), b) to obtain a bounded condition number for the diagonally preconditioned system and c) to obtain a sparse representation of the two-point correlation function (resp. the second moment) of the random solution density on the boundary which requires $\mathcal{O}(N \log N)$ rather than $\mathcal{O}(N^2)$ degrees of freedom while essentially retaining the asymptotic convergence rate of the full tensor product discretization. While boundary reduction and wavelet discretization thus ideally serves our purpose, we note that similar results can be obtained also with other so-called "fast" discretizations of the integral operators on unstructured meshes on the boundary as e.g. in [20]; essential ingredient, however, is a Galerkin discretization of the mean field problem in a hierarchic basis; such bases on surfaces in $\mathbb{R}^3$ can be obtained in various ways, see, for example, [10, 20, 27] for such bases on structured as well as on unstructured meshes.

The main result of this paper is a deterministic algorithm to compute, to third order in the boundary perturbation amplitude, the first and second moment of the stochastic potential at any interior point of D with a complexity that stays essentially asymptotically proportional to the number N of degrees of freedom for the discretization of the boundary ∂D of the nominal domain D.

The paper is organized as follows. Section 2 recapitulates results from shape calculus. In Section 3 we specify the stochastic domains under consideration. Then, in Section 4, we derive deterministic boundary value problems for the mean and two-point correlation of the associated stochastic potential. The reformulation of the boundary value problems as boundary integral equations is performed in Section 5. Then, Section 6 is devoted to the full tensor product discretization and corresponding error estimates. In Section 7 we introduce the fast wavelet based algorithm. Finally, in Section 8 we present numerical results which demonstrate the capability of the proposed algorithm.

Throughout this paper, in order to avoid the repeated use of generic but unspecified constants, by $C_1 \lesssim C_2$ we mean that C_1 can be bounded by a multiple of C_2, independently of parameters which C_1 and C_2 may depend on. Obviously, $C_1 \gtrsim C_2$ is defined as $C_2 \lesssim C_1$, and $C_1 \sim C_2$ as $C_1 \lesssim C_2$ and $C_1 \gtrsim C_2$.

2. Shape Calculus

In order to assess the impact of random boundary perturbations of a domain $D \subset \mathbb{R}^n$, $n = 2, 3$, on the solution of boundary value problems in D, we use shape calculus via boundary variations. For a general overview on shape calculus, mainly based on the perturbation of identity (Murat and Simon) or the speed method (Sokolowski and Zolesio), we refer the reader for example to Murat and Simon [14, 25], Pironneau [18], Sokolowski and Zolesio [26], Delfour and Zolesio [6], and the references therein.

We consider the model Dirichlet Problem for the Poisson equation

$$-\Delta u = f \text{ in } D, \qquad u = g \text{ on } \partial D, \tag{2.1}$$

where $D \subset \mathbb{R}^n$, is a given, bounded domain. For the sake of simplicity we assume $f \in C^\infty(\mathbb{R}^n)$ and that $g \in C^\infty(\partial D)$ is the restriction of some function $\bar{g} \in C^\infty(\mathbb{R}^n)$. Finally, we assume that $\partial D \in C^\infty$ which implies that $u \in C^\infty(\overline{D})$.

Consider a smooth, nontangential boundary variation field $\mathbf{U} : \partial D \to \mathbb{R}^n$ with $\|\mathbf{U}\|_{C^{3,\alpha}(\partial D)} \leq 1$ for some $\alpha > 0$ and define the perturbed boundary for sufficiently small $\varepsilon > 0$ by

$$\partial D_\varepsilon = \{\mathbf{x} + \varepsilon \mathbf{U}(\mathbf{x}) : \mathbf{x} \in \partial D\}.$$

For sufficiently small ε, the boundary curve ∂D_ε uniquely defines a perturbed domain $D_\varepsilon \in C^\infty$. Throughout the paper we restrict ourselves to variations $\mathbf{U}$ which are normal with respect to the domain D: denoting by $\mathbf{n}(\mathbf{x})$ the exterior unit normal vector to the reference domain D at the point $\mathbf{x} \in \partial D$, the boundary variation $\mathbf{U}(\mathbf{x})$ is given by

$$\mathbf{U}(\mathbf{x}) := \kappa(\mathbf{x})\mathbf{n}(\mathbf{x}), \quad \text{where} \quad \kappa(\mathbf{x}) \in \mathbb{R} \quad \text{satisfies} \quad \|\kappa\|_{C^{3,\alpha}(\partial D)} \leq 1. \tag{2.2}$$

Let us also remark that each boundary variation can be extended smoothly to a domain variation field, but for our purpose it suffices to consider only boundary variations (see, e.g., Section 2.8 of [26]).

The solution u of the model problem (2.1) is known to depend (Fréchet) differentiably on the shape of D (e.g. [18, 26, 14, 25] and the references there). Its first derivative, the so-called *local shape derivative du on the boundary perturbation field* $\mathbf{U}$, denoted by $du[\mathbf{U}]$, is given by the Dirichlet problem

$$\Delta du = 0 \text{ in } D, \qquad du = \langle \nabla(g - \bar{u}), \mathbf{U}\rangle = \langle \mathbf{U}, \mathbf{n}\rangle \frac{\partial(g - \bar{u})}{\partial \mathbf{n}} \text{ on } \partial D \tag{2.3}$$

where $\bar{u}$ denotes the solution of (2.1), The shape derivative is *formally* (see [14, 26] for a rigorous derivation) obtained by the pointwise limit

$$du(\mathbf{x}) := \lim_{\varepsilon \to 0} \frac{u_\varepsilon(\mathbf{x}) - u(\mathbf{x})}{\varepsilon}, \qquad \mathbf{x} \in D \cap D_\varepsilon,$$

where u_ε satisfies the boundary value problem (2.1) on the domain D_ε, see [7, 8, 19] for detailed calculations.

For a second order shape calculus we consider a second perturbation field $\mathbf{U}'$ defined analogously to $\mathbf{U}$ in (2.2): $\mathbf{U}'(\mathbf{x}) = \kappa'(\mathbf{x})\mathbf{n}(\mathbf{x})$, $\kappa'(\mathbf{x}) \in C^\infty(\partial D)$.

The second order shape derivative, the "shape Hessian", is a bilinear form on pairs of boundary perturbation fields $(\mathbf{U}, \mathbf{U}')$, denoted by $d^2u = d^2u[\mathbf{U}, \mathbf{U}']$. It is obtained from the Dirichlet problem

$$\begin{gathered} \Delta d^2 u = 0 \text{ in } D, \\ d^2u = \langle \mathbf{H}[g - \bar{u}])\mathbf{U}', \mathbf{U}\rangle - \langle \nabla du[\mathbf{U}], \mathbf{U}'\rangle - \langle \nabla du[\mathbf{U}'], \mathbf{U}\rangle \text{ on } \partial D, \end{gathered} \tag{2.4}$$

cf. [8, Theorem 1 and Remark 7] and [11], where $\mathbf{H}[\varphi]$ denotes the Hessian of φ.

With (2.3) and (2.4) at hand, we obtain for sufficiently small $\varepsilon > 0$ the "shape-Taylor expansion"

$$u_\varepsilon(\mathbf{x}) = u(\mathbf{x}) + \varepsilon du[\mathbf{U}](\mathbf{x}) + \frac{\varepsilon^2}{2} d^2u[\mathbf{U},\mathbf{U}](\mathbf{x}) + \mathcal{O}(\varepsilon^3), \quad \mathbf{x} \in K \subset\subset D \cap D_\varepsilon. \tag{2.5}$$

3. A Class of Stochastic Domains

We obtain a family of stochastic domains from the preceding shape calculus by admitting random fields $\mathbf{U}(\mathbf{x},\omega)$, $\mathbf{U}'(\mathbf{x},\omega)$ as domain variations.

To this end, we fix an unperturbed reference domain D. We assume it to be a bounded subdomain of $\mathbb{R}^n$, $n = 2,3$ with sufficiently smooth, closed and orientable $(n-1)$-dimensional boundary manifold ∂D ($\partial D \in C^k$ with $k > 4$ will suffice in what follows). Denote by $\mathbf{n}(\mathbf{x})$ the exterior unit normal vector to ∂D at the boundary point $\mathbf{x} \in \partial D$. Then for sufficiently small $\varepsilon_0 > 0$ and for some scalar function $\kappa(\mathbf{x}) \in C^k(\partial D, \mathbb{R})$ with $\|\kappa(\cdot)\|_{L^\infty(D)} \le 1$, the family of surfaces $\partial D_\varepsilon = \{\mathbf{x} + \varepsilon\kappa(\mathbf{x})\mathbf{n}(\mathbf{x}) | \mathbf{x} \in \partial D\}_{0 \le \varepsilon < \varepsilon_0}$ belongs to C^{k-1}. We denote the corresponding interior domains (which depend, of course, on κ) by D_ε.

To specify random domain variations, we assume that $\kappa(\cdot) : \partial D \to \mathbb{R}$ is a random field on ∂D taking values in $\mathbb{R}$. We denote by X a space of admissible boundary perturbation functions. The random perturbations of D will be described by a suitable probability space (Ω, Σ, P) consisting of a) a set Ω of realizations $\omega \mapsto \kappa(\omega) \in X$ (i.e., realizations of particular perturbations $\kappa(\cdot)$), b) a sigma algebra Σ and c) a probability measure on the space X.

In what follows, we take for X the space $C^k(\partial D, \mathbb{R})$ with k sufficiently large ($k > 4$ will do) and equip it with the usual norm and Σ as a sub-sigma algebra of the Borel sets of X. We then choose $P : \Sigma \to [0,1]$ to be a probability measure on (X, Σ) (see, e.g. [3] for more on measures on function spaces).

Example 3.1. *An important and widely used example for probability measures on X are the so-called Gaussian measures (see, e.g.* [3] *and the references there).*

Gaussian random fields u on a Banach space X are essentially specified by their mean fields $\mathrm{E}_u = \int_\Omega u(\omega) dP \in (X^*)'$ *and by their covariance kernels* Covar_u *which are defined by*

$$\mathrm{Covar}_u := \int_\Omega ((u - \mathrm{E}_u) \otimes (u - \mathrm{E}_u))\, dP(\omega) : (X^*)' \times (X^*)' \to \mathbb{R} \tag{3.1}$$

where $(X^*)'$ denotes the algebraic dual of X^* (see [3]*, Def. 2.2.7). Under sufficient regularity, E_u and* Covar_u *can be identified with objects in X resp. in $X \otimes X$.*

In what follows, we let thus (Ω, Σ, P) be a probability space on the space X of admissible boundary perturbation fields κ in (2.2).

Then we consider the random domain variation field $\mathbf{U}(\mathbf{x},\omega) = \kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x})$, where κ is a P-measurable mapping $\kappa(\mathbf{x},\omega) : \Omega \to X = C^k(\partial D, \mathbb{R})$, and assume finite second moments of $\kappa(\mathbf{x},\omega)$ with respect to P. We denote the set of all such κ by $L^2\big(\Omega, C^k(\partial D)\big)$.

With the random field $\kappa \in L^2\big(\Omega, C^k(\partial D)\big)$, and a perturbation parameter $\varepsilon > 0$ which is sufficiently small, we associate boundaries $\partial D_\varepsilon(\omega)$ through the parametric representation

$$\gamma_\varepsilon : \partial D \times \Omega \to \mathbb{R}^3, \quad \gamma_\varepsilon(\mathbf{x},\omega) := \mathbf{x} + \varepsilon\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x}) \tag{3.2}$$

where

$$\|\kappa(\cdot,\omega)\|_{C^k(\partial D)} \le 1 \quad \text{for P- almost all} \quad \omega \in \Omega, \tag{3.3}$$

which we assume in what follows. A realization of the stochastic domain $D_\varepsilon(\omega)$ is the interior of the boundary manifold

$$\partial D_\varepsilon(\omega) := \{\gamma_\varepsilon(\mathbf{x},\omega) : \mathbf{x} \in \partial D(\omega)\}.$$

The assumption (3.3) implies in particular that the domain $D_\varepsilon(\omega)$ does not degenerate $P - a.s.$ if $0 \le \varepsilon < \varepsilon_0$ for suffiently small ε_0 depending only on the curvature of ∂D. We assume that the mean field

$$\mathrm{E}_\kappa(\mathbf{x}) := \int_\Omega \kappa(\mathbf{x},\omega)dP(\omega) = \mathrm{E}\big(\kappa(\mathbf{x},\omega)\big), \quad \mathbf{x} \in \partial D,$$

and the two-point correlation

$$\mathrm{Cor}_\kappa(\mathbf{x},\mathbf{y}) := \int_\Omega \kappa(\mathbf{x},\omega)\kappa(\mathbf{y},\omega)dP(\omega) = \mathrm{E}\big(\kappa(\mathbf{x},\omega)\kappa(\mathbf{y},\omega)\big), \quad \mathbf{x},\mathbf{y} \in \partial D,$$

of the domain variation $\kappa(\mathbf{x},\omega)$ under consideration are pointwise finite and known. Here, the notation $\mathrm{E}(\cdot)$ denotes the expectation or "ensemble average" with respect to the probability measure $P(\omega)$. Then, since

$$\mathrm{E}\big(\gamma_\varepsilon(\mathbf{x},\omega)\big) = \mathbf{x} + \varepsilon\,\mathrm{E}_\kappa(\mathbf{x})\mathbf{n}(\mathbf{x}), \quad \mathbf{x} \in \partial D,$$

the reference domain $\mathrm{E}\big(D_\varepsilon(\omega)\big)$ is formally described via the reference boundary

$$\mathrm{E}\big(\partial D_\varepsilon(\omega)\big) = \{\mathbf{x} + \varepsilon\,\mathrm{E}_\kappa(\mathbf{x})\mathbf{n}(\mathbf{x}) : \mathbf{x} \in \partial D\}. \tag{3.4}$$

We assume below that the perturbation field $\kappa(\mathbf{x},\omega)$ is *centered*, i.e. that

$$\mathrm{E}_\kappa(\mathbf{x}) = 0. \tag{3.5}$$

The assumption (3.5) implies then in (3.4) that $\mathrm{E}\big(\partial D_\varepsilon(\omega)\big) = \partial D$ and that

$$\mathrm{Covar}_\kappa = \mathrm{Cor}_\kappa. \tag{3.6}$$

Next, exploiting once more (3.5), the covariance of the random boundary perturbation field is given by

$$\begin{aligned}\operatorname{Cor}_\gamma(\mathbf{x},\mathbf{y}) &= \operatorname{E}\big(\gamma(\mathbf{x},\omega)\otimes\gamma(\mathbf{y},\omega)\big)\\ &= \operatorname{E}\Big(\big(\mathbf{x}+\varepsilon\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x})\big)\otimes\big(\mathbf{y}+\varepsilon\kappa(\mathbf{y},\omega)\mathbf{n}(\mathbf{y})\big)\Big)\\ &= \mathbf{x}\otimes\mathbf{y}+\varepsilon^2\operatorname{Cor}_\kappa(\mathbf{x},\mathbf{y})\big(\mathbf{n}(\mathbf{x})\otimes\mathbf{n}(\mathbf{y})\big).\end{aligned}$$

Consequently, the correlation of the random domain variation can be either described by the two-point correlation kernel $\operatorname{Cor}_\kappa$ of the perturbation field κ in (3.2), (3.3) or, equivalently, by the following manifold of dimension $2(n-1)$ which is a submanifold of $\mathbb{R}^n\times\mathbb{R}^n=\mathbb{R}^{2n}$, $n=2,3$, given by

$$\big\{\mathbf{x}\otimes\mathbf{y}+\varepsilon^2\operatorname{Cor}_\kappa(\mathbf{x},\mathbf{y})\big(\mathbf{n}(\mathbf{x})\otimes\mathbf{n}(\mathbf{y})\big):\mathbf{x},\mathbf{y}\in\partial D\big\}\subset\mathbb{R}^{2n}$$

4. Expectation and Variance of the Random Solution

We are interested in the statistics of the random solution of the Poisson equation (2.1) defined on the stochastic domain $D_\varepsilon(\omega)$. More precisely, given $D_\varepsilon(\omega)$ and deterministic, smooth data $f,g\in C^\infty(\mathbb{R}^n)$ as in (2.1), we seek $u_\varepsilon(\omega)\in H^1(D_\varepsilon(\omega))$ such that

$$-\Delta u_\varepsilon(\omega)=f \text{ in } D_\varepsilon(\omega),\qquad u_\varepsilon(\omega)=g \text{ on } \partial D_\varepsilon(\omega). \tag{4.1}$$

We choose a fixed point $\mathbf{z}\in D$ such that

$$\operatorname{dist}(\mathbf{z},\partial D)>\varepsilon. \tag{4.2}$$

Then, due to (3.2), (3.3) it holds $P-a.s.$ that

$$\mathbf{z}\in D_\varepsilon:=\bigcap_{\omega\in\Omega}D_\varepsilon(\omega). \tag{4.3}$$

Our aim is the deterministic, approximate computation of the expectation $\operatorname{E}_u(\mathbf{z}):=\operatorname{E}\big(u(\mathbf{z},\omega)\big)$ and of the variance $\operatorname{Var}_u(\mathbf{z}):=\operatorname{Var}\big(u(\mathbf{z},\omega)\big)$ of the random solution $u(\mathbf{z},\omega)$ of (4.1) in the point $\mathbf{z}\in D_\varepsilon$. Since the random solution's dependence on the domain variation κ is nonlinear, we assume small perturbation amplitude ε and derive next approximations for these deterministic quantities under the assumption of sufficiently small domain perturbations, i.e. provided that $\varepsilon>0$ in (3.2) is sufficiently small.

A crucial tool in the derivation will be the Taylor expansion of the random solution $u_\varepsilon(\omega)$ in (4.1) with respect to the perturbation parameter ε. It is the stochastic analog of the “shape-Taylor expansion” (2.5).

Lemma 4.1. *Assume* (2.2) *and* (3.3). *Then, for sufficiently small* $\varepsilon > 0$, *the random solution* $u_\varepsilon(\omega)$ *of the boundary value problem (4.1) admits the asymptotic expansion*

$$u_\varepsilon(\mathbf{z},\omega) = \bar{u}(\mathbf{z}) + \varepsilon du(\mathbf{z},\omega) + \frac{\varepsilon^2}{2} d^2u(\mathbf{z},\omega) + \mathcal{O}(\varepsilon^3) \text{ for } P - a.e.\ \omega \in \Omega, \tag{4.4}$$

where $\bar{u} \in H^1(D)$ *denotes the solution of the deterministic Dirichlet problem*

$$-\Delta \bar{u} = f \text{ in } D, \qquad \bar{u} = g \text{ on } \partial D, \tag{4.5}$$

where we used the abbreviations

$$du(\mathbf{z},\omega) := du[\kappa(\cdot,\omega)\mathbf{n}](\mathbf{z}), \tag{4.6}$$

and

$$d^2u(\mathbf{z},\omega) := d^2u[\kappa(\mathbf{z},\omega)\mathbf{n}(\mathbf{z}), \kappa(\mathbf{z}',\omega)\mathbf{n}(\mathbf{z}')]|_{\mathbf{z}'=\mathbf{z}}. \tag{4.7}$$

The remainder term is $\mathcal{O}(\varepsilon^3)$ *for* $P - a.e.\ \omega \in \Omega$.

Proof. Applying the shape-Taylor expansion (2.5) for an arbitrary, fixed realization $\kappa(\cdot,\omega)$, $\omega \in \Omega$ yields with the assumptions (3.3) and (2.2) its stochastic counterpart (4.4). □

Based on the Taylor expansion (4.4) of the random solution $u_\varepsilon(\omega)$ of (4.1), we derive next two deterministic expressions for the first and second moment, i.e. the mean field and the two-point correlation kernel, of the random solution of (4.1). We emphasize that these expressions are *linear* in terms of the corresponding first and second moments of the boundary perturbation field $\kappa(\mathbf{x},\omega)$.

Lemma 4.2. *To second order, the expectation* $\mathrm{E}_u(\mathbf{z})$ *is obtained directly from the Poisson equation* (2.1) *with respect to the nominal domain* D. *Specifically, there holds*

$$\mathrm{E}_u(\mathbf{z}) = \bar{u}(\mathbf{z}) + \mathcal{O}(\varepsilon^2), \qquad \mathbf{z} \in D_\varepsilon. \tag{4.8}$$

where $\bar{u} \in H^1(D)$ *denotes the solution of the deterministic Dirichlet problem (4.5).*

Proof. If $\|\mathbf{U}(\cdot,\omega)\|_{C^{3,\alpha}(D)} \lesssim 1$ almost shure, we apply the Taylor expansion (4.4) to arrive at

$$u(\mathbf{z},\omega) = \bar{u}(\mathbf{z}) + \varepsilon du[\kappa(\cdot,\omega)\mathbf{n}](\mathbf{z}) + \mathcal{O}(\varepsilon^2) \quad a.e.\ \omega \in \Omega,$$

Thus, using the abbreviation (4.6), we conclude that

$$\mathrm{E}\big(u(\mathbf{z},\omega)\big) = \mathrm{E}\big(u(\mathbf{z}) + \varepsilon du(\mathbf{z},\omega) + \mathcal{O}(\varepsilon^2)\big) = \bar{u}(\mathbf{z}) + \varepsilon\, \mathrm{E}\big(du(\mathbf{z},\omega)\big) + \mathcal{O}(\varepsilon^2).$$

We claim

$$\mathrm{E}\big(du(\mathbf{z},\omega)\big) = 0. \tag{4.9}$$

To see this, we note that (2.3) and (2.2) yield for the shape derivative du in the direction $\mathbf{U} = \kappa(\mathbf{x}, \omega)\mathbf{n}$ the problem

$$\Delta du(\cdot, \omega) = 0 \text{ in } D, \qquad du(\cdot, \omega) = \kappa(\cdot, \omega)\frac{\partial(g - \bar{u})}{\partial \mathbf{n}} \text{ on } \partial D. \tag{4.10}$$

whence $\mathrm{E}_{du}(\mathbf{z}) := \mathrm{E}\big(du(\mathbf{z}, \omega)\big)$ is given by (cf. (2.3))

$$\Delta\,\mathrm{E}_{du} = 0 \text{ in } D, \qquad \mathrm{E}_{du} = \mathrm{E}_\kappa \frac{\partial(g - \bar{u})}{\partial \mathbf{n}} \text{ on } \partial D,$$

and since, by assumption (3.5), $E_\kappa \equiv 0$ on ∂D. □

Lemma 4.3. *For $\varepsilon > 0$ sufficiently small, the variance $\mathrm{Var}_u(\mathbf{z})$ of the random solution satisfies for all $\mathbf{z}$ with (4.2)*

$$\mathrm{Var}_u(\mathbf{z}) = \varepsilon^2\,\mathrm{Var}\big(du(\mathbf{z}, \omega)\big) + \mathcal{O}(\varepsilon^3) = \varepsilon^2\,\mathrm{E}\left(du(\mathbf{z}, \omega)^2\right) + \mathcal{O}(\varepsilon^3). \tag{4.11}$$

Proof. We start by noting that for every fixed $\mathbf{z} \in D$, it holds that

$$\mathrm{Var}\big(u(\mathbf{z}, \omega)\big) := \mathrm{E}\big(u(\mathbf{z}, \omega)^2\big) - \mathrm{E}^2\big(u(\mathbf{z}, \omega)\big). \tag{4.12}$$

Applying the stochastic Taylor expansion (4.4) yields

$$u(\mathbf{z}, \omega) = \bar{u}(\mathbf{z}) + \varepsilon du(\mathbf{z}, \omega) + \frac{\varepsilon^2}{2} d^2u(\mathbf{z}, \omega) + \mathcal{O}(\varepsilon^3) \quad a.e. \text{ in } \omega \in \Omega.$$

We expand both terms on the right hand side of (4.12) with respect to ε. On the one hand, we get

$$\begin{aligned}\mathrm{E}\big(u(\mathbf{z}, \omega)^2\big) &= \mathrm{E}\left(\left[\bar{u}(\mathbf{z}) + \varepsilon du(\mathbf{z}, \omega) + \frac{\varepsilon^2}{2} d^2u(\mathbf{z}, \omega) + \mathcal{O}(\varepsilon^3)\right]^2\right)\\ &= \bar{u}(\mathbf{z})^2 + \varepsilon^2\,\mathrm{E}\big(du(\mathbf{z}, \omega)^2\big) + 2\varepsilon\bar{u}(\mathbf{z})\,\mathrm{E}\big(du(\mathbf{z}, \omega)\big) + \varepsilon^2\bar{u}(\mathbf{z})\,\mathrm{E}\big(d^2u(\mathbf{z}, \omega)\big) + \mathcal{O}(\varepsilon^3).\end{aligned}$$

On the other hand we find

$$\begin{aligned}\mathrm{E}^2\big(u(\mathbf{z}, \omega)\big) &= \left(\bar{u}(\mathbf{z}) + \varepsilon\,\mathrm{E}\big(du(\mathbf{z}, \omega)\big) + \frac{\varepsilon^2}{2}\,\mathrm{E}\big(d^2u(\mathbf{z}, \omega)\big) + \mathcal{O}(\varepsilon^3)\right)^2\\ &= \bar{u}(\mathbf{z})^2 + \varepsilon^2\,\mathrm{E}^2\big(du(\mathbf{z}, \omega)\big) + 2\varepsilon\bar{u}(\mathbf{z})\,\mathrm{E}\big(du(\mathbf{z}, \omega)\big) + \varepsilon^2\bar{u}(\mathbf{z})\,\mathrm{E}\big(d^2u(\mathbf{z}, \omega)\big) + \mathcal{O}(\varepsilon^3).\end{aligned}$$

Subtracting both equations yields the desired result. □

The following question arises in view of (4.9), (4.11):

$$\text{how to compute } \mathrm{E}\big(du(\mathbf{z}, \omega)^2\big) \text{ deterministically?}$$

Observing that (4.9) implies

$$\mathrm{Var}\big(du(\mathbf{z}, \omega)\big) = \mathrm{Cor}\big(du(\mathbf{z}, \omega), du(\mathbf{z}', \omega)\big)\big|_{\mathbf{z}=\mathbf{z}'},$$

we approximate $\mathrm{Var}\big(du(\mathbf{z}, \omega)\big)$ as trace of the two-point correlation of the shape gradient, following [23, 17]. The next result shows that the deterministic two-point correlation function of the local shape derivative in the direction of the random boundary perturbation $\mathbf{U}(\mathbf{x},\omega)=\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x})$ satisfies, to leading order in perturbation size ε, a deterministic boundary value problem in higher dimension.

Theorem 4.4. *Let $\bar{u}$, the solution of (4.5), belong to $H^2(D)$. Then the two-point correlation*

$$\operatorname{Cor}_{du}(\mathbf{z},\mathbf{z}') := \operatorname{Cor}\big(du(\mathbf{z},\omega), du(\mathbf{z}',\omega)\big)$$

is the unique solution in $H^{1,1}(D\times D)$ of the following tensor product boundary value problem on $D\times D\subset\mathbb{R}^{2n}$

$$\begin{aligned} (\Delta_{\mathbf{z}}\otimes\Delta_{\mathbf{z}'})\operatorname{Cor}_{du}(\mathbf{z},\mathbf{z}') &= 0, && \mathbf{z},\mathbf{z}'\in D,\\ \operatorname{Cor}_{du}(\mathbf{x},\mathbf{y}) &= \operatorname{Cor}_{\kappa}(\mathbf{x},\mathbf{y})\left[\frac{\partial(g-\bar{u})}{\partial\mathbf{n}}(\mathbf{x})\otimes\frac{\partial(g-\bar{u})}{\partial\mathbf{n}}(\mathbf{y})\right], && \mathbf{x},\mathbf{y}\in\partial D. \end{aligned} \tag{4.13}$$

Moreover, $\operatorname{Cor}_{du}\in H^{s+1/2,s+1/2}(D\times D)$ *provided that $\partial(g-\bar{u})/\partial\mathbf{n}\in H^s(\partial D)$ for some $s\geq 1/2$.*

Proof. Observing (2.3) and the identity

$$\langle\mathbf{U}(\mathbf{x},\omega),\mathbf{n}(\mathbf{x})\rangle=\langle\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x}),\mathbf{n}(\mathbf{x})\rangle=\kappa(\mathbf{x},\omega),\quad \mathbf{x}\in\partial D,$$

one infers from (2.3), (4.4) and (4.6) that the local shape derivative $du(\cdot,\omega)$ in the direction $\mathbf{U}(\mathbf{x})=\kappa(\mathbf{x},\cdot)\mathbf{n}$ is the solution of (4.10). Equation (4.13) is now an immediate consequence of the linearity of the above boundary value problem. If $\partial(g-\bar{u})/\partial\mathbf{n}\in H^s(\partial D)$ for some $s\geq 1/2$ and if the perturbation field $\kappa\in L^2\big(\Omega,C^k(\partial D)\big)$, it holds that $\operatorname{Cor}_\kappa(\mathbf{x},\mathbf{y})\in C^k(\partial D)\otimes C^k(\partial D)$. Hence the Dirichlet data in (4.13) are in $H^{s,s}(\partial D\times\partial D)$ for $1/2\leq s\leq k$. By elliptic regularity, this implies as in [23] that $\operatorname{Cor}_{du}\in H^{s+1/2,s+1/2}(D\times D)$ in the range of s specified above. The unique solvability of the problem (4.13) in the space $H^{1,1}(D\times D)\sim H^1(D)\otimes H^1(D)$ was shown e.g. in [23]. □

Remark 4.5. Based on Lemma 4.3 and on Theorem 4.4, we obtain a third order accurate approximation to the variance of the random solution by solving the deterministic problems (4.5) and (4.13). On the other hand, based on Lemma 4.2, we see that the solution $\bar{u}$ of the mean field problem (4.5) is only a second order accurate approximation to $\mathbb{E}(u)$. To obtain a third order accurate approximation to the mean $\mathbb{E}(u(\mathbf{z},\omega))$ from (4.4), we need to obtain $\mathbb{E}(d^2u)$. To derive a deterministic boundary value problem for this quantity, we exploit the second order shape calculus. Evaluating the bilinear Hessian in (2.4) on two independent realizations of the perturbation density $\kappa(\mathbf{x},\omega)$, $\mathbf{U}(\mathbf{x})=\kappa(\mathbf{x},\omega)\mathbf{n}(\mathbf{x})$ and $\mathbf{U}'(\mathbf{x})=\kappa(\mathbf{x},\omega')\mathbf{n}(\mathbf{x})$, and taking expectations, we obtain the following deterministic problem for the mean of the shape Hessian $\mathbb{E}(d^2u)$ in terms of the (known) two-point correlation $\mathrm{Cor}_\kappa(\mathbf{x},\mathbf{y})$ of the boundary perturbation field $\kappa(\mathbf{x},\omega)$.

$$\Delta\,\mathbb{E}(d^2u) = 0 \quad \text{in} \quad D, \tag{4.14}$$

which is completed by the Dirichlet condition at $\mathbf{x}\in\partial D$

$$\begin{aligned} \mathbb{E}(d^2u)|_{\partial D}(\mathbf{x}) &= \mathrm{Cor}_\kappa(\mathbf{x},\mathbf{x})\frac{\partial^2(g-\bar{u})(\mathbf{x})}{\partial\mathbf{n}_\mathbf{x}^2} \\ &- \left\{(I_\mathbf{x}\otimes PS_\mathbf{y})\left(\mathrm{Cor}_\kappa(\mathbf{x},\mathbf{y})\frac{\partial(g-\bar{u})(\mathbf{y})}{\partial\mathbf{n}_\mathbf{y}}\right)\right\}\Big|_{\mathbf{y}=\mathbf{x}} \\ &- \left\{(PS_\mathbf{x}\otimes I_\mathbf{y})\left(\mathrm{Cor}_\kappa(\mathbf{x},\mathbf{y})\frac{\partial(g-\bar{u})(\mathbf{x})}{\partial\mathbf{n}_\mathbf{x}}\right)\right\}\Big|_{\mathbf{y}=\mathbf{x}} \end{aligned} \tag{4.15}$$

where PS denotes the Dirichlet-to-Neumann or Poincaré-Steklov Operator for the Laplacian in D. Equation (4.14) is once again a potential problem of the type (4.5), with homogeneous right hand side since f was assumed to be deterministic. The Dirichlet boundary condition (4.15), however, requires sufficient regularity of $\mathrm{Cor}_\kappa(\mathbf{x},\mathbf{x})$ and also of the mean field $\bar{u}$, the solution of (4.5) and of g, to ensure regularity of the second normal derivative of $\bar{u}-g$ to render (4.14), (4.15) well posed.

5. Boundary Reduction

To obtain a deterministic algorithm for the numerical computation of the second moments, we reformulate boundary value problems (2.1) and (4.13) as weakly singular boundary integral equations of the first kind over ∂D resp. $\partial D\times\partial D$. To this end, consider a Newton potential N_f satisfying the equation

$$-\Delta N_f = f \quad \text{in } \overline{D}. \tag{5.1}$$

Then, via the ansatz $\bar{u} = v + N_f$, we are seeking a function v that solves the Laplace equation

$$\Delta v = 0 \text{ in } D, \qquad v = g - N_f \text{ on } \partial D. \tag{5.2}$$

We next introduce the *single layer potential* $\mathcal{S}$ and the *double layer potential* $\mathcal{D}$,

$$\left.\begin{aligned} (\mathcal{S}\rho)(\mathbf{x}) &= \frac{1}{4\pi}\int_{\partial D}\frac{\rho(\mathbf{y})}{\|\mathbf{x}-\mathbf{y}\|}d\sigma_\mathbf{y}, \\ (\mathcal{D}\rho)(\mathbf{x}) &= \frac{1}{4\pi}\int_{\partial D}\frac{\langle\mathbf{x}-\mathbf{y},\mathbf{n}(\mathbf{y})\rangle}{\|\mathbf{x}-\mathbf{y}\|^3}\rho(\mathbf{y})d\sigma_\mathbf{y}, \end{aligned}\right\}\quad \mathbf{x}\in\mathbb{R}^n\backslash\partial D$$

and their traces on the boundary, the *single layer operator* $\mathcal{V}$ and *double layer operator* $\mathcal{K}$,

$$\mathcal{V} = \gamma_0\mathcal{S}, \qquad \mathcal{K} = \gamma_0\mathcal{D}$$

where $\gamma_0 : H^1(D) \to H^{1/2}(\partial D)$ denotes the trace operator. Then, we employ the Dirichlet-to-Neumann map

$$\mathcal{V}\frac{\partial v}{\partial \mathbf{n}} = (1/2 + \mathcal{K})(g - N_f) \quad \text{on } \partial D \tag{5.3}$$

to derive the solution of (2.1) via the potential evaluation

$$u = \mathcal{S}\frac{\partial v}{\partial \mathbf{n}} + \mathcal{D}(g - N_f) + N_f \quad \text{in } D. \tag{5.4}$$

In first instance we shall consider the solution of the boundary value problem (4.10) for fixed $\omega \in \Omega$ before we derive the boundary integral formulation of (4.13). Provided that we are only interested in the solution in a few points $\mathbf{x} \in D \cap D_\varepsilon$, we can employ the indirect method to compute $du(\cdot, \omega)$, namely the single layer potential ansatz

$$du(\cdot, \omega) = \mathcal{S}\sigma \quad \text{in } D \tag{5.5}$$

where σ solves the first kind boundary integral equation

$$\mathcal{V}\sigma = \kappa(\cdot, \omega)\frac{\partial(g - \bar{u})}{\partial \mathbf{n}} \quad \text{on } \partial D. \tag{5.6}$$

Notice that in the context of (5.3), (5.6) the single and double layer operators are operators of order -1 and 0, respectively, acting on ∂D,

$$\mathcal{V} : H^{-1/2}(\partial D) \to H^{1/2}(\partial D), \qquad 1/2 + \mathcal{K} : H^{1/2}(\partial D) \to H^{1/2}(\partial D),$$

while the single and double layer potentials satisfy (e.g. [13])

$$\mathcal{S} : H^{-1/2}(\partial D) \to H^1(D), \qquad \mathcal{D} : H^{1/2}(\partial D) \to H^1(D).$$

We are now in the position to derive the indirect method to solve the boundary value problem (4.13) by straightforward modification of (5.6) and (5.5). We find the tensor product first kind boundary integral equation

$$(\mathcal{V} \otimes \mathcal{V})\Sigma = \operatorname{Cor}_\kappa\left[\frac{\partial(g - \bar{u})}{\partial \mathbf{n}} \otimes \frac{\partial(g - \bar{u})}{\partial \mathbf{n}}\right] \quad \text{on } \partial D \times \partial D, \tag{5.7}$$

where the boundary integral operator

$$\mathcal{V} \otimes \mathcal{V} : \big(H^{1/2,1/2}(\partial D \times \partial D)\big)' \to H^{1/2,1/2}(\partial D \times \partial D)$$

is bounded and coercive in the space

$$H^{1/2,1/2}(\partial D \times \partial D) := H^{1/2}(\partial D) \otimes H^{1/2}(\partial D),$$

i.e. there is a constant $c > 0$ such that

$$\forall \Sigma \in H^{1/2,1/2}(\partial D \times \partial D) : \quad \langle \Sigma, (\mathcal{V} \otimes \mathcal{V})\Sigma \rangle \geq c\|\Sigma\|^2_{H^{1/2,1/2}(\partial D \times \partial D)}. \tag{5.8}$$

This follows from the positivity of $\mathcal{V}$ in $H^{-1/2}(\partial D)$ (cf. [15]) and a tensor product argument (cf. [17]).

Hence, $\mathcal{V} \otimes \mathcal{V}$ is boundedly invertible, and (5.7) admits a unique solution $\Sigma \in H^{1/2,1/2}(\partial D \times \partial D)$. Then Cor_{du} admits in $D \times D$ the representation

$$\mathrm{Cor}_{du} = (\mathcal{S} \otimes \mathcal{S})\Sigma \quad \text{in } D \times D, \tag{5.9}$$

where the potential evaluation

$$\mathcal{S} \otimes \mathcal{S} : \big(H^{1/2,1/2}(\partial D \times \partial D)\big)' \to H^{1,1}(D \times D) \sim H^1(D) \otimes H^1(D)$$

is bounded.

We close with a remark on the reformulation of (4.14), (4.15) as boundary integral equations. Due to the right hand side in (4.14) being zero, subtraction of a Newton potential is not necessary here and the potential ansatz (5.5) may be used here as well. A key issue in the boundary reduction of (4.14), (4.15), however, is the evaluation of the Dirichlet data in (4.15). It can be obtained directly from the boundary integral equation formulation of the mean field problem (5.2), by a so-called *extraction technique* (see [24] for details).

6. Tensor Product Galerkin Discretization

The numerical solution of the integral equation (5.7) on the $2(n-1)$-dimensional manifold $\partial D \times \partial D$ will be based on tensor product Galerkin discretization. Here, we consider so-called *full* tensor products of finite element spaces on ∂D. We give an error analysis of these discretizations leading to convergence rates of variances of the potentials at interior points $\mathbf{x} \in D$ in terms of the meshwidth h on ∂D. The number of degrees of freedom in this discretization scales as $O(h^{-2(n-1)})$.

For the feasibility of second moment computation, however, we will show in the next section that the maximal convergence rates we will in the next section show that essentially the same convergence rates can be achieved with so-called *sparse* tensor product subspaces with merely $O(h^{-(n-1)}|\log h|)$ degrees of freedom.

We consider a sequence of nested spaces

$$V_0 \subset V_1 \subset \ldots \subset V_J \ldots \subset L^2(\partial D), \tag{6.1}$$

consisting of piecewise polynomial ansatz functions $V_J = \operatorname{span}\{\varphi_{J,k} : k \in \Delta_J\}$, such that $\dim V_j \sim 2^{J(n-1)}$ and

$$L^2(\partial D) = \overline{\bigcup_{J \geq 0} V_J}.$$

Since we are going to use the spaces V_J as trial spaces for the approximate solution of (5.3) and (5.7), we shall assume that the following Jackson and Bernstein type estimates hold for $s \leq t < \gamma$, $t \leq q \leq d$,

$$\inf_{v_J \in V_J} \|u - v_J\|_{H^t(\partial D)} \lesssim h_J^{q-t} \|u\|_{H^q(\partial D)}, \quad u \in H^q(\partial D), \tag{6.2}$$

and

$$\|v_J\|_{H^t(\partial D)} \lesssim h_J^{s-t}\|v_J\|_{H^s(\partial D)}, \quad v_J \in V_J, \tag{6.3}$$

uniformly in J, where we set $h_J := 2^{-J}$. The parameter d refers to the maximal degree of polynomials which are locally contained in V_J while

$$\gamma := \sup\big\{t \in \mathbb{R} : V_J \subset H^t(\partial D)\big\} > 0$$

indicates the regularity or smoothness of the functions in the spaces V_J. The quantity h_J corresponds to the mesh width of the mesh on ∂D. Notice that for ansatz functions based on cardinal B-splines there holds $\gamma = d - 1/2$.

In what follows the basis $\Phi_J = \{\varphi_{J,k} : k \in \Delta_J\}$ will be viewed as a row vector, such that, for $\mathbf{v} = [v_k]_{k\in\Delta_J} \in \ell^2(\Delta_J)$, the function $v_J = \Phi_J\mathbf{v}$ is defined as $v_J = \sum_{k\in\Delta_J} v_k\varphi_{J,k}$.

For sake of simplicity, we shall assume that the Newton potential (5.1) is given analytically since we do not want to consider additional approximation errors induced by a numerical computation of N_f. However, let us remark that the Newton potential can be computed on a fairly simple domain G, containing D, with arbitrary boundary conditions, using finite elements or the dual reciprocity method.

We introduce the system matrices

$$\mathbf{V}_J = (\mathcal{V}\Phi_J, \Phi_J)_{L^2(\partial D)}, \qquad \mathbf{K}_J = (\mathcal{K}\Phi_J, \Phi_J)_{L^2(\partial D)}, \tag{6.4}$$

the load vector $\mathbf{g}_J = (g, \Phi_J)_{L^2(\partial D)}$ and the mass matrix $\mathbf{G}_J = (\Phi_J, \Phi_J)_{L^2(\partial D)}$. Then, making the ansatz $\rho_J = \Phi_J\boldsymbol{\rho}_J$ for the Neumann data $\rho := \partial v/\partial\mathbf{n}$ leads to the discrete Dirichlet-to-Neumann map (cf. (5.3))

$$\mathbf{V}_J\boldsymbol{\rho}_J = \mathbf{g}_J/2 + \mathbf{K}_J\mathbf{G}_J^{-1}\mathbf{g}_J. \tag{6.5}$$

Note that $g_J = \Phi_J\mathbf{G}_J^{-1}\mathbf{g}_J$ denotes the L^2-orthogonal projection of the Dirichlet data g onto the space V_J.

Lemma 6.1. *The Galerkin solution ρ_J defined in* (6.5) *satisfies the error estimate*

$$\|\rho - \rho_J\|_{H^{-d}(\partial D)} \lesssim h_J^{2d}\|\rho\|_{H^d(\partial D)} \tag{6.6}$$

provided that $\rho \in H^d(\partial D)$. The discrete potential evaluation (see (5.4)*) in a fixed point $\mathbf{x} \in D$ satisfies*

$$|u(\mathbf{x}) - u_J(\mathbf{x})| \le C(\mathbf{x})h_J^{2d}\|\rho\|_{H^d(\partial D)}. \tag{6.7}$$

Proof. Let Π_J denote the L^2-orthogonal projection onto V_J. Since for any $v \in L^2(\partial D)$ the function $\Pi_J v$ is the Galerkin solution of the equation $Ix = v$ with respect to V_J, we arrive at the error estimate

$$\|v - \Pi_J v\|_{H^t(\partial D)} \lesssim h_J^{d-t}\|v\|_{H^d(\partial D)}, \quad -d \le t \le 0, \tag{6.8}$$

provided that $v \in H^d(\partial D)$.

We will abbreviate $f := (1/2 + \mathcal{K})g$ and $f_J = (1/2 + \mathcal{K}\Pi_J)g$. Thus, we get the estimate

$$\|f - f_J\|_{H^{1+t}(\partial D)} = \|\mathcal{K}g - \mathcal{K}\Pi_J g\|_{H^{1+t}(\partial D)} \lesssim \|g - \Pi_J g\|_{H^t(\partial D)}, \quad -d \le t \le 0,$$

since $\mathcal{K} : H^t(\partial D) \to H^{t+1}(\partial D)$ is continuous if ∂D is sufficiently smooth. Hence, using (6.8), we arrive at

$$\|f - f_J\|_{H^{1+t}(\partial D)} \lesssim h_J^{d-t}\|g\|_{H^d(\partial D)} \lesssim h_J^{d-t}\|\rho\|_{H^{d-1}(\partial D)}, \quad -d \le t \le 0, \tag{6.9}$$

where the last estimate follows from the fact that the Dirichlet-to-Neumann map is a continuous operator of order 1.

For any $a \in H^{1/2}(\partial D)$ let ϕ^a denote the solution of the following adjoint problem

$$(\mathcal{V}\mu, \phi^a)_{L^2(\partial D)} = (a, \mu)_{L^2(\partial D)} \quad \text{for all } \mu \in H^{-1/2}(\partial D). \tag{6.10}$$

Then, we obtain

$$\begin{aligned}
\|\rho - \rho_J\|_{H^{-d}} &= \sup_{\|a\|_{H^d(\partial D)}=1} \big|(a, \rho - \rho_J)_{L^2(\partial D)}\big| = \sup_{\|a\|_{H^d(\partial D)}=1} \big|(\mathcal{V}(\rho - \rho_J), \phi^a)_{L^2(\partial D)}\big| \\
&\le \sup_{\|a\|_{H^d(\partial D)}=1} \big\{\big|(\mathcal{V}(\rho - \rho_J), \phi^a - \Pi_J\phi^a)_{L^2(\partial D)}\big| + \big|(\mathcal{V}(\rho - \rho_J), \Pi_J\phi^a)_{L^2(\partial D)}\big|\big\} \\
&\lesssim \sup_{\|a\|_{H^d(\partial D)}=1} \big\{\|\rho - \rho_J\|_{H^{-1/2}(\partial D)}\|\phi^a - \Pi_J\phi^a\|_{H^{-1/2}(\partial D)} + \big|(f - f_J, \Pi_J\phi^a)_{L^2(\partial D)}\big|\big\}.
\end{aligned}$$

We now estimate the terms on the right hand side of this inequality separately. By the First Strang Lemma we have

$$\|\rho - \rho_J\|_{H^{-1/2}(\partial D)} \lesssim h_J^{d+1/2}\|\rho\|_{H^d(\partial D)}$$

while from (6.8) we get

$$\|\phi^a - \Pi_J\phi^a\|_{H^{-1/2}(\partial D)} \lesssim h_J^{d-1/2}\|\phi^a\|_{H^{d-1}(\partial D)} \lesssim h_J^{d-1/2}\|a\|_{H^d(\partial D)}. \tag{6.11}$$

Here, the latter inequality follows from the fact that $\mathcal{V} = \mathcal{V}^\star : H^{d-1}(\partial D) \to H^d(\partial D)$ is bounded and boundedly invertible. Finally, invoking (6.8) and (6.9), the last term can be estimated by

$$\begin{aligned}
\big|(f - f_J, \Pi_J\phi^a)_{L^2(\partial D)}\big| &\le \big|(f - f_J, \phi^a - \Pi_J\phi^a)_{L^2(\partial D)}\big| + \big|(f - f_J, \phi^a)_{L^2(\partial D)}\big| \\
&\le \|f - f_J\|_{L^2(\partial D)}\|\phi^a - \Pi_J\phi^a\|_{L^2(\partial D)} + \|f - f_J\|_{H^{1-d}(\partial D)}\|\phi^a\|_{H^{d-1}(\partial D)} \\
&\lesssim h_J^{2d}\|\rho\|_{H^{d-1}(\partial D)}\|a\|_{H^d(\partial D)}.
\end{aligned}$$

Putting the last four inequalities together, we arrive at (6.6).

Finally, in view of (5.4), (6.7) follows now immediately from

$$|u(\mathbf{x}) - u_J(\mathbf{x})| = \left| \int_{\partial D} \frac{(\rho - \rho_J)(\mathbf{y})}{\|\mathbf{x} - \mathbf{y}\|} d\sigma_{\mathbf{y}} \right|$$
$$\lesssim \|\rho - \rho_J\|_{H^{-d}(\partial D)} \left\| \frac{1}{\|\mathbf{x} - \cdot\|} \right\|_{H^d(\partial D)} \lesssim h_J^{2d} \|\rho\|_{H^d(\partial D)}.$$

□

Next, we shall consider the discretization of (5.7), (5.9) in $V_J \otimes V_J$. Concerning the boundary integral equation (5.7) for the unknown density $\Sigma \in (H^{1/2,1/2}(\partial D \times \partial D))'$, the ansatz $\Sigma_J = (\Phi_J \otimes \Phi_J)\boldsymbol{\Sigma}_J \in V_J \otimes V_J$ leads to the linear system of equations

$$(\mathbf{V}_J \otimes \mathbf{V}_J)\boldsymbol{\Sigma}_J = \mathbf{Q}_J, \tag{6.12}$$

where the data vector $\mathbf{Q}_J$ is given by

(6.13)
$$\mathbf{Q}_J = \left(\operatorname{Cor}_\kappa \left\{ \left[\frac{\partial(g - N_f)}{\partial \mathbf{n}} - \rho_J \right] \otimes \left[\frac{\partial(g - N_f)}{\partial \mathbf{n}} - \rho_J \right] \right\}, \Phi_J \otimes \Phi_J \right)_{L^2(\partial D \times \partial D)}.$$

Lemma 6.2. *The approximate solution $\Sigma_J = (\Phi_J \otimes \Phi_J)\boldsymbol{\Sigma}_J \in V_J \otimes V_J$, derived from the tensor product equation* (6.12) *satisfies the estimate*

$$\|\Sigma - \Sigma_J\|_{(H^{d+1,d+1}(\partial D \times \partial D))'} \lesssim h_J^{2d} \big\{ \|\Sigma\|_{H^{d-1,d-1}(\partial D \times \partial D)} + A \big\}$$

provided that $\Sigma \in H^{d-1,d-1}(\partial D \times \partial D)$ and $\rho \in H^d(\partial D)$, where

$$A := \|\operatorname{Cor}_\kappa\|_{C^{d-1,1}(\partial D) \otimes C^{d-1,1}(\partial D)} \cdot \|\rho\|_{H^d(\partial D)} \cdot \left\{ \left\| \frac{\partial(g - N_f)}{\partial \mathbf{n}} \right\|_{H^d(\partial D)} + \|\rho\|_{H^d(\partial D)} \right\}.$$

Moreover, for $\mathbf{x}, \mathbf{y} \in D$ we have

$$|\operatorname{Cor}_{du}(\mathbf{x}, \mathbf{y}) - \operatorname{Cor}_{du,J}(\mathbf{x}, \mathbf{y})| \lesssim h_J^{2d} \big\{ \|\Sigma\|_{H^{d-1,d-1}(\partial D \times \partial D)} + A \big\}. \tag{6.14}$$

Proof. During this proof we shall abbreviate

$$q := \frac{\partial(g - \bar{u})}{\partial \mathbf{n}} \otimes \frac{\partial(g - \bar{u})}{\partial \mathbf{n}}, \qquad q_J := \left[\frac{\partial(g - N_f)}{\partial \mathbf{n}} - \rho_J \right] \otimes \left[\frac{\partial(g - N_f)}{\partial \mathbf{n}} - \rho_J \right].$$

We insert the numerically approximated Neumann data on ∂D into (6.13) and distinguish between the exact and the Galerkin approximated right hand side of (5.7)

$$Q := \operatorname{Cor}_\kappa q, \qquad Q_J := \operatorname{Cor}_\kappa q_J.$$

From the well known estimate $\|uv\|_{H^d(\partial D)} \lesssim \|u\|_{C^{d-1,1}(\partial D)} \|v\|_{H^d(\partial D)}$ (see eg. [12, 28]) we conclude by duality $\|uv\|_{H^{-d}(\partial D)} \lesssim \|u\|_{C^{d-1,1}(\partial D)} \|v\|_{H^{-d}(\partial D)}$. Hence, by standard tensor product arguments, we find for all $0 \leq t \leq d$

$$\|Q - Q_J\|_{(H^{t,t}(\partial D))'} \lesssim \|\operatorname{Cor}_\kappa\|_{C^{d-1,1}(\partial D) \otimes C^{d-1,1}(\partial D)} \|q - q_J\|_{(H^{t,t}(\partial D))'}.$$

In accordance with Lemma 6.1 we can further estimate

$$\|Q - Q_J\|_{(H^{t,t}(\partial D\times\partial D)))'} \lesssim h_J^{d+t} A, \qquad 0 \le t \le d. \tag{6.15}$$

Next, we a duality argument as in the proof of Lemma 6.1. We denote the solution of the adjoint equation by ϕ^a and the L^2-orthogonal projection onto $V_J \otimes V_J$ by Π_J^2. Thus, we get

$$\begin{aligned}\|\Sigma - \Sigma_J\|_{(H^{d-1,d-1}(\partial D\times\partial D))'} &= \sup_{\|a\|_{H^{d+1,d+1}(\partial D\times\partial D)}=1} \big|(a, \Sigma - \Sigma_J)_{L^2(\partial D\times\partial D)}\big| \\ \lesssim \sup_{\|a\|_{H^{d+1,d+1}(\partial D\times\partial D)}=1} &\Big\{\|\Sigma - \Sigma_J\|_{(H^{1/2,1/2}(\partial D\times\partial D))'}\|\phi^a - \Pi_J^2\phi^a\|_{(H^{1/2,1/2}(\partial D\times\partial D))'} \\ &+ \big|(Q - Q_J, \Pi_J^2\phi^a)_{L^2(\partial D\times\partial D)}\big|\Big\}.\end{aligned} \tag{6.16}$$

In view of (6.15) the First Strang Lemma gives

$$\|\Sigma - \Sigma_J\|_{(H^{1/2,1/2}(\partial D\times\partial D))'} \lesssim h_J^{d-1/2}\|\Sigma\|_{H^{d-1,d-1}(\partial D\times\partial D)}$$

while, likewise to (6.11), we deduce

$$\|\phi^a - \Pi_J^2\phi^a\|_{H^{1/2,1/2}(\partial D\times\partial D)} \lesssim h_J^{d+1/2}\|a\|_{H^{d+1,d+1}(\partial D\times\partial D)}.$$

Finally, the last term in (6.16) can be estimated in complete analogy to the corresponding expression in Lemma 6.1 by using (6.15)

$$\big|(Q - Q_J, \Pi_J^2\phi^a)_{L^2(\partial D\times\partial D)}\big| \lesssim h_J^{2d} A\|a\|_{H^{d+1,d+1}(\partial D\times\partial D)}.$$

The estimate (6.14) is derived similarly to estimate (6.7). □

7. Fast Second Moment Analysis

Using the traditional *single-scale bases* Φ_J to set up the system matrices (6.4) yields densely populated and ill conditioned system matrices. Then, we end up with at least complexity $O(N^2)$ (in the number N of unknowns needed to approximate the unperturbed boundary surface) for solving the discretized boundary integral equations (6.5) and complexity $O(N^4)$ for the second moment equation (6.12).

We shall introduce a wavelet basis associated with the multiscale hierarchy (6.1). The wavelets $\Psi_j = \{\psi_{j,k} : k \in \nabla_j\}$, where $\nabla_j := \Delta_j \setminus \Delta_{j-1}$, are the bases of complementary spaces W_j of V_{j-1} in V_j, i.e.,

$$V_j = V_{j-1} \oplus W_j, \quad V_{j-1} \cap W_j = \{0\}, \quad W_j = \operatorname{span}\{\psi_{j,k} : k \in \nabla_j\}.$$

Recursively we obtain

$$V_J = \bigoplus_{j=0}^{J} W_j, \quad W_0 := V_0,$$

and thus a wavelet basis in V_J

$$\Psi_J := \bigcup_{j=0}^{J} \Psi_j, \quad \Psi_0 := \Phi_0.$$

We assume that the wavelets are locally and isotropically supported with $\operatorname{diam}(\operatorname{supp}\psi_{j,k}) \sim 2^{-j}$ and that they provide a cancellation property of order $\widetilde{d} > d+1$, that is

$$\left|(v, \psi_{j,k})_{L^2(\partial D)}\right| \lesssim 2^{j((1-n)/2-\widetilde{d})} |v|_{W^{\widetilde{d},\infty}(\operatorname{supp}\psi_{j,k})}.$$

A final requirement is that the infinite collection $\Psi := \bigcup_{j\geq 0} \Psi_j$ forms a Riesz-basis of $L_2(\Gamma)$. Then, there exists also a biorthogonal, or dual, wavelet basis, see e.g. [4] for further details. Note that wavelet bases which satisfy the above properties have been constructed in several papers, see for example [10, 27] and the references therein.

Employing the wavelet basis Ψ_J in the Galerkin discretization, the system matrices in (6.4) become quasi-sparse, having only $\mathcal{O}(N_J)$ $(N_J := \dim V_J)$ relevant matrix coefficients. Moreover, if the regularity $\widetilde{\gamma}$ of the dual wavelets fulfills $\widetilde{\gamma} > 1/2$, the diagonally scaled system matrix arising from the single layer operator has a uniformly bounded condition number. Applying the matrix compression strategy developed in [5, 21] combined with an exponentially convergent *hp*-quadrature method [9], the wavelet Galerkin scheme produces the approximate solution of (6.5) and, as we will show, also of (6.12), with essentially the optimal convergence rates in work and memory which grows only log-linearly in N.

The main idea to achieve this is to solve (5.7) and (5.9) using instead of the full tensor product grid space

$$V_J^2 = V_J \otimes V_J = \bigoplus_{0\leq j,j'\leq J} W_j \otimes W_{j'}.$$

with N_J^2 degrees of freedom the sparse tensor product space defined by

$$\widehat{V}_J^2 = \bigoplus_{0\leq j+j'\leq J} W_j \otimes W_{j'} \subset V_J^2,$$

with $\dim \widehat{V}_J^2 \sim N_J \log N_J$ degrees of freedom. The basis of $\widehat{V}_J^2$ will be indicated by $\widehat{\Psi}_J$.

This leads to a restriction of (6.12),

$$(\widehat{\mathbf{V}_J \otimes \mathbf{V}_J})\widehat{\mathbf{\Sigma}}_J = \widehat{\mathbf{Q}}_J, \tag{7.1}$$

to all indices related to wavelet basis functions in the sparse tensor product space. Provided that stiffness matrix $\mathbf{V}_J$ for the Galerkin discretization of the mean field problem with the hierarchic wavelet basis is stored blockwise, we can use Algorithm 7.1 to compute the matrix-vector product of the sparse tensor product discretization (7.1) in an iterative solver without forming the stiffness matrix for the sparse tensor product discretization $(\widehat{\mathbf{V}_J \otimes \mathbf{V}_J})$ explicitly.

Combined with the above mentioned diagonal preconditioner we obtain an algorithm which solves (5.7) in complexity $\mathcal{O}(\dim \widehat{V}_J^2) = \mathcal{O}(N_J \log N_J)$, see [17, 23] for the details.

Algorithm 7.1 (Sparse tensor product matrix-vector multiplication)**.**
input: *blockwise stored sparse matrix* $\mathbf{V}_J = [\mathbf{V}_{j,j'}^J]_{0 \le j,j' \le J}$ *and*
vector $\widehat{\mathbf{x}}_J = [\widehat{\mathbf{x}}_{j,j'}^J]_{0 \le j+j' \le J}$
output: *blockwise stored vector* $\widehat{\mathbf{y}}_J = [\widehat{\mathbf{y}}_{j,j'}^J]_{0 \le j+j' \le J}$

for all $0 \le j_1 + j_2 \le J$ **do begin**
  initialize $\widehat{\mathbf{y}}_{j_1,j_2}^J := \mathbf{0}$
  for all $0 \le j_1' + j_2' \le J$ **do begin**
    if $(j_1 + j_2' \le j_1' + j_2)$ **then**
      $\widehat{\mathbf{y}}_{j_1,j_2}^J := \widehat{\mathbf{y}}_{j_1,j_2}^J + (\mathbf{Id}_{j_1,j_1} \otimes \mathbf{V}_{j_2,j_2'})(\mathbf{V}_{j_1,j_1'} \otimes \mathbf{Id}_{j_2',j_2'})\widehat{\mathbf{x}}_{j_1',j_2'}^J$
    else
      $\widehat{\mathbf{y}}_{j_1,j_2}^J := \widehat{\mathbf{y}}_{j_1,j_2}^J + (\mathbf{V}_{j_1,j_1'} \otimes \mathbf{Id}_{j_2,j_2})(\mathbf{Id}_{j_1',j_1'} \otimes \mathbf{V}_{j_2,j_2'})\widehat{\mathbf{x}}_{j_1',j_2'}^J$
    end
  end
end

However, since the right hand side $\widehat{\mathbf{Q}}_J$ of (7.1) involves the nonsmooth approximate function ρ_J (cf. (6.13)) a naive calculation will not lead to a (nearly) optimal overall algorithm. One option is to expand the function ρ_J into smooth basis functions like e.g. Legendre polynomials. However, we do not further pursue this option since optimal complexity is only achieved if ρ is piecewise analytic. So we decided to insert the L^2-orthogonal projection onto $\widehat{V}_J^2$ into the right hand side. Thus, we get

$$\widehat{\mathbf{Q}}_J \approx (\widehat{\mathbf{M}_J \otimes \mathbf{M}_J})(\widehat{\mathbf{G}_J \otimes \mathbf{G}_J})^{-1} \widehat{\mathbf{C}}_J, \tag{7.2}$$

where $\mathbf{G}_J = (\Psi_J, \Psi_J)_{L^2(\partial D)}$ is the mass matrix,

$$\mathbf{M}_J = \left(\left[\frac{\partial (g - N_f)}{\partial \mathbf{n}} - \rho_J \right] \Psi_J, \Psi_J \right)_{L^2(\partial D)}$$

is a multiplication operator, and $\widehat{\mathbf{C}}_J$ indicates the sparse tensor product approximation of

$$\mathbf{C}_J = (\mathrm{Cor}_\kappa, \Psi_J \otimes \Psi_J)_{L^2(\partial D\times\partial D)}.$$

Since the matrices $\mathbf{G}_J$, $\mathbf{M}_J$, and the vector $\widehat{\mathbf{Q}}_J$ can be assembled within nearly optimal complexity, the right hand side $\widehat{\mathbf{Q}}_J$ becomes now computable within nearly optimal complexity.

At least in the case of continuous ansatz functions of order $d > 1$ it is reasonably simple to prove that essentially no accuracy is lost by projecting the correlation onto $\widehat{V}_L^2$. To derive this result, we shall first address the L^2-orthogonal projection onto the sparse tensor product space $\widehat{V}_J^2$.

Lemma 7.2. *Let $\widehat{\Pi}_J^2$ denote the L^2-orthogonal projection onto the sparse tensor product space $\widehat{V}_J^2$. Then, for $0 \le s,t \le d$ there holds*

$$\|u - \widehat{\Pi}_J^2 u\|_{(H^{s,s}(\partial D\times\partial D))'} \lesssim \begin{cases} h_J^{(t-s)}\|u\|_{H^{t,t}(\partial D\times\partial D)}, & \text{for } 0 < s < t < d\\ h_J^{d-s}\sqrt{|\log h_J|}\|u\|_{H^{d,d}(\partial D\times\partial D)}, & \text{if } 0 \le s < d \text{ and } t = d,\\ h_J^d|\log h_J|\|u\|_{H^{d,d}(\partial D\times\partial D)}, & \text{if } s = 0 \text{ and } t = d,\end{cases}$$

Proof. Using the fact that $\widehat{\Pi}_J^2 u$ is the Galerkin solution of $Ix = u$ with respect to $\widehat{V}_J^2$ we can use the Galerkin orthogonality to arrive at

$$\begin{aligned}\|u - \widehat{\Pi}_J^2 u\|_{(H^{s,s}(\partial D\times\partial D))'} &= \sup_{\|g\|_{H^{s,s}(\partial D\times\partial D)}=1} (u - \widehat{\Pi}_J^2 u, g)_{L^2(\partial D\times\partial D)}\\ &= \sup_{\|g\|_{H^{s,s}(\partial D\times\partial D)}=1} (u - \widehat{\Pi}_J^2 u, g - \widehat{v}_J)_{L^2(\partial D\times\partial D)} \qquad (7.3)\\ &\lesssim \sup_{\|g\|_{H^{s,s}(\partial D\times\partial D)}=1} \|u - \widehat{\Pi}_J^2 u\|_{L^2(\partial D\times\partial D)}\|g - \widehat{v}_J\|_{L^2(\partial D\times\partial D)}\end{aligned}$$

for all $\widehat{v}_J \in \widehat{V}_J^2$. Next, we need that for a given function

$$u = \sum_{j,j'\ge 0}\sum_{k\in\nabla_j}\sum_{k'\in\nabla_{j'}} u_{(j,k),(j',k')}(\psi_{j,k}\otimes\psi_{j',k'}) \in L^2(\partial D\times\partial D)$$

the projection that truncates the wavelet expansion to the sparse tensor product space

$$P_J u := \sum_{0\le j+j'\le J}\sum_{k\in\nabla_j}\sum_{k'\in\nabla_{j'}} u_{(j,k),(j',k')}(\psi_{j,k}\otimes\psi_{j',k'}) \in \widehat{V}_J^2,$$

leads to the following estimate (cf. [16])

$$\|u - P_J u\|_{L^2(\partial D\times\partial D)} \lesssim \begin{cases} h_J^d\sqrt{|\log h_J|}\|u\|_{H^{d,d}(\partial D\times\partial D)}, & \text{if } t = d,\\ h_J^t\|u\|_{H^{t,t}(\partial D\times\partial D)}, & \text{otherwise.}\end{cases}$$

Thus, choosing $\widehat{v}_J := P_J g$ and using $\|u - \widehat{\Pi}_J^2 u\|_{L^2(\partial D\times\partial D)} \le \|u - P_J u\|_{L^2(\partial D\times\partial D)}$, one can estimate (7.3) further to derive the assertion. $\square$

We are now in the position to give the rate of convergence in negative norms of the the sparse approximation $\widehat{\Sigma}_J$ of the two-point correlation of the boundary flux Σ.

Theorem 7.3. *Assume that V_J is exact of order $d > 1$ consisting of contiuous ansatz functions (i.e. $\gamma > 1$) and assume that the Neumann data of* (2.1) *satisfy $\partial(g - \bar{u})/\partial\mathbf{n} \in C^{d-1,1}(\partial D)$. Then, the Galerkin solution $\widehat{\Sigma}_J \in \widehat{V}_J^2$ derived from the sparse tensor product equation* (7.1)*, using the right hand side approximation* (7.2)*, satisfies the estimate*

$$\|\Sigma - \widehat{\Sigma}_J\|_{(H^{d,d}(\partial D\times\partial D))'} \lesssim h_J^{2d}|\log h_J|\big\{\|\Sigma\|_{H^{d-1,d-1}(\partial D\times\partial D)} + B\big\}$$

provided that $\Sigma \in H^{d-1,d-1}(\partial D \times \partial D)$ and $\rho \in H^d(\partial D)$. The discrete potential satisfies for $\mathbf{x},\mathbf{y} \in D$ the pointwise estimate

$$|\operatorname{Cor}_{du}(\mathbf{x},\mathbf{y}) - \widehat{\operatorname{Cor}}_{du,J}(\mathbf{x},\mathbf{y})| \lesssim h_J^{2d}|\log h_J|\big\{\|\Sigma\|_{H^{d-1,d-1}(\partial D\times\partial D)} + B\big\}.$$

The constant B is defined as

$$B := \|\operatorname{Cor}_\kappa\|_{C^{d-1,1}(\partial D)\otimes C^{d-1,1}(\partial D)} \cdot \left[\left\|\frac{\partial(g-\bar{u})}{\partial\mathbf{n}}\right\|^2_{C^{d-1,1}(\partial D)} + \|\rho\|_{H^d(\partial D)}\left\{\left\|\frac{\partial(g-N_f)}{\partial\mathbf{n}}\right\|_{H^d(\partial D)} + \|\rho\|_{H^d(\partial D)}\right\}\right].$$

Proof. We denote the exact and approximate right hand sides by

$$Q := q\operatorname{Cor}_\kappa = \left(\left[\frac{\partial(g-N_f)}{\partial\mathbf{n}} - \rho\right] \otimes \left[\frac{\partial(g-N_f)}{\partial\mathbf{n}} - \rho\right]\right)\operatorname{Cor}_\kappa,$$
$$Q_J := q_J\widehat{\Pi}_J^2\operatorname{Cor}_\kappa = \left(\left[\frac{\partial(g-N_f)}{\partial\mathbf{n}} - \rho_J\right] \otimes \left[\frac{\partial(g-N_f)}{\partial\mathbf{n}} - \rho_J\right]\right)\widehat{\Pi}_J^2\operatorname{Cor}_\kappa.$$

Similarly to the proof of Lemma 6.2, we find for all $0 \le t \le d$

$$\begin{aligned}\|Q - Q_J\|_{(H^{t,t}(\partial D\times\partial D)'} &\le \|(q-q_J)\operatorname{Cor}_\kappa\|_{(H^{t,t}(\partial D\times\partial D))'} \\ &\quad + \|q_J(I - \widehat{\Pi}_J^2)\operatorname{Cor}_\kappa\|_{(H^{t,t}(\partial D\times\partial D))'} \\ &\lesssim \|q - q_J\|_{(H^{t,t}(\partial D\times\partial D))'}\|\operatorname{Cor}_\kappa\|_{C^{d-1,1}(\partial D)\otimes C^{d-1,1}(\partial D)} \\ &\quad + \sup_{\|a\|_{H^{t,t}(\partial D\times\partial D)}=1}\big(q_J(I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa, a\big)_{L^2(\partial D\times\partial D)}.\end{aligned} \tag{7.4}$$

The first term might be estimated by using

$$\|q - q_J\|_{(H^{t,t}(\partial D\times\partial D))'} \lesssim h_J^{d+t}\|\rho\|_{H^d(\partial D)}\left\{\left\|\frac{\partial(g-N_f)}{\partial\mathbf{n}}\right\|_{H^d(\partial D)} + \|\rho\|_{H^d(\partial D)}\right\}, \qquad 0 \le t \le d. \tag{7.5}$$

The second term is estimated as follows. Assume $t = d$, i.e. $a \in H^{d,d}(\partial D \times \partial D) \subset L^\infty(\partial D \times \partial D)$. Then, employing Galerkin orthogonality, we find

$$\begin{aligned}
&\big(q_J(I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa, a\big)_{L^2(\partial D\times\partial D)} \\
&\quad = \big((q_J-q)(I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa, a\big)_{L^2(\partial D\times\partial D)} + \big((I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa, qa\big)_{L^2(\partial D\times\partial D)} \\
&\quad \le \|(q-q_J)(I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa\|_{L^1(\partial D\times\partial D)}\|a\|_{L^\infty(\partial D\times\partial D)} \\
&\qquad\qquad + \big((I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa, (I-\widehat{\Pi}_J^2)(qa)\big)_{L^2(\partial D\times\partial D)} \\
&\quad \lesssim \|q-q_J\|_{L^2(\partial D\times\partial D)}\|(I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa\|_{L^2(\partial D\times\partial D)}\|a\|_{H^{d,d}(\partial D\times\partial D)} \\
&\qquad\qquad + \|(I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa\|_{L^2(\partial D\times\partial D)}\|(I-\widehat{\Pi}_J^2)(qa)\|_{L^2(\partial D\times\partial D)}.
\end{aligned}$$

In view of (7.5) and Lemma 7.2 we derive the estimate

$$\begin{aligned}
&\big(q_J(I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa, a\big)_{L^2(\partial D\times\partial D)} \lesssim h_J^{2d}|\log h_J|\|\operatorname{Cor}_\kappa\|_{H^{d,d}(\partial D\times\partial D)}\|a\|_{H^{d,d}(\partial D\times\partial D)} \\
&\qquad \cdot \left[\left\|\frac{\partial(g-\bar u)}{\partial\mathbf{n}}\right\|_{C^{d-1,1}(\partial D)}^2 + \|\rho\|_{H^d(\partial D)}\left\{\left\|\frac{\partial(g-N_f)}{\partial\mathbf{n}}\right\|_{H^d(\partial D)} + \|\rho\|_{H^d(\partial D)}\right\}\right],
\end{aligned}$$

and thus

$$\|Q-Q_J\|_{(H^{d,d}(\partial D\times\partial D))'} \lesssim h_J^{2d}|\log h_J|B. \tag{7.6}$$

Next, in the case $t = 0$, we can estimate

$$\begin{aligned}
&\big(q_J(I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa, a\big)_{L^2(\partial D\times\partial D)} \\
&\le \|q_J\|_{L^\infty(\partial D\times\partial D)}\|(I-\widehat{\Pi}_J^2)\operatorname{Cor}_\kappa\|_{L^2(\partial D\times\partial D)}\|a\|_{L^2(\partial D\times\partial D)} \\
&\lesssim h_J^d\sqrt{|\log h_J|}\|\operatorname{Cor}_\kappa\|_{H^{d,d}(\partial D\times\partial D)}\|a\|_{L^2(\partial D\times\partial D)} \\
&\qquad \cdot \left[\left\|\frac{\partial(g-\bar u)}{\partial\mathbf{n}}\right\|_{H^d(\partial D)}^2 + \|\rho\|_{H^d(\partial D)}\left\{\left\|\frac{\partial(g-N_f)}{\partial\mathbf{n}}\right\|_{H^d(\partial D)} + \|\rho\|_{H^d(\partial D)}\right\}\right]
\end{aligned}$$

since for all $\varepsilon > 0$ one has

$$\begin{aligned}
\|q_J\|_{L^\infty(\partial D\times\partial D)} &\lesssim (\|q\|_{H^{(n-1)/2+\varepsilon,(n-1)/2+\varepsilon}(\partial D\times\partial D)} + \|q_J-q\|_{H^{(n-1)/2+\varepsilon,(n-1)/2+\varepsilon}(\partial D\times\partial D)}) \\
&\lesssim \left[\left\|\frac{\partial(g-\bar u)}{\partial\mathbf{n}}\right\|_{H^d(\partial D)}^2 + \|\rho\|_{H^d(\partial D)}\left\{\left\|\frac{\partial(g-N_f)}{\partial\mathbf{n}}\right\|_{H^d(\partial D)} + \|\rho\|_{H^d(\partial D)}\right\}\right].
\end{aligned}$$

Consequently, we have

$$\|Q-Q_J\|_{L^2(\partial D\times\partial D)} \lesssim h_J^d\sqrt{|\log h_J|}B. \tag{7.7}$$

Using (7.6) and (7.7) together with Lemma 7.2 one can finish now the proof in complete analogy to the proof of Lemma 6.2. □

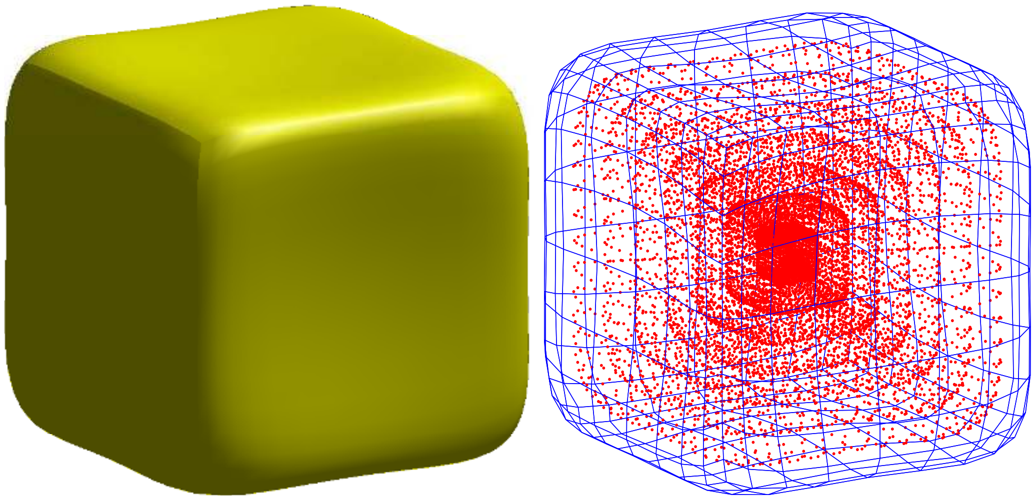

FIGURE 1. The domain D and the potential evaluation points.

8. Numerical Results

We shall first check the predicted orders of convergence. Let D be the smoothened cube presented in Fig. 1. We will choose the data f and g such that the solution of the Poisson equation (2.1) is known. That way we can measure the predicted rates of convergence in case of the mean field equation. Choosing the source term $f = 1$ and the Dirichlet data $g(x, y, z) = -x^2/2$, one readily infers that $u(x, y, z) = -x^2/2$ satisfies the Poisson equation. The Newton potential employed by our algorithm is analytically defined as $N_f(x, y, z) := -(x^2 + y^2 + z^2)/6$. We discretize the boundary integral operators by piecewise constant wavelets, that is the case $d = 1$.

First, we consider the mean field equation. The Neumann data of the solution u should converge in the $L^2(\partial D)$-norm with order $h_J \sim N_J^{-1/2}$, cf. (6.1). Moreover, due to (6.6), the error $|u(\mathbf{x}) - u_J(\mathbf{x})|$ in a single point $\mathbf{x} \in D$ should behave like $\mathcal{O}(h_J^2)$. However, the errors in a single point might oscillate extremely due to round-off errors. To be on save ground we compute the ℓ^∞-norm of the measurements in all points $\{\mathbf{x}_i\}_{i\in\mathcal{I}}$ specified in Fig. 1. The results are recorded in Table 1 and plotted in the double logarithmic plot in Fig. 1. The measured rates of convergence with respect to the potential are even slightly higher than predicted. A least squares fit yields $\|\mathbf{u} - \mathbf{u}_J\|_{\ell^\infty} = \mathcal{O}(h_J^{2.5})$, where $\mathbf{u} := [u(\mathbf{x}_i)]_{i\in\mathcal{I}}$ and $\mathbf{u}_J := [u_J(\mathbf{x}_i)]_{i\in\mathcal{I}}$.

Next, we consider the numerical solution of (4.13) by the sparse tensor product approximation (7.1). For comparison reasons we choose the correlation of κ such that $\mathrm{Cor}_\kappa(\mathbf{x}, \mathbf{y}) = F(\mathbf{x}) \cdot G(\mathbf{y})$. Consequently, (4.13) decouples into two boundary value

J	N_J	$\|\rho - \rho_J\|_{L^2(\partial D)}$	$\|\mathbf{u} - \mathbf{u}_J\|_\infty$	cpu-time
1	24	2.9e-1	5.6e-1	1
2	96	3.5e-1 (0.8)	5.1e-2 (11)	1
3	384	1.7e-1 (2.1)	2.0e-2 (2.5)	2
4	1536	8.4e-2 (2.0)	3.4e-3 (5.9)	9
5	6144	4.2e-2 (2.0)	4.4e-4 (7.9)	47
6	24576	2.1e-2 (2.0)	9.1e-5 (4.8)	413
7	98304	1.0e-2 (2.0)	1.6e-5 (5.6)	2002
8	393216	1.3e-2 (2.0)	3.7e-6 (4.3)	13097

TABLE 1. Numerical results with respect to the mean field equation.

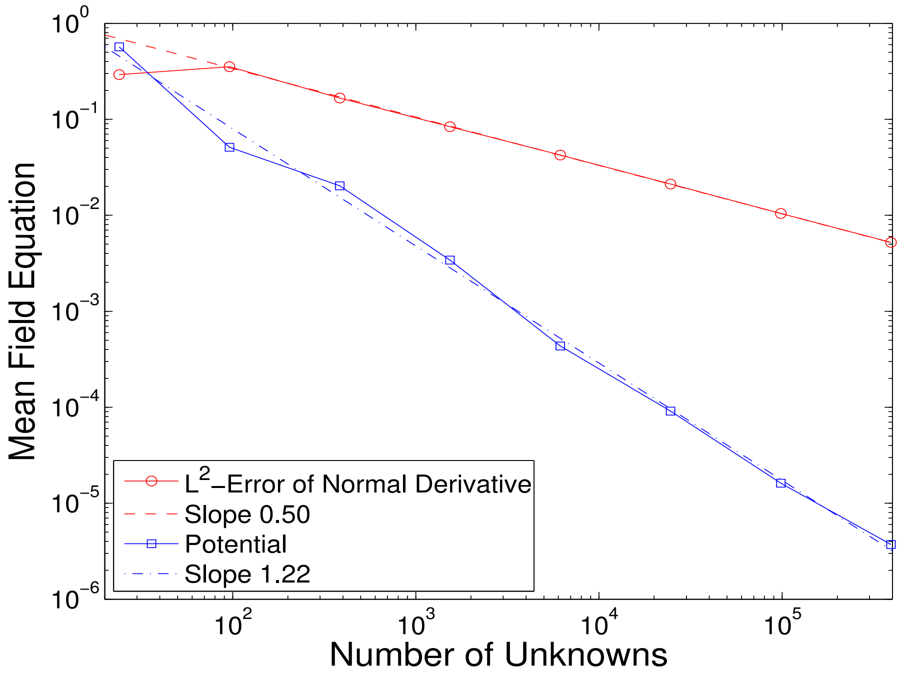

FIGURE 2. Asymptotic behaviour of the errors for the mean field equation.

problems depending only on $\mathbf{x}$ or $\mathbf{y}$. Therefore, the solution of the full tensor product space can be computed and compared to the sparse grid solution. Particularly, we choose $F(x, y, z) = e^{-x^2-y^2-z^2}$ and $G(x, y, z) = xyz$. For a full tensor product discretization in $L^2(\partial D \times \partial D)$ we would expect the rate of convergence $\mathcal{O}(h_J)$ for the approximate right hand side Q_J and the rate $\mathcal{O}(1)$ for the approximate density Σ_J. The discrete variance $\mathbf{C}_J := [\mathrm{Var}_{du,J}(\mathbf{x}_i)]_{i\in\mathcal{I}}$ should be approximated by the rate $\mathcal{O}(h_J^2)$, cf. Lemma 6.2.

To measure the rates of convergence that are realized by the sparse tensor product approximation, we use the solutions Q_J, Σ_J, and $\mathbf{C}_J$ associated with the full tensor product spaces as reference values since the exact solution is unknown. The errors of $\widehat{Q}_J$, $\widehat{\Sigma}_J$, and $\widehat{\mathbf{C}}_J := [\widehat{\mathrm{Var}}_{du,J}(\mathbf{x}_i)]_{i\in\mathcal{I}}$ with respect to the sparse tensor product spaces are tabulated in Table 2. In Fig. 3 these errors are plotted in a corresponding log-log-diagram. Since the convergence bebaviour exhibits oscillations we performed least squares fits (indicated by the dashed/dash-dotted/dotted lines) to estimate the orders of convergence. Even though the present discretization is not covered by Theorem 7.3, we observe essentially the rates of convergence of the full tensor product space.

J	$\widehat{N}_J$	$\|Q_J - \widehat{Q}_J\|_{L^2(\partial D\times\partial D)}$	$\|\Sigma_J - \widehat{\Sigma}_J\|_{L^2(\partial D\times\partial D)}$	$\|\mathbf{C}_J - \widehat{\mathbf{C}}_J\|_\infty$	cpu-time
1	252	1.2e-1	1.3e-1	1.6	1
2	1440	3.4e-1 (0.4)	7.3e-1 (0.2)	2.0e-1 (7.8)	1
3	7488	2.5e-1 (1.4)	7.2e-1 (1.0)	1.7e-1 (1.2)	3
4	36864	9.6e-2 (2.6)	5.2e-1 (1.4)	2.5e-2 (6.6)	14
5	175104	2.8e-2 (3.5)	4.2e-1 (1.2)	8.5e-3 (3.0)	124
6	811008	8.8e-3 (3.1)	3.7e-1 (1.1)	1.0e-3 (8.6)	1210
7	3.7 mio	4.2e-3 (2.1)	3.1e-1 (1.2)	1.6e-4 (6.4)	3 hrs
8	16.5 mio	2.1e-3 (2.0)	3.3e-1 (0.9)	9.4e-5 (1.6)	24 hrs

TABLE 2. Errors in the covariance approximation by the sparse tensor product approach.

The last column of Table 2 refers to the cpu-time consumed for computing the right hand side of (7.1) and solving the associated linear system of equations by Algorithm 7.1. Although we observe strong logarithmical factors, we are able to solve (7.1) on level 8 within 24 hours using 2.5 Gigabyte main memory and one processor of a Sun Fire V20z Server with two 2.2 MHz AMD Opteron processors and 4 GB main memory per processor. Notice that the full tensor product space on level $J = 8$ owns about $15 \cdot 10^{10}$ unknowns.

Finally, we shall present results for realistic data. We consider the Poisson equation (2.1) for the source term $f = 1$ and homogeneous Dirichlet data. We choose Gaussian correlation, i.e., $\mathrm{Cor}_\kappa(\mathbf{x},\mathbf{y}) = e^{-\|\mathbf{x}-\mathbf{y}\|^2}$. We compute the expectation and the variance of the solution on the two dimensional plane shown in Fig. 4. The approximate expectation and variation are presented on the left and right hand side of Fig. 5. One observes that the variance is small in the middle of the plane while it becomes larger if one tends to the edges. However, near the corners of the plane the variance keeps small. We like to mention that the approximate variance depends linearly on $\mathrm{Cor}_\kappa(\mathbf{x},\mathbf{y})$. Therefore, a scaling of $\mathrm{Cor}_\kappa(\mathbf{x},\mathbf{y})$ does not affect the qualitative behaviour of the approximate variance.

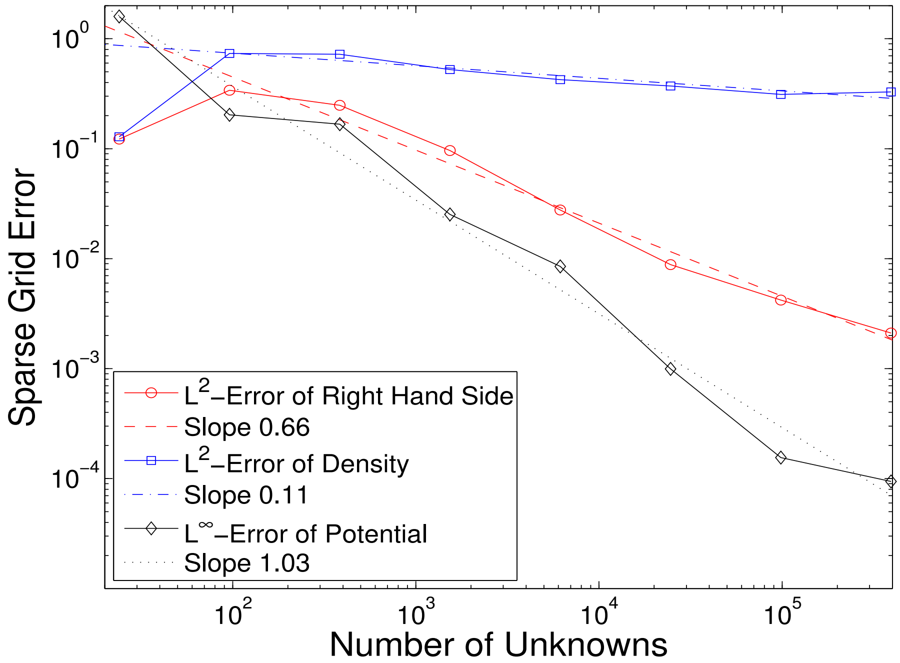

FIGURE 3. Asymptotic behaviour of the errors of the sparse tensor product approach.

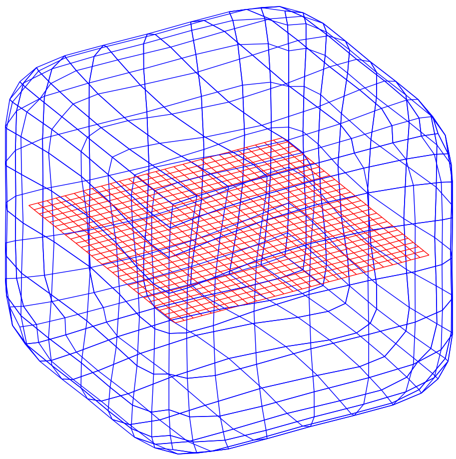

FIGURE 4. Sectional plane for evaluating expectation and variance.

9. CONCLUSIONS AND GENERALIZATIONS

We developed and analyzed a fast deterministic method for the second moment analysis of random solutions to the Dirichlet problem (2.1) in smooth, bounded nominal domains $D \subset \mathbb{R}^d$ subject to a class of random boundary perturbations in a space X.

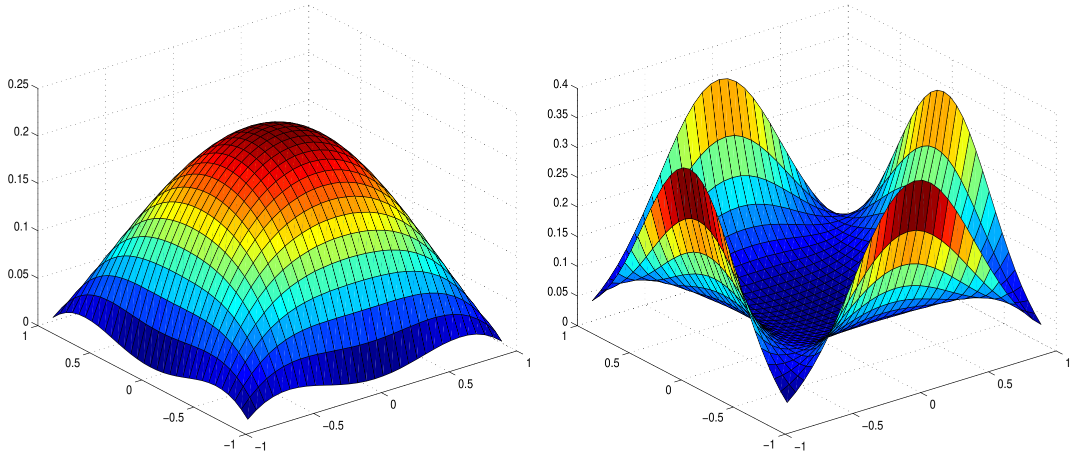

FIGURE 5. Expectation (left) and variance (right) of the solution.

Under the assumption of small perturbation amplitude $\varepsilon > 0$, almost shure with respect to a probability measure P on the space X of admissible perturbations, we showed using a domain sensitivity analysis how second order statistics of the random solution and functionals of it can be expressed, to third order in the perturbation size ε, through solutions of deterministic boundary value problems in D resp., for second moments, in $D \times D$, which are related to the nominal problem's shape gradient

Using boundary reduction of these problems to first kind, strongly elliptic boundary integral equations and wavelet Galerkin discretization of these integral equations on sparse tensor product spaces we obtained a deterministic algorithm for the computation of approximate mean field and second moments of the random solution and functionals of it whose work and memory scale log-linearly in N, the number of degrees of freedom on ∂D while converging at the optimal rates afforded by Galerkin BEM (e.g. [22]). The development in the present paper was performed for the model Poisson equation (2.1). It is, however, by no means limited to this model equation – our fast deterministic computation of the second order statistics of the random solution and functionals of it can be applied to any elliptic boundary value problem for which boundary reduction to integral equations (e.g. [13, 22]) and, at least, a *first order* shape calculus are available; we refer to [17] for the numerical analysis of sparse tensor product approximation schemes for the second (and higher) moment problems. For shape gradients of Dirichlet and Neumann problems for the Helmholtz and Maxwell equations, we refer to [19], Chapter 5.

In the present paper, we used classical shape calculus in D from [11, 14, 26] for the derivation of the Fréchet derivative of the solution with respect to perturbations of ∂D and obtained an integral equation formulation by boundary reduction of the shape gradients. A direct derivation of these integral equations consists of differentiating boundary integral operators with respect to ∂D. Details are available, also for time harmonic electromagnetic scattering, in [19].

We used the wavelet implementation of [9, 10] which use structured mesh hierarchies on ∂D to allow matrix compression, preconditioning and sparse second moment analysis in a unified fashion. We emphasize, however, that our approach could also be realized on unstructured surface meshes with the hierarchic bases of [27], in conjunction with a Fast Multipole Method for matrix-vector multiplication, as, e.g. in [20].

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