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A quasi-optimal sparse grids procedure for groundwater flows*

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Abstract

In this work we explore the extension of the quasi-optimal sparse grids method proposed in our previous work "*On the optimal polynomial approximation of stochastic PDEs by Galerkin and Collocation methods*" to

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a Darcy problem where the permeability is modeled as a lognormal random field. We propose an explicit a-priori/a-posteriori procedure for the construction of such quasi-optimal grid and show its effectivenenss on a numerical example. In this approach, the two main ingredients are an estimate of the decay of the Hermite coefficients of the solution and an efficient nested quadrature rule with respect to the Gaussian weight.

1 Introduction

Uncertainty quantification plays a crucial role in the area of groundwater flows where, given the time and length scale of most problems, it is quite common to have partial and fragmented knowledge about most of the system properties, e.g. on the permeability field, forcing terms, boundary conditions. Broad classes of applications of interest could be oil or water reservoir management, see e.g. [8, 10].

Given the complexity of the deterministic solvers for such problems, a non-intrusive computational approach to perform the uncertainty quantification analysis is quite appealing. In this work we consider a Darcy problem with uncertain permeability modeled as a lognormal random field, and we explore (rather heuristically) the possibility to extend to this problem the quasi-optimal sparse grid method that we proposed in [4] for problems depending instead on a set of uniform random variables.

The well-posedness of the lognormal problem has been thoroughly investigated in [7, 15]. The optimal convergence rate of its so-called Polynomial Chaos Expansion approximation has been analyzed theoretically in [18]. Although the deterministic Darcy problem is more commonly approximated numerically in its mixed form (see e.g. [1, 5, 9, 16]), in this work we will consider a standard Finite Element discretization of the primal elliptic formulation of the Darcy problem, in which the unknown is the water pressure p.

The rest of this work is organized as follows. In Section 2 we specify the model assumptions on the random permeability field, on the deterministic problem and on the quantity of interest. Section 3 deals with the finite dimensional Fourier expansion of the random field, and Section 4 with the derivation of the quasi-optimal sparse grid for the problem at hand. Finally, we present some numerical results in Section 5, and draw some conclusions in Section 6.

2 Problem setting

Let $(\Omega, \mathcal{F}, P)$ be a complete probability space, where Ω denotes the set of outcomes, $\mathcal{F}$ its σ-algebra, and $P : \mathcal{F} \to [0, 1]$ a probability measure. Following a standard notation, we denote with $H^1(D)$ the Sobolev space of square-intergrable functions in D with square integrable derivatives. $L^q_P(\Omega)$ will denote the Banach space of random functions with bounded q-th moment with respect

to the probability measure P, and $L^q_P(\Omega; H^1(D))$ the Bochner space of $H^1(D)$-valued random fields with q-th bounded moment with respect to P, that is

$$f \in L^q_P(\Omega; H^1(D)) \Leftrightarrow \int_\Omega \|f(\cdot,\omega)\|^q_{H^1(D)}\, dP(\omega) < \infty\,.$$

As mentioned in the introduction, the permeability field is supposed to be uncertain. Since hydrogeologycal applications deal in general with composite materials (sand, marl, clay), the pointwise permeability values can vary within several orders of magnitude. It is thus rather common to model the logarithm of the permeability as a random field, rather than the permeability itself. More in detail, we will make the following assumption.

Assumption 2.1 *The permeability $a(\mathbf{x},\omega) : \overline{D} \times \Omega \to \mathbb{R}$ is a lognormal field, that is*

$$a(\mathbf{x},\cdot) = e^{\gamma(\mathbf{x},\cdot)}, \quad \gamma(\mathbf{x},\cdot) \sim \mathcal{N}(\mu,\sigma^2) \quad \forall \mathbf{x} \in D, \tag{1}$$

where $\mathcal{N}(\mu,\sigma^2)$ denotes a Gaussian probability distribution with expected value μ and variance σ^2, and $\gamma(\mathbf{x},\omega) : \overline{D} \times \Omega \to \mathbb{R}$ is such that for $\mathbf{x},\mathbf{x}' \in D$ the covariance function $C_\gamma(\mathbf{x},\mathbf{x}') = \mathbb{C}\mathrm{ov}\,[\gamma(\mathbf{x},\cdot)\gamma(\mathbf{x}',\cdot)]$ depends only on the distance $\|\mathbf{x}-\mathbf{x}'\|$ ("isotropic" property). Moreover, $C_\gamma(\mathbf{x},\mathbf{x}') = C_\gamma(\|\mathbf{x}-\mathbf{x}'\|)$ is Lipschitz continuous, and is a positive definite function.

As for the choice of C_γ, several models have been proposed in the literature. While hydrogeological expertise seems to indicate that a reasonable choice for C_γ for isotropic media would be the exponential correlation function $C_\gamma(\mathbf{x},\mathbf{x}') = \sigma^2 \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|_1}{L_c^2}\right)$, it is intuitive that the spike featured by this choice will make the problem quite difficult to tackle. As a consequence, given the exploratory level of this work, we choose here to work with the more regular Gaussian covariance function,

Assumption 2.2 *The Gaussian field $\gamma(\mathbf{x},\omega)$ has a Gaussian covariance function,*

$$C_\gamma(\mathbf{x},\mathbf{x}') = \sigma^2 \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{L_c^2}\right). \tag{2}$$

where $L_c > 0$ is called "correlation length".

The Darcy problem will be set in a horizontal square domain $D = (0,L)^2$, $L = 1$, with no forcing terms. We impose a pressure gradient acting on the water by setting $p = 1$ on the left boundary $\mathcal{B}_1 = \{\mathbf{x} \in D : x_1 = 0\}$ and $p = 0$ on the right boundary $\mathcal{B}_2 = \{\mathbf{x} \in D : x_1 = L\}$. Finally, we consider a no-flux Neumann condition on the upper and lower boundaries $\mathcal{B}_3 = \{\mathbf{x} \in D : x_2 = 0\}$ and $\mathcal{B}_4 = \{\mathbf{x} \in D : x_2 = L\}$. The Darcy problem thus reads:

Strong Formulation 1 *Find a random pressure* $p : \overline{D} \times \Omega \to \mathbb{R}$ *such that* P*-almost everywhere the following equation holds*

$$\begin{cases} -\operatorname{div}(a(\mathbf{x},\omega)\nabla p(\mathbf{x},\omega)) = 0 & \mathbf{x} \in D, \\ p(\mathbf{x},\omega) = 1 & \mathbf{x} \in \mathcal{B}_1, \\ p(\mathbf{x},\omega) = 0 & \mathbf{x} \in \mathcal{B}_2, \\ a(\mathbf{x},\omega)\nabla p(\mathbf{x},\omega)\cdot\mathbf{n} = 0 & \mathbf{x} \in \mathcal{B}_3 \cup \mathcal{B}_4. \end{cases} \tag{3}$$

It is straightforward to see that, thanks to the Lax–Milgram lemma, (3) is well-posed for almost every $\omega \in \Omega$. Proving the well-posedness of (3) in the Bochner spaces $L^q_P(\Omega; H^1(D))$ for $q > 0$ is instead not trivial, since a is not uniformely bounded nor uniformely coercive with respect to ω. It is however possible to prove the following result (see e.g. [2, 7, 11, 15]):

Proposition 2.1 *For every* $q > 0$*, there exists a unique* $H^1(D)$*-valued random pressure* $p = p(\mathbf{x},\omega)$ *in* $L^q_P(\Omega; H^1(D))$ *solving* (3)*.*

As for quantities of interest, we aim at computing the expected value of the total flux crossing the right boundary $\mathcal{B}_2$. This is indeed a random variable,

$$Z_p(\omega) = \int_{\mathcal{B}_2} a(\mathbf{x},\omega)\partial_{\mathbf{n}} p(\mathbf{x},\omega) d\mathbf{x}\,, \tag{4}$$

and also represents the "effective permeability" of the random medium in D.

3 Series expansion of the log-permeability random field

To get to a computable representation of p we need to derive an approximation of a in terms of a finite set of N random variables $y_i(\omega)$, $i = 1, \ldots, N$ ("finite noise approximation"). Such approximation is usually obtained by suitably truncating a series expansion such as the Karhunen-Loève expansion, see e.g. [21]. As an alternative, we consider here a Fourier-based decompostion of γ, which uses trigonometric polynomials as basis functions in the physical space. This choice allows analytical computation of the expansion and highlights the contribution of each spatial frequency to the total field a.

Proposition 3.1 (Fourier expansion) *Let* $\gamma(\mathbf{x},\omega) : [0, L]^2 \times \Omega \to \mathbb{R}$ *be a weakly stationary gaussian random field as in Assumption 2.1, with pointwise variance* σ^2*. Then the covariance function can be expanded in cosine-Fourier series*

$$C_\gamma(\left\|\mathbf{x} - \mathbf{x}'\right\|) = \sigma^2 \sum_{\mathbf{k}=(k_1,k_2)\in\mathbb{N}_0^2} c_{\mathbf{k}} \cos(\omega_{k_1}(x_1 - x_1')) \cos(\omega_{k_2}(x_2 - x_2')), \tag{5}$$

with $\omega_{k_1} = \frac{k_1\pi}{L}$, $\omega_{k_2} = \frac{k_2\pi}{L}$, *and normalized Fourier coefficient* $c_{\mathbf{k}}$ *so that*

$$\sum_{\mathbf{k}\in\mathbb{N}_0^2} c_{\mathbf{k}} = 1. \tag{6}$$

In particular, for the Gaussian covariance function in Assumption 2.2, and for sufficiently small values of L_c, $c_{\mathbf{k}}$ *are well approximated by*

$$c_{\mathbf{k}} \approx \lambda_{k_1}\lambda_{k_2}, \text{ where } \lambda_k = \begin{cases} \dfrac{L_c\sqrt{\pi}}{2L} & \text{if } k = 0 \\ \dfrac{L_c\sqrt{\pi}}{L}\exp\left(-\dfrac{(k\pi L_c)^2}{4L^2}\right) & \text{if } k > 0\ . \end{cases} \tag{7}$$

The random field γ *admits then the following expansion*

$$\gamma(\mathbf{x},\omega) = \mathbb{E}\left[\gamma(\mathbf{x},\cdot)\right] + \sigma \sum_{\mathbf{k}\in\mathbb{N}^2}\sum_{i=1}^{4} \left(\sqrt{c_{\mathbf{k}}}\, y_{\mathbf{k},i}(\omega)\phi_{\mathbf{k},i}(\mathbf{x})\right) \tag{8}$$

where $y_{\mathbf{k},i}(\omega)$ *are identically distributed and independent standard Gaussian random variables, and* $\phi_{\mathbf{k},i}$ *are defined as* $\phi_{\mathbf{k},1}(\mathbf{x}) = \cos(\omega_{k_1}x_1)\cos(\omega_{k_2}x_2)$, $\phi_{\mathbf{k},2}(\mathbf{x}) = \sin(\omega_{k_1}x_1)\sin(\omega_{k_2}x_2)$, $\phi_{\mathbf{k},3}(\mathbf{x}) = \cos(\omega_{k_1}x_1)\sin(\omega_{k_2}x_2)$, $\phi_{\mathbf{k},4}(\mathbf{x}) = \sin(\omega_{k_1}x_1)\cos(\omega_{k_2}x_2)$.

Proof. See [27, Chapter 4]. □

A good approximation of γ, γ_N, can be achieved by retaining in (8) only the N random variables corresponding to the frequencies $\mathbf{k}$ in the set

$$\mathcal{K}_\kappa = \left\{\mathbf{k}\in\mathbb{N}_0^2 : k_1^2 + k_2^2 \le \kappa^2, \kappa\in\mathbb{N}\right\}. \tag{9}$$

Following the argument of [7], it can be shown in particular that γ_N converges to γ almost surely in $\mathcal{C}^0(D)$.

Example 3.1 *Table 1 shows the number of random variables that need to be included into* (8) *to take into account a fraction* α *of the total variance of* γ *for different correlation lengths* L_c. *This has been computed by noting that, thanks to* (6), *if* $\sum_{\mathbf{k}\in\mathcal{K}} c_{\mathbf{k}} = \alpha$ *then* γ_N *is taking into account* $\alpha\%$ *of the total variance of the field. The need to include a high number of random variables in the approximation of the random field* γ, *and hence the high-dimensionality of the vector* $\mathbf{y}$ *of input random variables clearly emerges. In practice, the level of truncation should be related to the error in the variance of the solution of the PDE.*

Let us now denote $\Gamma_i = \mathbb{R}$ the support of $y_i(\omega)$, $\Gamma = \Gamma_1 \times \ldots \times \Gamma_N$ the support of $\mathbf{y} = [y_1, \ldots, y_N]$, $\rho_i(y_i) : \Gamma_i \to \mathbb{R}$ the probability density function of y_i and $\rho(\mathbf{y}) : \Gamma \to \mathbb{R}$ the joint probability density function of $\mathbf{y}$, with $\rho(\mathbf{y}) = \prod_{n=1}^{N}\rho_i(y_i), \rho_i(y_i) = \frac{1}{\sqrt{2\pi}}e^{-\frac{y_i^2}{2}}$. Having introduced the random variables y_i, we can replace the abstract probability space $(\Omega, \mathcal{F}, P)$

	$\boldsymbol{\alpha = 0.7}$	$\boldsymbol{\alpha = 0.9}$	$\boldsymbol{\alpha = 0.99}$
$\mathbf{L_c = 0.35}$	$N = 13$	$N = 25$	$N = 49$
$\mathbf{L_c = 0.25}$	$N = 25$	$N = 49$	$N = 97$
$\mathbf{L_c = 0.1}$	$N = 161$	$N = 293$	$N = 593$

Table 1: Random variables needed to represent $\alpha\%$ of the total variance of a random field with Gaussian covariance function for different correlation lengths L_c.

with $(\Gamma, \mathscr{B}(\Gamma), \rho(\mathbf{y})d\mathbf{y})$, where $\mathscr{B}(\Gamma)$ denotes the Borel σ-algebra, and hence $L^q_P(\Omega)$ with $L^q_\rho(\Gamma)$ and $L^q_P(\Omega; H^1(D))$ with $L^q_\rho(\Gamma; H^1(D))$.

Moreover, the permeability and pressure fields can now be seen as functions of $\mathbf{x}$ and $\mathbf{y}$, $a(\mathbf{x}, \omega) \approx a_N(\mathbf{x}, \mathbf{y}) = e^{\gamma_N(\mathbf{x},\mathbf{y})}$, $p(\mathbf{x}, \omega) \approx p_N(\mathbf{x}, \mathbf{y})$ and the quantity of interest (4) becomes a random function $Z_p : \Gamma \to \mathbb{R}$. We will not however address here the study on the convergence of p_N to p, see e.g. [7] to this end. Here we just mention that, following again the argument in [7], it is possible to show that the almost sure convergence of γ_N to γ guarantees the almost sure convergence of a_N to a in $\mathcal{C}^0(D)$, and that for any $q > 0$ there holds $\|a_{N(\kappa)} - a\|_{L^q(\Omega, \mathcal{C}^0(D))} \leq C_1(q)\kappa e^{-C_2(L,L_c)\kappa^2}$, $N(\kappa)$ being the cardinality of the set $\mathcal{K}_\kappa$ defined in (9). In the rest of this work, with a slight abuse of notation, we will therefore omit subscript $\cdot_N$ if no confusion arise. Moreover, the quasi-optimal Sparse Grid Collocation technique that we will present in the next Section is able to automatically select the "most important" random variables that should be retained for the approximation of p. This would allow us to work with formally $N \to \infty$ random variables.

The previous results on the well-posedness of the problem still hold after having replaced ω with $\mathbf{y}$, and we can write the problem in weak form.

Weak Formulation 1 *Find* $p \in H^1(D) \otimes L^2_\rho(\Gamma)$ *such that* $p = 1$ *on* $\mathcal{B}_1$, $p = 0$ *on* $\mathcal{B}_2$ *and* $\forall\, v \in H^1_{dir}(D) \otimes L^2_\rho(\Gamma)$

$$\int_\Gamma \int_D a(\mathbf{x}, \mathbf{y}) \nabla p(\mathbf{x}, \mathbf{y}) \cdot \nabla v(\mathbf{x}, \mathbf{y})\, \rho(\mathbf{y})\, d\mathbf{x}\, d\mathbf{y} = 0. \tag{10}$$

where $H^1_{dir}(D)$ is the subset of $H^1(D)$ functions that vanish on the Dirichlet boundary $\mathcal{B}_1 \cup \mathcal{B}_2$.

4 Quasi-Optimal sparse grid approximation

As highlighted in Example 3.1, both the permeability a and the pressure p depend on a high number of random variables y_i. To obtain efficiently an approximation of p over Γ we then resort to the sparse grid method [2, 3, 6, 23, 24, 28], that allows to obtain an accurate representation of p while keeping the number of interpolation points considerably lower than what would be needed if a full

tensor grid approximation was employed. In formulae, the sparse grid approximation of p is written as

$$p_{\mathrm{w}}(\mathbf{y}) = \mathcal{S}^m_{\mathcal{I}(\mathrm{w})}[p](\mathbf{y}) = \sum_{\mathbf{i}\in\mathcal{I}(\mathrm{w})} \bigotimes_{n=1}^{N} \Delta_n^{m(i_n)}[p](\mathbf{y}), \tag{11}$$

where

- $\mathbf{i} \in \mathbb{N}_+^N$ is a multiindex with non-zero components;
- $\Delta_n^{m(i_n)} = \mathcal{U}_n^{m(i_n)} - \mathcal{U}_n^{m(i_n-1)}$ is called "detail operator", and is the difference between two consecutive one-dimensional interpolants, using $m(i)$ and $m(i-1)$ points respectively;
- $\Delta^{m(\mathbf{i})}[p] = \bigotimes_{n=1}^{N} \Delta^{m(i_n)}[p]$ is called "hierarchical surplus";
- $\{\mathcal{I}(\mathrm{w})\}_{\mathrm{w}\in\mathbb{N}}$ denotes a sequence of index sets. Each of these sets has to be *admissible* in the following sense for the sparse grid to be consistent (see e.g. [14]):

$$\forall\, \mathbf{i} \in \mathcal{I},\ \mathbf{i} - \mathbf{e}_j \in \mathcal{I} \text{ for } 1 \le j \le N,\ i_j > 1, \tag{12}$$

$\mathbf{e}_j$ being the j-th canonical vector. Roughly speaking, the sparse grid approximation of p can be understood as a linear combination of tensor grid approximations of p over Γ, each one built over "few" points.

The efficiency of the sparse grid depends on the choice of the interpolation points used in $\mathcal{U}_n^{m(i)}$ and of the index sets $\mathcal{I}(\mathrm{w})$. As for the interpolation points, they should be chosen in agreement with the probability measure over Γ, a good choice being given e.g. by the Gauss-Hermite points (see e.g. [26]).

Regarding the index sets $\mathcal{I}(\mathrm{w})$, the best strategy is to include in (11) only the hierarchical surpluses with the highest profits [4, 14, 17]. The latter is defined as the ratio between the expected error decrease by adding a given hierarchical surplus to the sparse grid approximation and the corresponding cost, quantified here by the number of interpolation points in the hierarchical surplus,

$$\mathcal{I}(\mathrm{w}) = \left\{ \mathbf{i} \in \mathbb{N}_+^N : \frac{\Delta E(\mathbf{i})}{\Delta W(\mathbf{i})} \ge \epsilon(\mathrm{w}) \right\} \tag{13}$$

with $\{\epsilon(\mathrm{w})\}_{\mathrm{w}\in\mathbb{N}} \downarrow 0$ and $\Delta E(\mathbf{i})$, $\Delta W(\mathbf{i})$ representing the error and work contribution of each hierarchical surplus respectively. Note that $\mathcal{I}(\mathrm{w})$ in (13) may not satisfy the admissibility condition (12), that has to be explicitely enforced.

This criterion can be implemented in an adaptive procedure [14, 19] that explores the space of hierarchical surpluses and adds to $\mathcal{I}(\mathrm{w})$ the most profitable according to (13). As an alternative, in [4] we have detailed an a-priori/a-posteriori procedure to detect $\mathcal{I}(\mathrm{w})$ based on estimates of $\Delta E(\mathbf{i})$ and $\Delta W(\mathbf{i})$. On the one hand, the a-priori approach saves the computational cost of the exploration of the space of hierarchical surpluses, but on the other hand it will

be effective only if the estimates of $\Delta E(\mathbf{i})$ and $\Delta W(\mathbf{i})$ are sufficiently sharp. In [4] only the case of uniform random variables has been investigated. Deriving sharp estimates for the problem at hand, that depends on Gaussian random variables, is the goal of the present work.

We begin with the estimate of the work contribution corresponding to an additional index $\mathbf{i}$, which can be easily computed if the considered interpolant operators $\mathcal{U}_n^{m(i_n)}$ are nested and the set $\mathcal{I}(\mathrm{w})$ is admissible:

$$\Delta W(\mathbf{i}) = \prod_{n=1}^{N} (m(i_n) - m(i_n - 1)). \tag{14}$$

The estimate of the error contribution requires instead more effort. As a preliminary step, we need to introduce a spectral basis for $L^2_\rho(\Gamma)$. To this end, let $\{H_p(y_n)\}_{p\in\mathbb{N}}$ be the family of orthonormal Hermite polynomials relative to the weight $e^{-y^2/2}/\sqrt{2\pi}$ in the n-th direction [12]. The set of multidimensional Hermite polynomials $\mathcal{H}_{\mathbf{q}}(\mathbf{y}) = \prod_{n=1}^{N} H_{q_n}(y_n), \forall \mathbf{q} \in \mathbb{N}^N$ is an orthonormal basis for $L^2_\rho(\Gamma)$, that can be used to formally construct the spectral expansion of $p(\mathbf{y})$

$$p(\mathbf{y}) = \sum_{\mathbf{q}\in\mathbb{N}^N} p_{\mathbf{q}} \mathcal{H}_{\mathbf{q}}(\mathbf{y}), \quad p_{\mathbf{q}} = \int_\Gamma p(\mathbf{y}) \mathcal{H}_{\mathbf{q}}(\mathbf{y}) \rho(\mathbf{y}) d\mathbf{y}. \tag{15}$$

We can now state a heuristic estimate for the error contribution of the hierarchical surplus $\Delta^{m(\mathbf{i})}$ in the spirit of what was done in [4], eq. (4.9):

$$\Delta E(\mathbf{i}) \approx B(\mathbf{i}) \left\| p_{m(\mathbf{i}-\mathbf{1})} \right\|_{H^1(D)}, \tag{16}$$

where $p_{m(\mathbf{i}-\mathbf{1})}$ is the $m(\mathbf{i}-\mathbf{1})$-th coefficient of the spectral expansion (15), and $B(\mathbf{i})$ is a factor that depends on the interpolation points only, in the spirit of the Lebesgue constant. This is a reasonable heuristic assumption, since in this way the error contribution estimate "encodes" information on both the quality of the solution (through the decay of the spectral coefficients), and the quality of the interpolant operator itself. Numerical results in the next section will also show the effectiveness of (16).

To make estimates (14) and (16) computable we still need to:

1. choose a family of nested univariate interpolant operators for the Gaussian measure;
2. provide an estimate for the factor $B(\mathbf{i})$ in (16);
3. provide an estimate for the coefficients $p_{m(\mathbf{i}-\mathbf{1})}$ in (15), (16).

4.1 Nested quadrature formulae for Gaussian measure

The family of nested points we choose is the so-called "Kronrod-Patterson-Normal" (*KPN* in short, see Figure 1). Such family of interpolation/quadrature

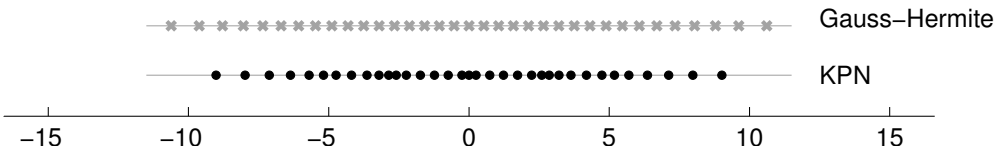


Figure 1: First 35 *KPN* and Gauss-Hermite knots.

points is due to Genz and Keister, see [13], that applied the Kronrod-Patterson procedure [20, 25] to the classical Gauss-Hermite quadrature points (i.e. the roots of the Hermite polynomials $H_p(y_n)$). We recall that the Kronrod-Patterson procedure is a way to modify a quadrature rule, by adding new points in a nested fashion retaining the highest degree of exactness possible. The knots and the corresponding quadrature weights are tabulated up to level 5 (35 nodes) and can be found e.g. at `http://www.sparse-grids.de/`. For such family of points there holds

$$m(i_n) = 1, 3, 9, 19, 35 \quad \text{for } i_n = 1, \dots, 5 \tag{17}$$

i.e. consecutive interpolants are built over $1, 3, 9, 19, 35$ points respectively.

4.2 Estimate for $B(\mathbf{i})$

In [4] the constant $B(\mathbf{i})$ in equation (16) was chosen to be equal to the product of the Lebesgue constants of interpolant operators in each direction, $B(\mathbf{i}) = \prod_{n=1}^{N} \mathbb{L}_n^{m(i_n)}$. Such an estimate is also supported by numerical verification.

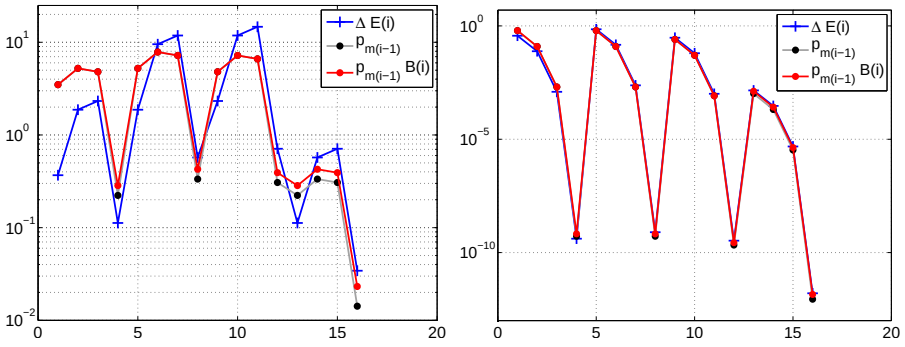
However, it is not easy to obtain a sharp bound for the Lebesgue constant in case of interpolation in spaces with Gaussian measure. Thus, we propose here a different estimate for $B(\mathbf{i})$, which on the one hand gives good numerical results when tested on model problems (see Figure 2) and on the other hand is close to the original choice when applied to a problem with uniform random variables.

To this end, we go back to the definition of error contribution for a hierarchical surplus, and exploit the fact that p admits a Hermite expansion. To improve the readibility we will use $\|\cdot\|_{\otimes}$ to denote the norm $\|\cdot\|_{H^1(D)\otimes L^2_\rho(\Gamma)}$.

$$\begin{aligned} \Delta E(\mathbf{i}) &= \left\| \left(p - \mathcal{S}^m_{\{\mathcal{J}\cup\mathbf{i}\}}[p]\right) - \left(p - \mathcal{S}^m_{\mathcal{J}}[p]\right) \right\|_{\otimes} = \left\| \Delta^{m(\mathbf{i})}[p] \right\|_{\otimes} \\ &= \left\| \Delta^{m(\mathbf{i})}\Big[\sum_{\mathbf{q}\in\mathbb{N}^N} p_{\mathbf{q}}\mathcal{H}_{\mathbf{q}}\Big] \right\|_{\otimes} = \Big\| \sum_{\mathbf{q}\in\mathbb{N}^N} p_{\mathbf{q}} \Delta^{m(\mathbf{i})}[\mathcal{H}_{\mathbf{q}}] \Big\|_{\otimes}. \end{aligned} \tag{18}$$

Observe now that by construction of hierarchical surplus there holds $\Delta^{m(\mathbf{i})}[\mathcal{H}_{\mathbf{q}}] = 0$ for polynomials such that $\exists\, n : q_n < m(i_n - 1)$. Next, we apply the triangular inequality and get to

$$\Delta E(\mathbf{i}) \leq \sum_{\mathbf{q}\geq m(\mathbf{i}-\mathbf{1})} \|p_{\mathbf{q}}\|_{H^1(D)} \left\| \Delta^{m(\mathbf{i})}[\mathcal{H}_{\mathbf{q}}] \right\|_{L^2_\rho(\Gamma)}. \tag{19}$$



(a) $p(y_1, y_2) = e^{-1-1.5y_1-1.5y_2}$. (b) $p(y_1, y_2) = e^{-1-y_1-0.2y_2}$.

Figure 2: Numerical comparison between $\Delta E(\mathbf{i})$ and $|p_{m(\mathbf{i-1})}|$ for p of the form $p(y_1, y_2) = e^{-1-b_1 y-1-b_2 y_2}$. The quantities $\Delta E(\mathbf{i})$ for $\mathbf{i}$ s.t. $\max\{i_1, i_2\} \leq 4$ have been computed with a standard Smolyak sparse grid, with $\mathcal{I}(\mathrm{w}) = \{\mathbf{i} \in \mathbb{N}_+^N : |\mathbf{i} - \mathbf{1}| \leq \mathrm{w}\}$, $\mathrm{w} = 10$, and "doubling" function $m(i)$: $m(0) = 0, m(1) = 1, m(i) = 2^{i-1}+1$. The Hermite coefficients $|p_{m(\mathbf{i-1})}|$ have been computed analytically with the formula stated in Lemma 4.1.

Therefore, the error estimate (16) is equivalent to assuming that the summation on the right-hand side of (19) is dominated by the first term, with

$$B(\mathbf{i}) = \left\| \Delta^{m(\mathbf{i})}[\mathcal{H}_{m(\mathbf{i-1})}] \right\|_{L^2_\rho(\Gamma)} = \prod_{n=1}^{N} B_n(i_n)\,, \tag{20}$$
$$B_n(i_n) = \left\| \Delta^{m(i_n)}[H_{m(i_n)}] \right\|_{L^2_{\rho_n}(\Gamma_n)}.$$

The quantity $B_n(i_n)$ can be easily computed numerically, and has a moderate growth with respect to i_n:

$$B_n(i_n) = 1,\ 1,\ 1,\ 1.28,\ 5.46 \quad \text{for } i = 1, \ldots, 5. \tag{21}$$

Finally, we test estimate (16) on the model function $p(y_1, y_2) = 1/\exp(1 + b_1 y_1 + b_2 y_2)$, so that we can compute each $\Delta E(\mathbf{i})$ as

$$\Delta E(\mathbf{i}) = \left\| \Delta^{m(\mathbf{i})}[p] \right\|_{L^2_\rho(\Gamma)} = \left\| \mathcal{S}^m_{\{\mathcal{J} \cup \mathbf{i}\}}[p] - \mathcal{S}^m_{\mathcal{J}}[p] \right\|_{L^2_\rho(\Gamma)}$$

using a sufficiently accurate sparse grid quadrature. The Hermite coefficients of p can be computed either numerically or analytically, see Lemma 4.1 in the next section. Once such quantities are available, we can verify the accuracy of (16), with $B(\mathbf{i})$ as in (20). The results are shown in Figure 2: the proposed estimate is thus seen to be quite reasonable.

Remark 4.1 *As mentioned earlier, the procedure used here to derive an estimate for $B(\mathbf{i})$ could be applied to the problems investigated in [4] as well. It can be seen numerically (see [27]) that estimating $B(\mathbf{i})$ in this way would end up in results not significantly different from the original choice, namely $B(\mathbf{i}) = \prod_{n=1}^{N} \mathbb{L}_n^{m(i_n)}$.*

4.3 Convergence of Hermite expansions

To derive an estimate for $\|p_{\mathbf{q}}\|_{H^1(D)}$ we first consider a simplified Darcy problem with a lognormal permeability field a constant over D, $a = a(\mathbf{y}) = \exp\left(b_0 + \sum_{i=1}^{N} b_i y_i\right)$ and with homogeneous Dirichlet boundary conditions,

$$\begin{cases} -\operatorname{div}\left(a(\mathbf{y})\nabla p(\mathbf{x},\mathbf{y})\right) = f(\mathbf{x}) & \mathbf{x} \in D, \\ p(\mathbf{x},\mathbf{y}) = 0 & \mathbf{x} \in \partial D. \end{cases} \tag{22}$$

Furthermore, let $h(\mathbf{x})$ be the solution of the Poisson problem $-\Delta h = f$ with homogeneous Dirichlet boundary conditions. We can then write the analytic expression for p solving (22), which is separable with respect to $\mathbf{y}$, $p(\mathbf{x},\mathbf{y}) = h(\mathbf{x})e^{-b_0}\prod_{n=1}^{N}\exp\left(-b_n y_n\right)$, and further derive the exact expression of the coefficients of the Hermite expansion.

Lemma 4.1 *Given problem* (22)*, the $H^1(D)$ norm of the Hermite coefficients* (15) *of p can be estimated as*

$$\|p_{\mathbf{q}}\|_{H^1(D)} = C_{\mathcal{H}} \prod_{n=1}^{N} \frac{e^{-g_n q_n}}{\sqrt{q_n!}}\,, \tag{23}$$

with $C_{\mathcal{H}} = \|h\|_{H^1(D)}\, e^{-b_0} \prod_{n=1}^{N} e^{b_n^2/2}$ and $g_n = -\log(b_n)$.

Proof. See [27] for details. □

Our numerical experience shows that estimate (23) is satisfactory even in the more general case where $a(\mathbf{x},\mathbf{y}) = e^{\gamma(\mathbf{x},\mathbf{y})}$, and the boundary conditions are those specified in eq. (3); on the other hand, the more general estimate $\|p_{\mathbf{q}}\|_{H^1(D)} = Ce^{-\sum_n g_n\sqrt{q_n}}$ that applies to analytic (but not entire) functions seems to be too pessimistic in this context.

As pointed out in [4], it is generally better to estimate the rates g_n numerically to get sharper bounds. This is achieved by freezing all the variables y_i but the n^*-th one e.g. at the midpoint of their support, and computing the solution $p_{\mathrm{w}}^{n^*}$ of such reduced problem increasing the sparse grid level w from 1 to i^*. If the quadrature points are accurate enough (i.e. Gaussian quadrature points), then the intermediate solutions $p_{\mathrm{w}}^{n^*}$ will converge to $p_{i^*}^{n^*}$ with the same rate, and the same holds for any quantity of interest $Z_p = Z_p(\mathbf{y})$ depending on p_{w}, that is

$$\left\|p_{\mathrm{w}}^{n^*} - p_{i^*}^{n^*}\right\|_{\otimes} \leq C\,\frac{e^{-g_n m(\mathrm{w})}}{\sqrt{m(\mathrm{w})!}}, \quad \left\|Z_{p,\mathrm{w}}^{n^*} - Z_{p,i^*}^{n^*}\right\|_{L^2_\rho(\Gamma)} \leq C\,\frac{e^{-g_n m(\mathrm{w})}}{\sqrt{m(\mathrm{w})!}}\,. \tag{24}$$

It is then possible to use a least square fitting on the computed errors to derive an estimated value for g_n. Figure 3 in next Section shows the results of such procedure applied to a test case, and confirms the quality of the method proposed. Alternative estimates for the decay of the Hermite coefficients are available in [18].

4.4 A computable expression for $\mathcal{I}(\mathrm{w})$

We are now in position to write a computable expression for the quasi-optimal set (13). Combining together the work contribution (14), the error contribution estimate (16), the estimate (23) for $\left\|p_{m(\mathbf{i}-\mathbf{1})}\right\|_{H^1(D)}$ and the numerical values obtained for $m(i_n)$, $B_n(i_n)$ and g_n, see respectively eq. (17), (21), and (24), we obtain the following expression

$$\mathcal{I}(\mathrm{w}) = \left\{ \mathbf{i} \in \mathbb{N}_+^N : \frac{\displaystyle\prod_{n=1}^{N} B_n(i_n) \frac{e^{-g_n m(i_n-1)}}{\sqrt{m(i_n-1)!}}}{\displaystyle\prod_{n=1}^{N} (m(i_n) - m(i_n-1))} \geq \epsilon(\mathrm{w}) \right\}, \tag{25}$$

with e.g. $\epsilon(\mathrm{w}) = e^{-\mathrm{w}}$. Again, note that (25) may not satisfy the admissibility condition (12), that has to be enforced by adding the missing multiindices.

5 Numerical results

In this section we test on an example the effectiveness of the proposed sparse grid. We consider the case of a stratified material in the direction transversal to the flow: that is, the log-permeability field γ depends only on x_1 and is constant along x_2. Thus the covariance function is

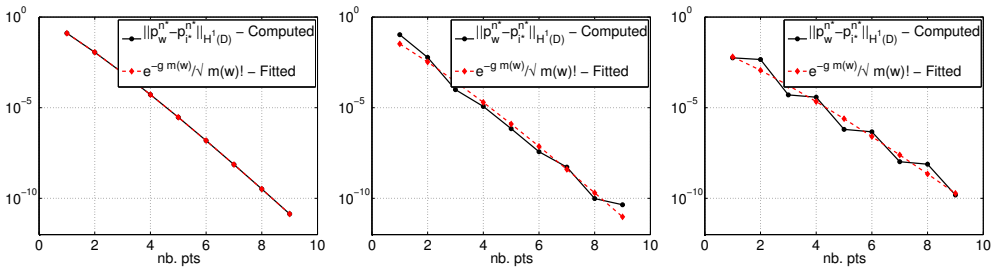
$$C_\gamma(s,t) = \sigma^2 \exp\left(-\frac{|s-t|^2}{L_c^2}\right), \quad s,t \in [0,1],$$

and the truncated Fourier expansion of γ (8) simplifies to

$$\gamma(x_1, \mathbf{y}) = \mathbb{E}\left[\gamma(\mathbf{x}, \cdot)\right] + \sigma\sqrt{c_0} y_0 + \sigma \sum_{k=1}^{K} \sqrt{c_k}\, [\, y_{2k-1} \cos(\omega_k x_1) + y_{2k} \sin(\omega_k x_1)]. \tag{26}$$

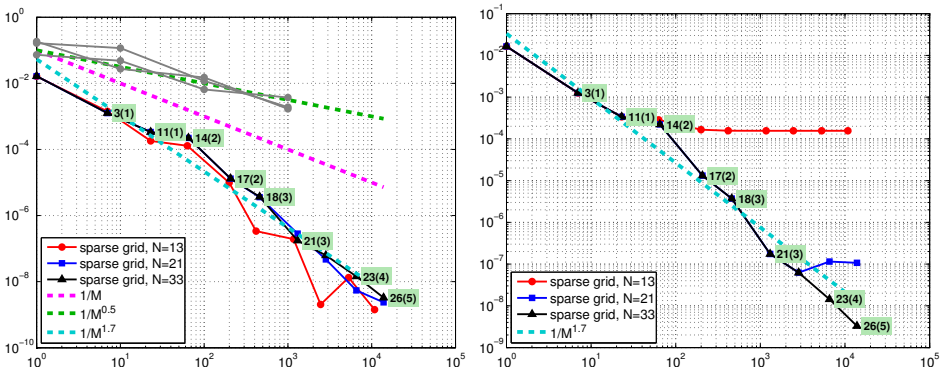
As in Proposition 3.1, we have $y_k \sim \mathcal{N}(0,1)$, $\omega_k = k\pi/L$, $L = 1$, and λ_k as in equation (7). Obviously, in this case it holds $c_k \approx \lambda_k$ rather than $c_{\mathbf{k}} \approx \lambda_{k_1}\lambda_{k_2}$, due to the layer structure of γ. We set the correlation length to $L_c = 0.2$ and the pointwise standard deviation to $\sigma = 0.3$.

We consider three different levels of truncation for γ in (26): $K = 6, 10, 16$ corresponding to $N = 13, 21, 33$ random variables. With these truncation we



(a) y_0, constant, $g = 1.96$. (b) y_2, $\sin(\pi x/L)$, $g = 1.90$. (c) y_5, $\cos(3\pi x/L)$,$g = 1.39$.

Figure 3: Assessment of the rates g_n, $n = 0, 2, 5$, used to build the quasi-optimal set (25), estimated according to equation (24). For each random variable y_n the corresponding harmonic in the Fourier expansion (26) is specified. The plots show the decay of $\left\| Z^{n^*}_{p,\mathrm{w}} - Z^{n^*}_{p,i^*} \right\|_{H^1(D)}$ as a function of the number of point $m(\mathrm{w})$ and its fitting according to the proposed estimate $e^{-g_n m(\mathrm{w})}/\sqrt{m(\mathrm{w})!}$.



(a) Convergence of quasi-optimal sparse grid approximations.

(b) Convergence with respect to the reference solution with $N = 33$ random variables.

Figure 4: Convergence for MC and sparse grid methods.

take into account up to 1%,10^{-2}% and 10^{-9}% respectively of the total variance of γ. For each truncation we compute the quasi-optimal sparse grid approximation $p_{N,\mathrm{w}}$ using the sets (25), and then compute the expected value for the total outgoing flux Z, using the resulting sparse grid quadrature rule. We also perform a classical Monte Carlo simulation, repeated three times. The deterministic problems are solved with $\mathbb{P}1$ finite elements on an unstructured regular mesh with approximately 1400 vertices.

We first fix the number of random variables N and study the convergence of the sparse grid approximation as the number of points in the sparse grid increases. Since we do not have an exact solution, we compute errors with respect to a reference solution, i.e. we measure the error as $\left|\mathbb{E}\left[Z_{p_{N,\mathrm{w}}}\right] - \mathbb{E}\left[Z_{p_{N,\mathrm{w}^*}}\right]\right|$. Results are shown in Figure 4(a). The Monte Carlo simulations converge with the expected rate 1/2; we also show the convergence rate 1 that would be obtained with a quasi-Monte Carlo method, like Sobol' sequences (see e.g. [22]). As for the sparse grids approximation, it is important to observe that not only they all converge with a rate higher than 1/2, but such rate seems to be independent of the truncation level. This would mean that the strategy detailed in Section 4 is quite effective in reducing the deterioration of the performance of the standard sparse grids as the number of random variables increases. Indeed, the selection of the most profitable hierarchical surpluses manages to "activate" (i.e. to put interpolation points) only in those directions that are most useful in explaining the total variance of the solution, so that the less influent random variables get activated only for small approximation errors. Beside the number of "active" variables, another interesting indicator is the number of "interacting" variables in the sparse grid. As was previously mentioned, a sparse grid is indeed a linear combinations of a number of "small" tensor grids, that put interpolation points only in some of the directions $y_1, \ldots, y_N$ at a time, say $\bar{n}$ directions out of N. We call the largest $\bar{n}$ in a sparse grid the number of interacting variables, that could be much lower than the number of active ones. This approach could also be seen as an "anisotropic ANOVA" analysis. In Figure 4(a) for each sparse grid we show the number of active variables followed by the number of interacting variables in parenthesis. For instance, the sparse grid labeled 18(3) places collocation points in 18 variables, but each tensor grid covers 3 dimensions at most.

We then repeat the analysis by computing the error for all the three approximation corresponding to $N = 13, 21, 33$ with respect to the same reference solution, i.e. p_{33,w^*}. Results are shown in 4(b): as expected, the convergence of the solutions with $N = 13$ and 21 stagnates when the error due to the truncation of the random field becomes predominant. However, the convergence rate up to the stagnation is again independent of the number of random variables.

6 Conclusions

In this work we have considered a Darcy problem with uncertain permeability, modeled as a lognormal random field with Gaussian covariance function, and we have applied the quasi-optimal sparse grid paradigm derived in [4] to the problem at hand. To this end, we have introduced a nested quadrature/interpolation rule and we have estimated the proportionality constant $B(\mathbf{i})$ between error contribution of the sparse grids and the coefficients of the Hermite expansion of the solution, for which we have derived an estimate as well.

We have applied our quasi-optimal sparse grid thus obtained to a test case describing a layered material, that has been discretized with a Fourier expansion with $N = 13, 21$ and 33 random variables. Numerical results on this preliminary test seem to suggest that the quasi-optimal sparse grid procedure achieves a convergence rate higher than the ones of the most common sampling methods. Moreover, it is quite effective in reducing considerably the degradation of the performance suffered by the standard sparse grids approach when the number of input random variables increases.

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