Bayesian Numerical Homogenization

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Abstract

Numerical homogenization, i.e. the finite-dimensional approximation of solution spaces of PDEs with arbitrary rough coefficients, requires the identification of accurate basis elements. These basis elements are oftentimes found after a laborious process of scientific investigation and plain guesswork. Can this identification problem be facilitated? Is there a general recipe/decision framework for guiding the design of basis elements? We suggest that the answer to the above questions could be positive based on the reformulation of numerical homogenization as a Bayesian Inference problem in which a given PDE with rough coefficients (or multi-scale operator) is excited with noise (random right hand side/source term) and one tries to estimate the value of the solution at a given point based on a finite number of observations. We apply this reformulation to the identification of bases for the numerical homogenization of arbitrary integro-differential equations and show that these bases have optimal recovery properties. In particular we show how Rough Polyharmonic Splines can be re-discovered as the optimal solution of a Gaussian filtering problem.

1 Bayesian Numerical Analysis

This paper is inspired by a curious (and, perhaps, overlooked) link between Bayesian Inference and Numerical Analysis [20], known as Bayesian Numerical Analysis [20, 56, 49, 50], and that can be traced back to Poincaré’s course on Probability Theory [55]. We will recall Diaconis’ compelling example [20] as an illustration of this link.

Let \( f : [0, 1] \to \mathbb{R} \) be a given function and assume that we are interested in the numerical approximation of \( \int_0^1 f(t) \, dt \). The Bayesian approach to this quadrature problem is to (1) Put a prior (probability distribution) on continuous functions \( \mathcal{C}[0, 1] \) (2) Calculate \( f \) at \( x_1, x_2, \ldots, x_n \) (3) Compute a posterior (4) Estimate \( \int_0^1 f(t) \, dt \) by the Bayes rule.

If the prior on \( \mathcal{C}[0, 1] \) is that of a Brownian Motion (i.e. \( f(t) = B_t \) where \( B_t \) is a Brownian motion and \( B_0 \) is normal), then \( \mathbb{E}[f(x) | f(x_1), \ldots, f(x_n)] \) is the piecewise linear interpolation of \( f \) between the points \( x_1, \ldots, x_n \) and one re-discovers the trapezoidal quadrature rule.

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If the prior on $C[0,1]$ is that of the first integral of a Brownian Motion (i.e. $f(t) \sim \int_0^t B_s \, ds$) then the posterior $\mathbb{E}[f(x)|f(x_1),\ldots,f(x_n)]$ is the cubic spline interpolant and integrating $k$ times yields splines of order $2k + 1$. Although this link has lead to the identification of new quadrature rules for numerical integration [49], it appears to have remained little known and our paper is prompted by the question of the existence of similar link between Bayesian Inference and Numerical Homogenization.

As a prototypical example, consider the numerical homogenization of the PDE

$$
\begin{align*}
-\text{div} \left( a(x) \nabla u(x) \right) &= g(x) \quad x \in \Omega; \ g \in L^2(\Omega), \\
\ u &= 0 \quad \text{on} \quad \partial \Omega,
\end{align*}
$$

(1.1)

where $\Omega$ is a bounded subset of $\mathbb{R}^d$ with piecewise Lipschitz boundary, $a$ is a symmetric, uniformly elliptic $d \times d$ matrix on $\Omega$ and with entries in $L^\infty(\Omega)$.

Recall that numerical homogenization concerns the approximation of the solution space of (1.1) with a finite-dimensional space. Although classical homogenization concepts [12, 46, 57, 36, 54, 44] might be present in some instances of this problem [43, 42, 3, 25, 2, 37, 15, 16, 31, 11, 32, 1], one of the main objectives of numerical homogenization is to achieve a numerical approximation of the solution space of (1.1) with arbitrary rough coefficients, i.e., in particular, without the assumptions found in classical homogenization, such as scale separation, ergodicity at fine scales and $\epsilon$-sequences of operators. In this situation, piecewise linear finite-elements can perform arbitrarily badly [10] and the numerical approximation of the solution space involves the identification of accurate basis elements adapted to the microstructure $a(x)$ [62, 9, 6, 51, 28, 27, 5, 4, 48, 18, 17, 19, 13, 7, 52, 26, 45, 39].

As for the identification of quadrature rules in the numerical homogenization, the identification of accurate basis elements in numerical homogenization has been based on a difficult process of scientific investigation. Let us now turn our attention to the Bayesian approach to this problem. An immediate question is where do we place the prior? (1) If the prior is placed on $u$ then posterior values do not see (depend on) the microstructure. (2) If the prior is placed on $a$ then the microstructure becomes random whereas our purpose is the numerical homogenization of a given deterministic microstructure. Let us also note that the randomization of the microstructure, as investigated by Polynomial Chaos Approximation/Stochastic Expansion methods [35, 34, 64, 8, 30, 21], does not lead to the simplification in the homogenization process but to increased complexity with the dimension of input stochastic variables [58, 14] (although Stochastic Expansion methods have been used successfully to beat Monte-Carlo sampling they do not lead to averaging results seen in homogenization). (3) If the prior is placed on $g$ then the noise propagates through the microstructure and the posterior value of $u$ contains that information.

This observation motivates us to place the prior on the source term $g$ in (1.1), e.g., replace it by white noise (i.e. a centered Gaussian field on $\Omega$ with covariance function
\[ \delta(x - y) \) and consider the stochastic PDE

\[
\begin{aligned}
- \text{div} \left( a(x) \nabla u(x) \right) &= \xi(x) \quad x \in \Omega, \\
u &= 0 \quad \text{on} \quad \partial \Omega,
\end{aligned}
\] (1.2)

Observe that the solution (1.2) at the point \( x, u(x) \), is a random variable and its best (mean squared) approximation given \( u(x_1), \ldots, u(x_N) \) (its values at the points \( x_1, \ldots, x_N \)) is its conditional expectation \( E[u(x)|u(x_1), \ldots, u(x_N)] \). One result of this paper is that

\[
E[u(x)|u(x_1), \ldots, u(x_N)] = \sum_{i=1}^{N} u_i(x) \phi_i(x)
\] (1.3)

where the functions \( \phi_i \) are Rough Polyharmonic Splines [53] (RPS) which have been identified as accurate basis elements for the numerical homogenization of (1.1) having noteworthy variational, optimal recovery and localization properties. The discovery of these Rough Polyharmonic Splines has required a significant amount of work and trial and errors but here, they are identified after a single step of Bayesian conditioning.

This observation motivates us to investigate what the same process of Bayesian conditioning would give under different different priors and under other observations than the values of \( u \) at individual points. In particular, we will use this link between Bayesian Inference and Numerical Homogenization to identify bases for the numerical homogenization of arbitrary linear integro-differential equations. Our purpose is to show that this link is generic and could in principle be used, beyond numerical homogenization, as a guiding principle for the coarse-graining of multi-scale systems. The Bayesian approach to this problem is to (1) Put a prior on the degrees of freedom of the system (2) Select a finite number of coarse variables (3) Compute the posterior value of the state of the system conditioned on the coarse variables.

### 2 General setup

Let \( \mathcal{L} \) and \( \mathcal{B} \) be linear integro-differential operators on \( \Omega \) and \( \partial \Omega \) such that (1) \( (\mathcal{L}, \mathcal{B}) : \mathcal{H}(\Omega) \to \mathcal{H}_L(\Omega) \times \mathcal{H}_B(\partial \Omega) \), where \( \mathcal{H}(\Omega), \mathcal{H}_L(\Omega) \) and \( \mathcal{H}_B(\partial \Omega) \) are Hilbert spaces of Generalized functions on \( \Omega \) and \( \partial \Omega \) (2) \( \mathcal{H}(\Omega) \) and \( \mathcal{H}_L(\Omega) \) contain \( L^2(\Omega) \).

Consider the integro-differential equation

\[
\begin{aligned}
\mathcal{L}u(x) &= g(x) \quad x \in \Omega; \\
\mathcal{B}u &= 0 \quad \text{on} \quad \partial \Omega.
\end{aligned}
\] (2.1)

As with (1.1) the numerical homogenization of (2.1) will require the assumption that \( g \) belongs to a strict subspace of \( \mathcal{H}_L(\Omega) \).

We will assume that \( \mathcal{L} \) and \( \mathcal{B} \) are such that (2.1) (1) admits a unique solution in \( \mathcal{H}(\Omega) \) (2) and a Green’s function \( G \). Recall that \( G \) is defined as the solution of

\[
\begin{aligned}
\mathcal{L}G(x, y) &= \delta(x - y) \quad x \in \Omega, \\
\mathcal{B}G(x, y) &= 0 \quad \text{for} \quad x \in \partial \Omega.
\end{aligned}
\] (2.2)
where $\delta(\cdot - y)$ is the Delta mass of Dirac at the point $y$.

**Example 2.1.** Note that for the prototypical example (1.1) we have

$$L u(x) := - \text{div} \,(a(x) \nabla u(x)) \text{ and } B u(x) = u(x),$$

(2.3)

Our purpose is to identify a good basis for the numerical homogenization or coarse-graining of (2.1).

## 3 Bayesian Numerical Homogenization

Our Bayesian approach to the numerical homogenization of (2.1) is to replace the source term $g$ by a Gaussian field $\xi$. More precisely we introduce $\xi$, a centered Gaussian field on $\Omega$ with covariance function

$$\Lambda(x, y) := \mathbb{E}[\xi(x)\xi(y)]$$

(3.1)

and consider the stochastic integro-differential equation

$$\begin{cases}
L u(x) = \xi(x) & x \in \Omega; \\
B u = 0 & \text{on } \partial \Omega,
\end{cases}$$

(3.2)

**Proposition 3.1.** The solution of (3.2) is a Gaussian field on $\Omega$ whose covariance function $\Gamma(x, y) := \mathbb{E}[u(x)u(y)]$ is

$$\Gamma(x, y) = \int_{\Omega^2} G(x, z)\Lambda(z, z')G(y, z') \, dz \, dz'$$

(3.3)

**Remark 3.2.** Observe that if $\xi$ is white noise (i.e. $\Lambda(x - y) = \delta(x - y)$) then

$$\Gamma(x, y) = \int_{\Omega} G(x, z)G(y, z) \, dz$$

(3.4)

which is the Kernel of $L^*L$ (i.e., $L^*L \Gamma(x, y) = \delta(x - y)$, where $L^*$ is the adjoint of $L$).

**Proof.** Since $L$ and $B$ are linear operators, $u$ is a linear function of $\xi$ and is therefore a Gaussian field. Moreover its covariance function is given by

$$\Gamma(x, y) = \mathbb{E}[u(x)u(y)] = \mathbb{E}\left[ \int_{\Omega^2} G(x, z)\xi(z)G(y, z')\xi(z') \, dz \, dz' \right]$$

$$= \int_{\Omega^2} G(x, z)G(y, z')\mathbb{E}[\xi(z)\xi(z')] \, dz \, dz'$$

(3.5)

which finishes the proof.

**Remark 3.3.** Beyond Bayesian Homogenization, equations with random right hand side can also be of interest in practical applications, for instance in the modeling of the electrostatics in nanoscale field-effect sensors, where fluctuations arise from random charge concentrations [41].
3.1 On the choice of the noise

We will show that the choice of the noise $\xi$ is determined by the regularity of the source term $g$ in the right hand side of (2.1). More precisely if $\xi$ is white noise then the resulting accuracy estimates will be obtained under the assumption that $g \in L^2(\Omega)$ and as a function of $\|g\|_{L^2(\Omega)}$.

If $\xi$ is not white noise (i.e. if its covariance function is not $\delta(x - y)$) then we assume that there exists two linear integro-differential operators $L_\Lambda$ and $B_\Lambda$ such that $\xi$ is the stochastic solution of the following equation with white noise $\xi'$ as source term:

$$
\begin{align*}
L_\Lambda \xi(x) &= \xi'(x) & x \in \Omega; \\
B_\Lambda \xi &= 0 & \text{on } \partial \Omega,
\end{align*}
$$

(3.6)

In what follows, if $\xi$ is not white noise then we assume it to be obtained as in (3.6) and the resulting accuracy estimates will be obtained under the assumption that $L_\Lambda g \in L^2(\Omega)$ and as a function of $\|L_\Lambda g\|_{L^2(\Omega)}$. A prototypical example corresponds to the situation where $\xi$ is obtained as the regularization of white noise via a power of the Laplace Dirichlet operator on $\Omega$ and this allows us to identify optimal recovery bases under the assumption that $g \in H^s(\Omega)$ with $s \geq 0$ or $s < 0$.

3.2 Identification of basis elements via conditioning

Let $N$ be a strictly positive integer. Our Bayesian approach is based on the conditioning of the solution of (3.2) posterior to the observation of $N$ linear functions of $u(x)$, expressed as

$$
\int_\Omega u(x)\psi_i(x) \, dx \quad i \in \{1, \ldots, N\}
$$

(3.7)

where $\psi_1, \ldots, \psi_N$ are $N$ linearly independent generalized functions on $\Omega$ such that for all $i$

$$
\int_{\Omega^2} \psi_i(x)\Gamma(x, y)\psi_i(y) \, dx \, dy < \infty
$$

(3.8)

Let $\Theta$ be the $N \times N$ symmetric matrix defined by

$$
\Theta_{i,j} := \int_{\Omega^2} \psi_i(x)\Gamma(x, y)\psi_j(y) \, dx \, dy
$$

(3.9)

Note that (3.8) implies that if $u$ is the solution of (3.2) then

$$
\Psi := \left( \int_\Omega u(x)\psi_1(x) \, dx, \ldots, \int_\Omega u(x)\psi_N(x) \, dx \right)
$$

(3.10)

is a well defined center Gaussian random vector with covariance matrix $\Theta$.

Lemma 3.4. The $N \times N$ matrix $\Theta$ is symmetric positive definite. Furthermore for all $l \in \mathbb{R}^N$,

$$
l^T \Theta l = \|v\|_{L^2(\Omega)}^2
$$

(3.11)
where \( v \) is the solution of

\[
\begin{cases}
L v(x) = \sum_{j=1}^{N} l_j \psi_j(x) & \text{for } x \in \Omega; \\
\mathcal{B} v(x) = 0 & \text{for } x \in \partial \Omega.
\end{cases}
\] (3.12)

**Proof.** Let \( l \in \mathbb{R}^N \), write

\[
v(x) := \sum_{i=1}^{N} \int_{\Omega} G(x, y) \psi_i(y) l_i
\] (3.13)

Observe that since \( v \) is the solution of (3.12) and \( \|v\|_{L^2(\Omega)}^2 = l^T \Theta l \), it follows that \( \Theta \) is symmetric positive definite. Indeed if \( \Theta \) is not positive definite, then there would exist a non zero vector \( l \in \mathbb{R}^N \) such that \( \Theta l = 0 \). This would imply \( \|v\|_{L^2(\Omega)} = 0 \) which is a contradiction since the equation (3.12) has a non zero solution (since \( l \neq 0 \) and the \( \psi_i \) are linearly independent).

Our motivation for using Gaussian noise in (3.2) lies in the fact that for Gaussian fields, conditional expected values can be computed via linear projection. Henceforth our approach is also akin to Gaussian filtering for numerical homogenization and the following Theorem shows that this approach allows for the identification of a (projection) basis \( \phi_i \).

**Theorem 3.5.** Let \( u \) be the solution of (3.2) and \( \Psi \) defined by (3.10), then

\[
\mathbb{E}[u(x)\mid \Psi] = \sum_{i=1}^{N} \Psi_i \phi_i(x)
\] (3.14)

with

\[
\Psi_i := \int_{\Omega} u(y) \psi_i(y) \, dx
\] (3.15)

and

\[
\phi_i(x) := \sum_{j=1}^{N} \Theta_{i,j}^{-1} \int_{\Omega} \Gamma(x, y) \psi_j(y) \, dy
\] (3.16)

Furthermore, \( u(x) \) conditioned on the value of \( \Psi \) is a Gaussian random variable with mean (3.14) and variance

\[
\sigma(x)^2 = \Gamma(x, x) - \sum_{i,j=1}^{N} \Theta_{i,j}^{-1} \int_{\Omega} \Gamma(x, y) \psi_j(y) \int_{\Omega} \Gamma(x, y) \psi_i(y)
\] (3.17)

**Proof.** Let

\[
u_\Psi(x) := \mathbb{E}[u(x)\mid \Psi]
\] (3.18)

Since \( u \) and \( \Psi \) belong to the same Gaussian space, it follows that \( u_\Psi \) is a linear function of \( \Psi \) obtained by minimizing the mean squared error

\[
\mathbb{E}[(u(x) - c \cdot \Psi)^2] = \Gamma(x, x) - 2 \sum_{i=1}^{N} c_i \int_{\Omega} \Gamma(x, y) \psi_i(y) \, dy + \sum_{i,j=1}^{N} c_i c_j \Theta_{i,j}
\] (3.19)
with respect to \( c \in \mathbb{R}^N \), where \( \Theta \) is defined by (3.9). We conclude the proof by identifying the minimizer in \( c \), using Lemma 3.4 for the invertibility of \( \Theta \) and noting that (3.17) is simply (3.19) at the minimum in \( c \).

**Example 3.1.** If \( \mathcal{L} \) and \( \mathcal{B} \) correspond to the prototypical example (1.1) (see also Example 2.1), if \( \xi \) is white noise (i.e. if its covariance matrix is \( \Lambda(x,y) = \delta(x - y) \)), and if the observable functions are masses of Diracs at points \( x_i \in \Omega \) (and \( d \leq 3 \) which is required for (3.8)), then Theorem 3.5 implies (1.3) and the basis elements \( \phi_i \) are the RPS elements of [53] which are a generalization of Polyharmonic Splines to PDEs with rough coefficients. Recall that Polyharmonic splines can be traced back to the seminal work of Harder and Desmarais [40] and Duchon [22, 23, 24].

Note also that according to Theorem (3.5) the process of Bayesian conditioning gives us the whole posterior distribution of \( u(x) \) and not only its (conditional) expected value. In particular, the distribution of \( u(x) \) conditioned on \( u(x_1),...,u(x_N) \) is a Gaussian random variable with mean (1.3) and variance

\[
\sigma^2(x) = \Gamma(x,x) - \sum_{i,j=1}^{N} \Theta^{-1}_{ij} \Gamma(x,x_j) \Gamma(x,x_i)
\]

and this observation can be used to compute the probability of deviation of the RPS interpolation from \( u(x) \) by a given margin and guide the addition of interpolation points (note that \( \sigma^2(x) = 0 \) at the interpolation points \( x_1,...,x_N \)).

**Remark 3.6.** We will show in Theorem 5.1 that \( \sigma(x) \) also controls the pointwise error between the solution of the original integro-differential equation (2.1) and the approximation \( \sum_{i=1}^{N} \phi_i(x) \int_{\Omega} u(y) \psi_i(y) \mathrm{d}y \).

4 Variational properties of basis elements

In this section we will show that as for RPS [53], the basis elements \( \phi_i \) from Bayesian Inference have remarkable variational and optimal recovery properties that can be used (1) for their practical computation (2) for the derivation of accuracy estimates.

4.1 White Gaussian noise

In this subsection we will assume that \( \xi \) is white noise (i.e. \( \Lambda(x,y) = \delta(x - y) \)). Define

\[
V := \{ \phi \in H(\Omega) | \mathcal{L}\phi \in L^2(\Omega) \text{ and } \mathcal{B}\phi = 0 \text{ on } \partial\Omega \} \tag{4.1}
\]

and let \( \langle \cdot, \cdot \rangle \) be the (scalar) product on \( V \) defined by: for \( u,v \in V \),

\[
\langle u,v \rangle := \int_{\Omega} (\mathcal{L}u(x))(\mathcal{L}v(x)) \, dx \tag{4.2}
\]
Note in particular that \( \langle v, v \rangle = 0 \) if and only if \( v = 0 \) and we write
\[
\|v\|_V := \langle v, v \rangle^{\frac{1}{2}}
\] (4.3)
the corresponding norm.

**Theorem 4.1.** **If** \( \Gamma(x, x) < \infty \) **then for** \( v \in V \) **and** \( x \in \Omega \)
\[
|v(x)| \leq (\Gamma(x, x))^{\frac{1}{2}} \|v\|_V
\] (4.4)
and the space \( V \) with the reproducing Kernel \( \Gamma(x, y) \) forms a Reproducing Kernel Hilbert Space. **In particular,** for all \( v \in V \)
\[
\langle v, \Gamma(\cdot, x) \rangle = v(x)
\] (4.5)

**Proof.** Theorem 4.1 is a direct consequence of the fact that
\[
\langle v, \int \Omega \Gamma(\cdot, y)f(y)dy \rangle = \int \Omega v(y)f(y)dy
\] (4.6)
and (by Cauchy-Schwartz inequality and \( \langle \Gamma(\cdot, \cdot), \int \Omega \Gamma(\cdot, x) \rangle = \Gamma(x, x) \))
\[
\langle v, \Gamma(\cdot, x) \rangle \leq \langle v, v \rangle^{\frac{1}{2}} (\Gamma(x, x))^{\frac{1}{2}}
\] (4.7)

Define
\[
V_i := \{ \phi \in V | \int \Omega \phi(x)\psi_i(x)dx = 1 \text{ and } \int \Omega \phi(x)\psi_j(x)dx = 0 \text{ for } j \in \{1, \ldots, N\} \text{ such that } j \neq i \}
\] (4.8)

and consider the the following optimization problem over \( V_i \):
\[
\begin{cases}
\text{Minimize } \langle \phi, \phi \rangle \\
\text{Subject to } \phi \in V_i.
\end{cases}
\] (4.9)

**Proposition 4.2.** \( V_i \) is a non-empty closed affine subspace of \( V \). **Problem (4.9) is a**
strictly convex quadratic optimization problem over \( V_i \). **The unique minimizer of (4.9)**
is \( \phi_i \) as defined by (3.16).

**Proof.** Let us first prove that \( \phi_i \in V_i \). Let
\[
\theta_i(x) := \int \Omega \Gamma(x, y)\psi_i(y)dy
\] (4.10)
First observe that for all \( j \in \{1, \ldots, N\} \),
\[
\mathcal{L}\theta_i(x) = \int \Omega G(y, x)\psi_i(y)dy
\] (4.11)
and $B\theta_i(x) = 0$ on $\partial\Omega$. Noting that $\|\mathcal{L}\theta_i\|_{L^2(\Omega)}^2 = \Theta_i,i$ we deduce from Lemma 3.4 that $\theta_i \in V$. We conclude from (3.16) that $\phi_i \in V$. Now observing that

$$\Theta_{i,j} = \int_{\Omega} \psi_i(x) \Gamma(x,y) \psi_j(y)$$

we deduce that

$$\int_{\Omega} \phi_i(x) \psi_j(x) = (\Theta^{-1} \cdot \Theta)_{i,j} = \delta_{i,j}.$$  

where $\delta_{i,i} = 1$ and $\delta_{i,j} = 0$ for $j \neq i$. We conclude that $\phi_i \in V_i$ which implies that $V_i$ is non-empty (it is easy to check that it is a closed affine sub-space of $V$).

Now let us prove that problem (4.9) is a strictly convex optimization problem over $V_i$. Let $v, w \in V_i$ such that $v \neq w$. Write for $\lambda \in [0, 1],

$$f(\lambda) := \langle v + \lambda(w - v), v + \lambda(w - v) \rangle$$

and we need to show that $f(\lambda)$ is a strictly convex function. Observing that $f(\lambda) = \langle v, v \rangle + 2\lambda\langle v, w - v \rangle + \lambda^2\langle v - w, v - w \rangle$

and noting that $\langle v - w, v - w \rangle > 0$ (otherwise one would have $v = w$) we deduce that $f$ is strictly convex in $\lambda$. We conclude that (see, for example, [29, pp. 35, Proposition 1.2]) that Problem (4.9) is a strictly convex optimization problem over $V_i$ and that it admits a unique minimizer in $V_i$. We will postpone the proof of the fact that $\phi_i$ is the minimizer of (4.9) to the proof of Theorem 4.6. 

**Remark 4.3.** It is important to note that in practical (numerical) applications each element $\phi_i$ would be obtained by solving the quadratic optimization problem (4.9) rather than through the representation formula (3.16). Note also that, if $u$ is the (stochastic) solution of (3.2), then $\phi_i$ is also equal to the expected value of $u(x)$ conditioned on $\int_{\Omega} u(x) \psi_i(x) = 1$ and $\int_{\Omega} u(x) \psi_j(x) = 0$ for $j \neq i$, i.e.

$$\phi_i(x) = \mathbb{E}[u(x)| \int_{\Omega} u(x) \psi_i(x) = 1 \text{ and } \int_{\Omega} u(x) \psi_j(x) = 0 \text{ for } j \neq i]$$  

**Remark 4.4.** A simple calculation allows us to show that $\phi_i$ is also the solution of the following nested equations

$$\begin{cases}
\mathcal{L}\phi_i(x) = \chi_i(x) & x \in \Omega; \\
B\phi_i = 0 & \text{on } \partial\Omega,
\end{cases}$$

$$\begin{cases}
\mathcal{L}^*\chi_i(x) = \sum_{j=1}^{N} \Theta_{i,j}^{-1} \psi_j(x) & x \in \Omega; \\
B^*\chi_i(x) = 0 & \text{on } \partial\Omega,
\end{cases}$$

where $(\mathcal{L}^*, B^*)$ is the adjoint operator associated with $G(y,x)$ (the transpose of $G(x,y)$).
Remark 4.5. Another simple calculation allows us to show that $\phi_i$ is also the solution of the following nested equations

$$
\begin{align*}
\mathcal{L}_i \phi_i(x) &= \chi_i(x) \quad x \in \Omega; \\
\mathcal{B}_i \phi_i &= 0 \quad \text{on} \quad \partial \Omega, \\
\int_{\Omega} \phi_i(x) \psi_j(x) \, dx &= \delta_{i,j} \quad \text{for } j \in \{1, \ldots, N\}
\end{align*}
$$

where $c \in \mathbb{R}^N$ is an unknown vector determined by the third equation in (4.19).

Write $V_0$ the subset of $V$ defined by

$$
V_0 := \{ v \in V : \int_{\Omega} v(x) \psi_i(x) \, dx = 0, \forall i \in \{1, \ldots, N\} \} \quad (4.21)
$$

Theorem 4.6. It holds true that

- The basis $\phi_i$ is orthogonal to $V_0$ with respect to the product $\langle \cdot, \cdot \rangle$, i.e.
  $$
  \langle \phi_i, v \rangle = 0, \quad \forall i \in \{1, \ldots, N\} \text{ and } \forall v \in V_0 \quad (4.22)
  $$

- $\sum_{i=1}^{N} w_i \phi_i$ is the unique minimizer of $\langle v, v \rangle$ over all $v \in V$ such that $\int_{\Omega} v(x) \psi_i(x) \, dx = w_i$.

- For all $i \in \{1, \ldots, N\}$ and for all $v \in V$,
  $$
  \langle \phi_i, v \rangle = \sum_{j=1}^{N} \Theta_{i,j}^{-1} \int_{\Omega} v(x) \psi_j(x) \, dx \quad (4.23)
  $$

- For all $i, j \in \{1, \ldots, N\}$,
  $$
  \langle \phi_i, \phi_j \rangle = \Theta_{i,j}^{-1} \quad (4.24)
  $$

Remark 4.7. Theorem and its proof is analogous to the optimal property of strictly conditionally positive definite kernels [61] when used as interpolant solutions of the optimal recovery problem [38].

Proof. We have, using (4.10), (3.16) and (4.11)

$$
\langle \phi_i, v \rangle = \sum_{j=1}^{N} \Theta_{i,j}^{-1} \int_{\Omega} \mathcal{L}_j(x) \mathcal{L} v(x) \, dx = \sum_{j=1}^{N} \Theta_{i,j}^{-1} \int_{\Omega} \psi_j(y) v(y) = 0
$$

Which implies (4.22), (4.23) and (4.24).

Let $w \in \mathbb{R}^N$ and $\phi_w := \sum_{i=1}^{N} w_i \phi_i$. Let $v \in V$ such that $\int_{\Omega} v(x) \psi_i(x) \, dx = w_i$ for all $i \in \{1, \ldots, N\}$. Since $\phi_w - v \in V_0$, it follows that

$$
\langle v, v \rangle = \langle \phi_w, \phi_w \rangle + \langle v - \phi_w, v - \phi_w \rangle
$$

It follows that $\sum_{i=1}^{N} w_i \phi_i$ is the unique minimizer of $\langle v, v \rangle$ over all $v \in V$ such that $\int_{\Omega} v(x) \psi_i(x) \, dx = w_i$. Note that this also implies that $\phi_i$ is the minimizer of (4.9).
4.2 Non-white Gaussian noise

If $\xi$ is not white noise (i.e. $\Lambda(x, y) \neq \delta(x - y)$) then Theorem 4.1, Theorem 4.6 and Proposition 4.2 remain true provided that the definitions of the space $V$ and scalar product $\langle \cdot, \cdot \rangle$ are changed to

\[
V := \{ \phi \in \mathcal{H}(\Omega) | \mathcal{L}_\Lambda \mathcal{L} \phi \in L^2(\Omega), \mathcal{B} \phi = 0 \text{ and } \mathcal{B}_\Lambda \phi = 0 \text{ on } \partial \Omega \} \quad (4.27)
\]

\[
\langle u, v \rangle := \int_\Omega (\mathcal{L}_\Lambda \mathcal{L} u(x)) (\mathcal{L}_\Lambda \mathcal{L} v(x)) \, dx \quad (4.28)
\]

where $\mathcal{L}_\Lambda$ and $\mathcal{B}_\Lambda$ are defined in (3.6).

5 Accuracy of the basis elements $\phi_i$

5.1 Pointwise estimates

Let $\|v\|_V$ be defined as in (4.3).

**Theorem 5.1.** Assume that $\Gamma(x, x) < \infty$. Let $v \in V$. It holds true that for $x \in \Omega$

\[
\left| v(x) - \sum_{i=1}^{N} \phi_i(x) \left( \int_\Omega v(y) \psi_i(y) \, dy \right) \right| \leq \sigma(x) \|v\|_V \quad (5.1)
\]

where $\sigma^2(x)$ is the variance of $u(x)$ (solution of (3.2)) conditioned on $\int_\Omega u(y) \psi_1(y) \, dy, \ldots, \int_\Omega u(y) \psi_N(y) \, dy$ as defined by (3.17). In particular if $u$ is the solution of the original integro-differential equation (2.1), then

\[
\left| u(x) - \sum_{i=1}^{N} \phi_i(x) \left( \int_\Omega u(y) \psi_i(y) \, dy \right) \right| \leq \sigma(x) \|g\|_{L^2(\Omega)} \quad (5.2)
\]

if $\phi_i, \sigma$ are derived from white noise, and

\[
\left| u(x) - \sum_{i=1}^{N} \phi_i(x) \left( \int_\Omega u(y) \psi_i(y) \, dy \right) \right| \leq \sigma(x) \|\mathcal{L}_\Lambda g\|_{L^2(\Omega)} \quad (5.3)
\]

if $\phi_i, \sigma$ are derived from the noise with covariance function $\Lambda$ described in (3.6).

**Proof.** Let $v \in V$ and $x \in \Omega$. Using the reproducing kernel property of Theorem 4.1 we obtain that

\[
\left| v(x) - \sum_{i=1}^{N} \phi_i(x) \int_\Omega v(y) \psi_i(y) \, dy \right| = \left| \langle v, \Gamma(\cdot, x) - \sum_{i=1}^{N} \phi_i(x) \int_\Omega \Gamma(\cdot, y) \psi_i(y) \, dy \rangle \right| \quad (5.4)
\]

Therefore, using Cauchy-Schwartz inequality

\[
\left| v(x) - \sum_{i=1}^{N} \phi_i(x) \int_\Omega v(y) \psi_i(y) \, dy \right| \leq \|v\|_V \|\Gamma(\cdot, x) - \sum_{i=1}^{N} \phi_i(x) \int_\Omega \Gamma(\cdot, y) \psi_i(y) \, dy\|_V \quad (5.5)
\]
We conclude by expanding the right hand side of (5.5) and the definition \( \phi_i(x) = \sum_{j=1}^{N} \Theta_{i,j}^{-1} \int_{\Omega} \Gamma(x,y) \psi_i(y) \, dy \).

**Remark 5.2.** \( \sigma^2(x) \) is also known as the Power function in radial basis function interpolation [61, 33]. The proof of Theorem is similar to the one used to derive local error estimates for radial basis function interpolation of scattered data (see [63] in which \( \sigma^2(x) \) was referred to as the Kriging function, a terminology coming from geostatistics [47]).

### 5.2 \( \mathcal{H}(\Omega) \)-norm estimates

Let \( V_0 \) be the subset of \( V \) defined by (4.21). Write

\[
\rho(V_0) := \sup_{v \in V_0} \frac{\|v\|_{\mathcal{H}(\Omega)}}{\|v\|_V} \tag{5.6}
\]

Where \( \|\cdot\|_{\mathcal{H}(\Omega)} \) is the natural norm associated with the space on which the operator \( \mathcal{L} \) is defined.

**Theorem 5.3.** We have for all \( v \in V \)

\[
\left\| v - \sum_{i=1}^{N} \phi_i \left( \int_{\Omega} v(y) \psi_i(y) \, dy \right) \right\|_{\mathcal{H}(\Omega)} \leq \rho(V_0) \|v\|_V \tag{5.7}
\]

and \( \rho(V_0) \) is the smallest constant for which (5.7) holds for all \( v \in V \).

**Proof.** Write \( v_\psi(x) := \sum_{i=1}^{N} \phi_i(x) \left( \int_{\Omega} v(y) \psi_i(y) \, dy \right) \)

Observing that \( v - v_\psi \) belongs to \( V_0 \) implies that

\[
\|v - v_\psi\|_{\mathcal{H}(\Omega)} \leq \rho(V_0) \langle v - v_\psi, v - v_\psi \rangle^{\frac{1}{2}} \tag{5.8}
\]

Theorem 4.6 implies that

\[
\langle v, v \rangle = \langle v_\psi, v_\psi \rangle + \langle v - v_\psi, v - v_\psi \rangle \tag{5.9}
\]

which leads to

\[
\langle v - v_\psi, v - v_\psi \rangle = \langle v, v \rangle - \langle v_\psi, v_\psi \rangle \leq \langle v, v \rangle \tag{5.10}
\]

which concludes the proof. \qed

**Remark 5.4.** Observe that Theorem 5.3 implies that if \( u \) is the solution of the original integro-differential equation (2.1) and \( \phi_i, \sigma \) are derived from white noise, then

\[
\left\| u - \sum_{i=1}^{N} \phi_i \left( \int_{\Omega} u(y) \psi_i(y) \, dy \right) \right\|_{\mathcal{H}(\Omega)} \leq \rho(V_0) \|g\|_{L^2(\Omega)} \tag{5.11}
\]

Similarly, if \( \phi_i, \sigma \) are derived from the noise with covariance function \( \Lambda \) described in (3.6), then

\[
\left\| u - \sum_{i=1}^{N} \phi_i \left( \int_{\Omega} u(y) \psi_i(y) \, dy \right) \right\|_{\mathcal{H}(\Omega)} \leq \rho(V_0) \|\mathcal{L}g\|_{L^2(\Omega)} \tag{5.12}
\]
Example 5.1. If $\mathcal{L}$ and $\mathcal{B}$ correspond to the prototypical example (1.1) (Example 2.1), if $\xi$ is white noise, and if the observable functions are masses of Diracs at points $x_i \in \Omega$ (and $d \leq 3$), then [53],
\[ \rho(V_0) \leq CH \quad (5.13) \]
where $C$ depends only on $\lambda_{\min}(a), \lambda_{\max}(a)$ and $H$ where $\lambda_{\max}(a) := \sup_{x \in \Omega, t \neq 0} |\nabla a(x)| |t|^2$, $\lambda_{\min}(a) := \inf_{x \in \Omega, t \neq 0} |\nabla a(x)| |t|^2$ and $H$ is the mesh-norm
\[ H := \sup \min_{x \in \Omega} \|x - x_i\| \quad (5.14) \]
and
\[ \|u - \sum_{i=1}^N \phi_i(x)u(x_i)\|_{H^1(\Omega)} \leq CH \|\nabla (a\nabla u)\|_{L^2(\Omega)} \quad (5.15) \]
Let us also recall that the proof of (5.13) is based on the following Poincaré inequality (Lemma 3.1 of [53])

Lemma 5.5. Let $d \leq 3$ and $B_1$ be the open ball of center 0 and radius 1. There exists a finite strictly positive constant $C_{\lambda_{\min}(a), \lambda_{\max}(a)}$ such that for all $v \in H^1(B_1)$ such that $\nabla (a\nabla v) \in L^2(B_1)$ it holds true that
\[ \|v - v(0)\|^2_{L^2(B_1)} \leq C_{\lambda_{\min}(a), \lambda_{\max}(a)} \left( \|\nabla v\|^2_{L^2(B_1)} + \|\nabla (a\nabla v)\|^2_{L^2(B_1)} \right) \quad (5.16) \]

Example 5.2. If $\mathcal{L}$ and $\mathcal{B}$ correspond to the prototypical example (1.1) (Example 2.1), if $\xi$ is white noise, and if the observable functions are indicator functions of Voronoï cells around points in $x_i \in \Omega$ or of tetrahedra of a regular tessellation of the points $x_i \in \Omega$ then (5.13) remains valid as a simple consequence of localized Poincaré inequalities. Indeed for $v \in V_0$, writing $C_i$ the Voronoï cells the points $x_i \in \Omega$, we have (assuming $\Omega$ is the union of those Voronoï cells)
\[ \|v\|^2_{H^1(\Omega)} = \int_{\Omega} v(-\nabla (a\nabla v)) \leq \|v\|^2_{L^2(\Omega)} \|\nabla (a\nabla v)\|^2_{L^2(\Omega)} \quad (5.17) \]
and we conclude by applying Poincaré inequality to the $L^2$-norm of $v$ within each cell $C_i$, i.e.
\[ \|v\|^2_{L^2(\Omega)} = \sum_i \|v\|^2_{L^2(C_i)} \leq CH^2 \sum_i \|\nabla v\|^2_{L^2(C_i)} = CH^2 \|\nabla v\|^2_{L^2(\Omega)} \quad (5.18) \]
We will give the last example as a theorem.

Theorem 5.6. Let $\mathcal{L}$ and $\mathcal{B}$ be as in the prototypical example (1.1) (Example 2.1), let $\xi$ be white noise, and let $x_i \in \Omega$ be $N$ arbitrary points of $\Omega$ with mesh norm $H$ (see (5.14)). Let $\psi_1, \ldots, \psi_N$ be linearly independent generalized probability densities on $\Omega$ with (possibly overlapping) support $\text{support}(\psi_i)$. Define
\[ H := \sup \min_{x \in \Omega} \sup_{y \in \text{support}(\psi_i)} \|x - y\| \quad (5.19) \]
Then, it holds true that
\[
\rho(V_0) \leq CH \quad (5.20)
\]
where \( C \) depends only on \( \lambda_{\min}(\alpha), \lambda_{\max}(\alpha) \) and \( C_0 \). Henceforth, for \( u \in V \)
\[
\|u - \sum_{i=1}^{N} \phi_i(x) \int_{\Omega} u(y) \psi_i(y) \, dy\|_{H^1_0(\Omega)} \leq CH \|\text{div}(a \nabla u)\|_{L^2(\Omega)} \quad (5.21)
\]

**Remark 5.7.** Observe that if for all \( i \) the support of \( \psi_i \) is contained in a ball of center \( x_i \) and radius \( H' \), then
\[
H \leq H' + \sup_{x \in \Omega} \min_i \|x - x_i\| \quad (5.22)
\]

**Proof.** The proof of (5.20) is simply based on the observation that if \( v \in V_0 \) then (since \( \int_{\Omega} v(x) \psi_i(x) \, dx = 0 \)) there exists \( N \) points \( y_1, \ldots, y_N \) such that \( v(y_i) = 0 \) and the mesh norm of those points is bounded by \( H \). Therefore we can apply the result of Example 5.1.

## 6 Statistical Decision Theory

Another motivation for exploring Bayesian approximations of the solution space, lies in the decision theory/game theory approach to numerical homogenization. In this approach one looks at the numerical homogenization problem (1.1) as a game where player A chooses a function \( \theta \) of the observable \( u(x_1), \ldots, u(x_N) \) and player B chooses a source term \( g \) in a class/set \( A \). These two choices combine and form an error term
\[
E(\theta, g) = \left\| u(x) - \theta(u(x_1), \ldots, u(x_N)) \right\| \quad (6.1)
\]
Player’s A objective is to minimize the error (6.1) while player’s B objective is to maximize it. A surprising result from Wald’s Decision Theory \([60]\) (stemming out of Von Neumann’s Game Theory \([59]\)) is that, although such games are deterministic, under weak regularity conditions, the optimal strategy for player B is to play at random by placing an optimal prior distribution on the set of candidates for \( g \) and, similarly, the best strategy for player A lives in the Bayesian class obtained by placing an (optimal) prior on the set of candidates for \( g \).

Of course, in the present work we do not know, nor have investigated the optimality of the Gaussian prior (on \( g \)) in the game theoretic sense described above. Our choice has been motivated by the simplicity (linearity) of calculations associated Gaussian filtering and the fact that such a choice allows for the identification of accurate numerical homogenization bases with optimal recovery properties (Theorem 4.6).

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