A multi level Monte Carlo method with control variate for elliptic PDEs with log-normal coefficients

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Abstract

We consider the numerical approximation of the stochastic Darcy problem with log-normal permeability field and propose a novel Multi Level Monte Carlo approach with a control variate variance reduction technique on each level. We model the log-permeability as a stationary Gaussian random field with a covariance function belonging to the so called Matérn family, which includes both fields with very limited and very high spatial regularity. The control variate is obtained starting from the solution of an auxiliary problem with smoothed permeability coefficient and its expected value is effectively computed with a Stochastic Collocation method on the finest level in which the control variate is applied. We analyze the variance reduction induced by the control variate, and the total mean square error of the new estimator. To conclude we present some numerical examples and a comparison with the standard Multi Level Monte Carlo method, which shows the effectiveness of the proposed method.

Key Words: Log-normal random-fields, Multi Level Monte Carlo, Control Variate, Stochastic Collocation, Matérn covariance, Stochastic Darcy Problem

AMS subject classification: 60H35, 65C05, 65N30, 65N15, 35R60

1 Introduction

We consider the numerical approximation of an elliptic Partial Differential Equation (PDE) with random diffusion coefficients, modeled as a random field with limited spatial regularity. This problem arises e.g. in the study of groundwater flows, and has a great importance in hydrology: in this context the diffusion coefficient is given by the permeability of the subsoil and it is often modeled as a lognormal random field.

Several models for its covariance function have been proposed in literature, which lead to realizations having different spatial smoothness. We consider in this work covariance functions belonging to the so called Matérn family [21] which includes models having a whole range of possible regularity. Among these, a widely used covariance model belonging to this family is the exponential one which has realizations that are only Hölder continuous with exponent smaller than $\frac{1}{2}$, hence not even differentiable and featuring the same roughness as a Brownian motion. On the other extreme, the Matérn family also includes the “double exponential” (or Gaussian) covariance, which has infinitely differentiable realizations.

In the case of smooth random fields, great attention has been devoted in the last decades to methods employing polynomial chaos expansions of the solution, either in their Galerkin or Collocation versions (see e.g. [1, 2, 4, 10, 12, 13, 14]). The first step in setting up these methods
consists in expanding the input random field in series; one could use, for instance, a Karhunen-Loève or Fourier expansion. By this way, the random field is parametrized by a countable sequence of (hopefully independent) random variables. In practice, the series expansion will have to be truncated to high accuracy, so as to work only with a finite number of random variables, and a global multivariate polynomial approximation of the solution to each one of the retained random variables is sought. This approach has been shown to be very effective in the case of smooth highly correlated random fields, when only a moderate number of random variables can be retained in the expansion [3, 11]. On the other hand, the performance strongly degrades in the case of rough random fields and/or fields with a short correlation length which require a very large number of random variables to obtain accurate solutions. In such cases, a polynomial chaos approach may not be competitive with other sampling methods such as Monte Carlo or Quasi Monte Carlo.

A more traditional approach, better suited to treat the rough case, is offered by Monte Carlo type methods [5, 8, 17], which, however, feature a very slow convergence rate. Their computational cost is often unaffordable since, to obtain an accurate solution, many PDE solves will be needed, each one requiring a very fine mesh due to the roughness of the coefficient. Multi Level Monte Carlo methods (MLMC) have been recently proposed in literature (see e.g. [6, 13, 16]) in order to reduce the variance of the Monte Carlo estimator, and consequently reduce the number of solves on the fine grid.

The goal of this work is to combine the power of polynomial chaos methods in treating the smooth coefficient case, with the robustness of the MLMC approach in treating the rough coefficient case. This will be done in the framework or a control variate technique. The control variate is obtained as the solution of the PDE with a regularized version of the lognormal random field as input random datum and its mean can be successfully computed with a Stochastic Collocation method, using for instance the quasi optimal sparse grid procedure illustrated in [3]. The solution of this regularized problem being highly positively correlated with the solution of the original problem, allows us to achieve substantial variance reduction.

In our Multi Level Monte Carlo method with Control Variate (MLCV) the choice of a suitable regularized version of the input random field is crucial: a highly smoothed problem will be easily approximated by Stochastic Collocation but might fail to achieve good variance reduction. On the other hand, a poorly smoothed problem will provide substantial variance reduction in MLMC but will not be effectively approximated by Stochastic Collocation. In this work we regularize the log-permeability field by convolution with a Gaussian kernel with properly tuned variance.

We analyze the mean square error of the estimator and the overall complexity of the algorithm. We also propose possible choices of the regularization parameter and of the number of samples per grid so as to equilibrate the space discretization error, the statistical error and the error in the computation of the expected value of the control variate by Stochastic Collocation.

The outline of the paper is the following: after introducing some notation in Section 2, in Section 3 we present the problem setting and we recall the most important results concerning the well posedness of the continuous problem and its finite elements approximation. In Section 4 we recall the standard Multi Level Monte Carlo method and its associated mean square error. Section 5 is the core of the paper. Here, we introduce the new MLMC method with control variate (MLCV) and present a complete analysis of the statistical error associated to the MLCV estimator. We also present the practical algorithm we have used to calibrate the parameters appearing in the MLCV method and to optimize the number of samples per level as well as the size of the sparse grid to use in the Stochastic Collocation to achieve a given tolerance; the main result is given in Theorem 5.1; for easiness of exposition the most technical proofs have been confined to several appendices to the paper. In Section 6 we present some numerical results and a comparison with the standard MLMC method. Finally, we draw some conclusions in Section 7.

2 Notation

Given a bounded Lipschitz domain $D \in \mathbb{R}^d$, we introduce the following notation. For any $k \in \mathbb{N}$ we denote with $C^k(D)$ the space of continuously $k$ times differentiable functions with the usual
norms. For any positive real $\alpha$ we set $\alpha = k + s$ with $k \in \mathbb{N}$ and $s \in (0, 1]$ and we indicate $C^\alpha$ the Hölder space for which the following norm is bounded

$$
\|v\|_{C^\alpha(\Omega)} = \|v\|_{C^k(\Omega)} + \|v\|_{C^\alpha(\Omega)} = \sum_{j=1}^{k} \max_{|i|=j} |D^i v|^\alpha_{C^0(D)} + \max_{|i|=k} \sup_{x,y \in D} \frac{|D^i v(x) - D^i v(y)|}{|x-y|^s},
$$

where $i$ is a multi-index of $\mathbb{N}^d$ with $|i| = \sum_{k=1}^{d} i_k$, $D^i v = \frac{\partial^{i_1}}{\partial x_1^{i_1}} \cdots \frac{\partial^{i_d}}{\partial x_d^{i_d}} v$ and $|\cdot|$ denotes the euclidean norm in $\mathbb{R}^d$. Notice that with this definition, the space $C^1$ denotes the space of Lipschitz continuous functions and not the usual space $C^1$ of continuously differentiable functions. We will also use the usual Sobolev spaces $H^k(D)$, $k \in \mathbb{N}$, characterized by corresponding norm and seminorm

$$
|v|_{H^k(D)}^2 = \int_D \sum_{|i|=k} |D^i v(x)|^2 \, dx,
$$

as well as the fractional Sobolev spaces $H^\alpha(D)$, $\alpha \in \mathbb{R}$, using the Sobolev-Slobodetskii seminorm $|v|_{H^\alpha(D)}$:

$$
|v|_{H^\alpha(D)}^2 = |v|_{H^0(D)}^2 + |v|_{H^{-\alpha}(D)}^2 = \|v\|_{H^k(D)}^2 + \sum_{|i|=k} \int_{D \times D} \frac{|D^i v(x) - D^i v(y)|^2}{|x-y|^{2s}} \, dx dy.
$$

In the following, whenever possible, instead of the usual $H^1(D)$ norm, we will use the equivalent $H^1_0(D)$ norm, defined as

$$
\|v\|_{H^1_0(D)} = \int_D |\nabla v|^2 \, dx.
$$

Given a Banach space $B$ and a complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$, it is also useful to introduce the Bochner space $L^2_B(\Omega, B)$ as the Banach valued space of $q$-integrable functions equipped with the norm $\|v\|_{L^2_B(\Omega, B)} = \mathbb{E}[\|v\|_{B}^2]^{\frac{1}{2}}$, where $\mathbb{E}$ denotes the expectation operator $\mathbb{E}[v] = \int_{\Omega} v \, d\mathbb{P}$.

Finally, to simplify the notation, sometimes we will use the symbol $\lesssim$ to indicate a bound in which the hidden constant is just a positive real number that does not depend on anything (mesh size $h$, regularity of the random field $a$, etc.).

### 3 Problem setting

In this work we consider the groundwater flow problem in a highly heterogeneous saturated porous medium which is well described by the Darcy law relating the velocity field to the pressure gradient, together with a mass balance equation:

$$
\begin{cases}
\mathbf{u} = -a \nabla p & \text{in } D,
\div(\mathbf{u}) = f & \text{in } D,
p = g_j & \text{on } \Gamma_j^D, \ j = 1, \ldots, m_D,
\mathbf{u} \cdot \mathbf{n} = 0 & \text{on } \Gamma_j^N, \ j = 1, \ldots, m_N,
\end{cases}
$$

where $\Gamma_D = \bigcup_{j=1}^{m_D} \Gamma_j^D$ denotes the Dirichlet boundary, $\Gamma_N = \bigcup_{j=1}^{m_N} \Gamma_j^N$ denotes the Neumann boundary and $\bigcup D \cup \bigcup N = \partial D$, $\bigcap D \cap \bigcap N = \emptyset$. Here $p$ is the pressure, $\mathbf{u}$ the velocity field and $a = \frac{k}{\mu}$ represents the intrinsic permeability, i.e., the ratio between the permeability of the medium $k$ and the dynamic viscosity $\mu$; $f$ is an external source or sink term and $D \in \mathbb{R}^d$ a bounded open domain. In the following, since the dynamic viscosity $\mu$ is assumed to be constant, we will refer to $a$ as a permeability. A key issue in the study of groundwater flows in heterogeneous media concerns the characterization of the subsurfaces proprieties. In many cases we have only a very limited
knowledge of the input data of the problem and particularly the permeability field. In order to deal with this uncertainty the permeability is often modeled as a spatially correlated random field depending on a random event \( \omega \) of a suitable probability space \((\Omega, \mathcal{F}, \mathbb{P})\) [21]. Hence also the solution \((p, u)\) of (1) will depend on \( \omega \) and the problem (1) is interpreted in a probabilistic sense as

\[
\begin{align*}
\begin{cases}
  u(x, \omega) &= -a(x, \omega)\nabla p(x, \omega) & \text{in } D, \\
  \text{div}(u(x, \omega)) &= f(x) & \text{in } D, \\
  p(x, \omega) &= g_j(x) & \text{on } \Gamma^D_j, j = 1, \ldots, m_D, \\
  u(x, \omega) \cdot n &= 0 & \text{on } \Gamma^N_j, j = 1, \ldots, m_N,
\end{cases}
\end{align*}
\]

where \( a \) means “almost surely”. A widely used model for the permeability field \( a \) describes it as a lognormal random field [6, 3, 21], namely \( a(x, \omega) = e^{\gamma(x, \omega)} \) with \( \gamma(x, \omega) \) a Gaussian random field having mean \( \mu(x) = \mathbb{E}[\gamma(x, \cdot)] \) and covariance function \( \text{cov}_\omega(x_1, x_2) = \mathbb{E}[\gamma(x_1, \cdot) \gamma(x_2, \cdot)] - \mu(x_1)\mu(x_2) \). The choice of the covariance function is a delicate issue. It directly relates to the spatial smoothness of the random field realizations and strongly influences the choice of the numerical method to use. Equations (2) have been extensively studied during the last few years from both the theoretical and numerical point of view. Denoting \( V_g = \{ v \in H^1(D) : v = g \text{ on } \Gamma_D \} \), the variational formulation associated to problem (2) is: find \( p \in V_g \) such that

\[
b_\omega(p, v) = L(v) \quad \forall v \in V_0, \tag{3}
\]

where the bilinear form \( b_\omega \) (parametrized by \( \omega \)) and the linear functional \( L \) are defined as:

\[
\begin{align*}
b_\omega(u, v) &= \int_D a(x, \omega)\nabla p(x, \omega)\nabla v(x)dx, \\
L(v) &= \int_D f(x)v(x)dx.
\end{align*}
\]

Well posedness results for the problem (3) can be found in [5, 22, 23] where it is shown that the solution \( p \) is unique in the space \( L^2_\omega(\Omega, V_g) \), \( \forall q \in \mathbb{R}_+ \). Moreover, the following regularity result is shown in [5, 6]:

**Lemma 3.1.** Let \( D \) be a convex Lipschitz domain and let \( f \in H^{\alpha-1}(D) \) and \( g = 0 \) on \( \Gamma_D = \partial D \). Let \( a(x, \omega) \) be the input random field of problem (3) and denote \( a_{\min}(\omega) = \min_{x \in D} a(x, \omega) \) and \( a_{\max}(\omega) = \min_{x \in D} a(x, \omega) \). If

\[
\begin{itemize}
  \item \( a_{\min}(\omega) \in L^2_\omega(\Omega), \forall q \in \mathbb{R}_+ \),
  \item \( a(x, \omega) \in L^2_\omega(\Omega, C^\alpha(\overline{D})) \) for some \( 0 < \alpha \leq 1 \) and \( \forall q \in \mathbb{R}_+ \);
\end{itemize}

then for the problem (3) the following regularity result holds:

\[
\|p(\cdot, \omega)\|_{H^{1+\beta}(D)} \lesssim \frac{1}{\alpha - \beta} C_{3, 1}(\omega, \alpha)\|f\|_{H^{\beta-1}(D)}, \quad \forall 0 < \beta < \alpha \quad \text{a.s. in } \Omega.
\]

If the hypothesis hold also for \( \alpha > 1 \) then

\[
\|p(\cdot, \omega)\|_{H^2(D)} \lesssim C_{3, 1}(\omega, \alpha)\|f\|_{L^2(D)}, \quad \text{a.s. in } \Omega,
\]

where

\[
C_{3, 1}(\omega, \alpha) = \begin{cases}
  \frac{a_{\max}(\omega)}{a_{\min}(\omega)} & \text{if } \alpha \leq 1, \\
  \frac{a_{\max}(\omega)}{a_{\min}(\omega)} & \text{if } \alpha > 1.
\end{cases}
\tag{4}
\]

Moreover the constant \( C_{3, 1}(\omega, \alpha) \) is \( q \)-integrable for any \( q \in \mathbb{R}_+ \), i.e. \( C_{3, 1}(\omega, \alpha) \in L^q_\omega(\Omega) \) \( \forall q \in \mathbb{R}_+ \).
where $V$ solves the problem $p$imation $Q$ functional $\mathcal{F}$ to the Matérn family satisfies the hypothesis of Lemma 3.1.

Remark. This result may seem slightly different than the one presented in [6] but actually it is not; in fact in our work we use the $C^\alpha$ norm instead of the usual $C^\alpha$ one: this makes possible to recover a bound for the $H^2$ norm only when $\alpha$ is strictly larger than one. Secondly here we explicitly write the dependence of the constant with respect to the degenerating part which is $O(\frac{1}{c^2})$ when $\beta \to \alpha$.

In what follows we focus on the case in which the log-permeability Gaussian random field $\gamma$ is stationary and has a covariance function belonging to the Matérn family:

$$
\text{cov}_\gamma(x, y) = \tilde{\text{cov}}_\gamma(|x - y|) = \frac{\sigma^2}{\Gamma(\nu) 2^{\nu-1}} \left( \sqrt{2\nu} \frac{|x - y|}{L_c} \right)^\nu K_\nu \left( \sqrt{2\nu} \frac{|x - y|}{L_c} \right), \quad \nu \geq 0.5,
$$

(5)

where $\sigma^2$ is the pointwise variance, $L_c$ is a correlation length, $\Gamma$ is the gamma function, $K_\nu$ is the modified Bessel function of the second kind and $\nu$ is a parameter that governs the regularity of the covariance function and, consequently, of the realizations of the random field. In particular the following holds:

- the covariance function is H"older continuous, namely $\tilde{\text{cov}}_\gamma \in C^{2\nu}(\bar{D} \times \bar{D})$ (see appendix C, Lemma C.1),

- the realizations of the random field are a.s. Hölder continuous, $\gamma(\cdot, \omega) \in C^\alpha(\bar{D})$, $\forall \, 0 < \alpha < \nu$ (see appendix C, Lemma C.2).

Hence for $\nu = 0.5$ the covariance function is only Lipschitz continuous and the field is Hölder continuous $\gamma(\cdot, \omega) \in C^\alpha(\bar{D})$ with $\alpha < 0.5$. On the other hand, for $\nu \to \infty$ the covariance function as well as the field are continuous with all their derivates, namely $\tilde{\text{cov}}_\gamma(\cdot) \in C^\infty(\bar{D} \times \bar{D})$ and $\gamma(\cdot, \omega) \in C^\infty(\bar{D})$ a.s. in $\Omega$. It is important to notice that every log-normal random field $\alpha$ that can be obtained starting from a Gaussian log-permeability $\gamma$ having a covariance function belonging to the Matérn family satisfies the hypothesis of Lemma 3.1.

The goal of the analysis is to compute statistics of some quantities of interest given by a linear functional $Q(p) \in \mathbb{R}$ related to the solution of (2).

In order to numerically solve problem (3) we consider a piecewise linear finite element approximation $p_h$ of $p$ on a regular triangulation $\mathcal{T}_h$ of the domain. The approximate solution $p_h \in V_{h, g}$ solves the problem

$$
b_\omega(p_h, v) = L(v) \quad \forall v \in V_{h, 0},
$$

(6)

where $V_{h, g} = \{ v_h \in C^0(\bar{D}) : v_h|_{\partial K} \in \mathbb{P}_1 \, \forall K \in \mathcal{T}_h \text{ and } v_h = I_h g \text{ on } \Gamma_D \}$, and $I_h g$ is a suitable interpolation of the Dirichlet boundary datum.

Concerning the finite element approximation error of the original problem (2) the following result holds:

Lemma 3.2. Let $D$ be a convex Lipschitz domain and let $a(x, \omega)$ be a log-normal stationary random field with realizations a.s. in $C^\alpha(\bar{D})$, $\Gamma_D = \partial D$, $g = 0$ and $f \in L^2(\bar{D})$. If $\alpha \leq 1$, by using linear finite elements for the spatial discretization, and assuming all integrals are computed exactly in (6), it holds:

$$
\| p(\cdot, \omega) - p_h(\cdot, \omega) \|_{H^1(D)} \lesssim \frac{1}{\alpha - \beta} C_{3, 2}(\omega, \alpha) \| f \|_{L^2(D)} h^\beta, \quad \forall 0 \leq \beta < \alpha \quad \text{a.s. in } \Omega,
$$

where

$$
C_{3, 2}(\omega, \alpha) = \sqrt{\frac{a_{\max}(\omega)}{a_{\min}(\omega)}} C_{3, 1}(\omega, \alpha).
$$
If \( \alpha > 1 \) it holds
\[
\|p(\cdot, \omega) - p_h(\cdot, \omega)\|_{H^1_0(D)} \lesssim C_{3,2}(\omega, \alpha)\|f\|_{L^2(D)} h \quad \text{a.s. in } \Omega.
\]

Moreover the random variable \( C_{3,2}(\omega, \alpha) \) is \( q \)-integrable for any \( q \in \mathbb{R}_+ \), i.e. \( C_{3,2}(\omega, \alpha) \in L^q_\mathbb{P}(\Omega) \) \( \forall q \in \mathbb{R}_+ \).

**Remark.** Since \( C_{3,2}(\omega, \alpha) \in L^q_\mathbb{P}(\Omega) \) \( \forall q \in \mathbb{R}_+ \), we deduce immediately from Lemma 3.2 in the case \( \alpha \leq 1 \) the bound
\[
\|p - p_h\|_{L^q_\mathbb{P}(\Omega; H^1_0(D))} \lesssim \frac{c_{3,2}(\omega, q)}{\alpha - \beta}\|f\|_{L^2(D)} h^\beta, \quad \forall 0 \leq \beta < \alpha,
\]
where \( c_{3,2}(\alpha, q) = \|C_{3,2}(\cdot, \alpha)\|_{L^q_\mathbb{P}(\Omega)} \), and in the case \( \alpha > 1 \) the bound
\[
\|p - p_h\|_{L^q_\mathbb{P}(\Omega; H^1_0(D))} \lesssim c_{3,2}(\alpha, q)\|f\|_{L^2(D)} h.
\]

For the methods proposed in this work we need to expand the input random field in a countable number of independent identically distributed standard normal random variables \( y_n \), namely
\[
\gamma(x, \omega) = \mu(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} y_n(\omega) b_n(x),
\]
where \( \lambda_n \) are coefficients whose decay depends on the smoothness of the covariance function and \( b_n \) are suitably normalized functions in \( D \), which may be for instance Fourier modes or Karhunen-Loève modes, namely the eigenfunctions of the covariance operator \( T_\gamma : L^2(D) \rightarrow L^2(D) \) given by
\[
T_\gamma v(x) = \int_D v(y)\text{cov}_\omega(x, y)dy.
\]
In order to use numerical methods to solve the problem we will consider truncated versions of the random field:
\[
\gamma_N(x, \mathbf{y}(\omega)) = \mu(x) + \sum_{n=1}^{N} \sqrt{\lambda_n} y_n(\omega) b_n(x) \quad \text{where } \mathbf{y} = (y_1, \ldots, y_N),
\]
with \( N \) chosen so that the error due to the truncation (see [7]) of the input random field is sufficiently small compared to the space discretization error induced by the finite element approximation. In the case of a random field with limited regularity, since the decay of the coefficients \( \lambda_n \) in (7) is slow, many terms will have to be included in (8) to have a truncation error sufficiently small. In the following, for simplicity we will write \( \gamma \) instead of \( \gamma_N \) every time we will be dealing with a numerical discretization of equations (2).

## 4 Monte Carlo and Multi Level Monte Carlo Methods

In this section we review briefly the idea of Monte Carlo and Multi Level Monte Carlo sampling: let us denote by \( Q_h(\omega) \) the quantity of interest computed by finite elements on the triangulation \( T_h \) and for the random elementary event \( \omega \in \Omega \). The mean of the quantity of interest can be approximated by generating a sufficiently large random sample of size \( M \). To generate independent realizations of the log-permeability we can use expansion (8), possibly with a very large \( N \). Then the Monte Carlo (MC) estimator \( \hat{Q}_{h,M}^{MC} \) of the mean of \( Q \) associated to a particular spatial mesh of size \( h \) and a sample size \( M \) is defined as:
\[
\hat{Q}_{h,M}^{MC} = \frac{1}{M} \sum_{i=1}^{M} Q_h(\omega_i),
\]
where \( Q_h(\omega_i) \) are independent random variables all distributed as \( Q_h \). The mean square error of this estimator is given by:

\[
e(\hat{Q}_{h,M}^{MC})^2 := E[(\hat{Q}_{h,M}^{MC} - E[Q])^2] = \frac{\text{Var}(Q_h)}{M} + (E[Q_h] - Q)^2.
\]

Hence the error naturally splits in two terms: a statistical error given by the variance of the estimator and a bias term related to the finite element approximation of the PDE and the quantity of interest. The Monte Carlo approach is straightforward to implement, but unfortunately presents a rather slow convergence rate with respect to the sample size \( M \) which makes the computation of accurate solutions very demanding.

Multi Level Monte Carlo methods \([6, 8, 9, 13, 16]\) have been recently proposed and studied in order to reduce the variance of the MC estimator and its overall computational cost needed to meet a given tolerance. The basic idea is to consider a sequence of consecutive meshes of spatial step size \( h_0 > ... > h_l > ... > h_L \) and to use the linearity of the expectation operator to write the mean of the quantity of interest on the finest grid \( h_L \) as a telescopic sum of the mean of the quantity of interest on the coarsest level plus a sum of correcting terms given by the difference on two consecutive levels:

\[
E[Q_{h_L}] = E[Q_{h_0}] + \sum_{l=1}^{L} E[Q_{h_l} - Q_{h_{l-1}}].
\]

Hence, the idea of independently estimating via standard MC estimators the terms on each level, with suitably chosen sample sizes, in order to minimize the overall complexity. Given a sequence \( \{M_l\}_{l=0}^{L} \) of sample sizes to be used on each level, the Multi Level Monte Carlo (MLMC) estimator is given by

\[
\hat{Q}_{\{h_l\},\{M_l\}}^{MLMC} = \sum_{l=0}^{L} \frac{1}{M_l} \sum_{i=1}^{M_l} (Q_{h_l}(\omega_{l,i}) - Q_{h_{l-1}}(\omega_{l,i})), \text{ where } Q_{h_{-1}} = 0;
\]

whose mean square error is:

\[
e(\hat{Q}_{\{h_l\},\{M_l\}}^{MLMC})^2 = E[(\hat{Q}_{\{h_l\},\{M_l\}}^{MLMC} - E[Q])^2] = \sum_{l=0}^{L} \frac{\text{Var}(Q_{h_l} - Q_{h_{l-1}})}{M_l} + (E[Q_{h_L} - Q])^2.
\]

In the construction of the method a key point is the choice of the sample sizes \( M_l \) on each level and the choice of the mesh sizes \( h_l \). Several strategies have been proposed by different authors. Just to mention a few, Giles, Scheichl et al. in their works \([8, 16]\) consider a continuous minimization problem in \( M_0, ..., M_L \) to determine the sample sizes on each level given the mesh hierarchy \( \{h_l\}_{l=0}^{L} \): the finest level of the hierarchy is chosen so that the bias term meets half of the prescribed tolerance. Alternatively Schwab et al. in \([13]\) select the samples sizes to equilibrate all the \( L + 1 \) terms in the right hand side of (10). A global optimization of the MLMC strategy has been investigated in \([18]\) where the authors show that geometric sequences of \( h_l = h_0 \beta^{-l} \), with \( \beta > 1 \), lead to nearly optimal MLMC samples; however, the corresponding meshes are in general not nested. Also, optimal strategies might not split equally the prescribed tolerance into the discretization error and the statistical one.

5 Multi Level Monte Carlo method with Control Variate (MLCV)

As mentioned in the introduction, sparse grid collocation methods are very effective in solving the stochastic Darcy problem (2) in case of smooth input random fields. On the other hand, the Multi Level Monte Carlo method is more effective for problems with rough coefficients. We discuss here how these two strategies can be combined to further improve the performance of the
MLMC method in case of rough coefficients by exploiting the well known control variate variance reduction technique (see e.g. [26]). The idea is to introduce an auxiliary problem having a smoothed coefficient, which can be effectively approximated by a deterministic method as, for instance, a Stochastic Galerkin or a Stochastic Collocation one, and use the quantity of interest, computed from the corresponding solution, as control variate in the Multi Level Monte Carlo sampling.

Let $\gamma(x, \omega)$ and $\gamma^\epsilon(x, \omega)$ be the input random fields obtained respectively by considering a covariance function of the Matérn family and the convolution of $\gamma(x, \omega)$ with a smooth kernel (e.g. Gaussian), namely:

$$
\gamma^\epsilon(\cdot, \omega) = \gamma(\cdot, \omega) * \phi_\epsilon(\cdot) \quad \text{where} \quad \phi_\epsilon(x) = e^{-\frac{|x|^2}{2\epsilon^2}} / (2\pi\epsilon)^{\frac{D}{2}}, \quad (11)
$$

analogously let $a^\epsilon = e^{\gamma^\epsilon}$ and let $p(x, \omega)$ and $p^\epsilon(x, \omega)$ denote the solutions corresponding to the two (highly correlated) input random fields. Let us assume for the moment that we know exactly the

![Figure 1: Three different regularizations of the same realization of $a$. $\nu = 0.5$, $L_c = 0.5$, $\sigma = 1$.](image)

mean of the control variate $Q^\epsilon = Q(p^\epsilon(\cdot, \omega))$ obtained starting from the solution of the auxiliary problem having $a^\epsilon$ as input datum. We define

$$
\tilde{Q}^{CV}(\omega) := Q(\omega) - Q^\epsilon(\omega) + E[Q^\epsilon].
$$

This new variable is such that $E[\tilde{Q}^{CV}] = E[Q]$ and

$$
\text{Var}(\tilde{Q}^{CV}) = \text{Var}(Q) + \text{Var}(Q^\epsilon) - 2\text{cov}(Q, Q^\epsilon),
$$

showing that the more positively correlated the two random fields are the more positively correlated the corresponding quantities of interest are and the larger the variance reduction achievable. In
order to apply this strategy to solve the stochastic Darcy problem we should know the exact 
mean of $Q'(\omega)$. Actually we do not have this information available but, since $a'(x, \omega)$ has smooth 
realizations, we can successfully use a sparse grids Stochastic Collocation method to compute it 
accurately as long as the smoothing parameter $\epsilon$ remains sufficiently large. Denoting by $E^{SC}[Q'(\cdot)]$ 
the sparse grid approximation of the mean of $Q'$, the final variable on which we apply our MLMC 
algorithm is 

$$Q^{CV}(\omega) := Q(\omega) - Q'(\omega) + E^{SC}[Q'].$$ 

In this work we always consider a nested sequence of spatial grids that halves the mesh size at 
each level, $h_l = h_0 2^{-l}$. The mean of $Q^{CV}$ on the finest mesh can be written as a telescopic sum 
following the Multi Level idea: 

$$E[Q_{h_L}^{CV}] = E[Q_{h_0}^{CV}] + \sum_{l=1}^{L} E[Q_{h_l}^{CV} - Q_{h_{l-1}}^{CV}],$$

and the Multi Level Monte Carlo estimator with control variate (MLCV) is then defined as 

$$\hat{Q}^{MLCV}_{\{h_l\},\{M_l\}} = \sum_{l=0}^{L} \frac{1}{M_l} \sum_{i=1}^{M_l} \left(Q_{h_l}^{CV}(\omega_{l,i}) - Q_{h_{l-1}}^{CV}(\omega_{l,i})\right),$$

with $Q_{h_{l-1}}^{CV} = 0$ and $Q_{h_l}^{CV}(\omega_{l,i}) = Q_{h_l}(\omega_{l,i}) - Q_{h_l}'(\omega_{l,i}) + E^{SC}[Q_{h_l}']$. It can be equivalently rewritten as 

$$\hat{Q}^{MLCV}_{\{h_l\},\{M_l\}} = \sum_{l=0}^{L} \frac{1}{M_l} \sum_{i=1}^{M_l} \left(Q_{h_l}(\omega_{l,i}) - Q_{h_{l-1}}(\omega_{l,i}) - (Q_{h_l}'(\omega_{l,i}) - Q_{h_{l-1}}'(\omega_{l,i}))\right) + E^{SC}[\hat{Q}_{h_L}'],$$

where again $Q_{h_{l-1}}, Q_{h_{l-1}}' = 0$. Concerning the mean square error associated to the estimator (13), 
the following result generalizes (10): 

**Lemma 5.1.** The mean square error of the estimator (13) can be bounded as 

$$e(\hat{Q}^{MLCV}_{h_L,M_l})^2 \leq \sum_{l=0}^{L} \frac{\text{Var}(Q_{h_l'} - Q_{h_{l-1}}')}{M_l} + 2 \left(E[Q_{h_L}'] - E^{SC}[Q_{h_L}']\right)^2 + 2E[Q_{h_L} - Q]^2.$$ 

**Proof.** The mean square error associated to this estimator naturally splits into a variance and a 
bias term as 

$$e(\hat{Q}^{MLCV}_{h_L,M_l})^2 = E[(\hat{Q}^{MLCV}_{h_L,M_l} - E[\hat{Q}])^2] = \sum_{l=0}^{L} \frac{\text{Var}(Q_{h_l'} - Q_{h_{l-1}}')}{M_l} + E[Q_{h_L}^{CV} - Q]^2.$$ 

The second term on the right hand side represents the bias and can further be bounded as 

$$E[Q_{h_L}^{CV} - Q] = E[Q_{h_L} - Q_{h_L}'] + E^{SC}[Q_{h_L}'] - Q \leq 2 \left(E[Q_{h_L}'] - E^{SC}[Q_{h_L}']\right)^2 + 2E[Q_{h_L} - Q]^2.$$ 

The first term on the right hand side of (14), represents the variance of the estimator $\hat{Q}^{MLCV}_{h_L,M_l}$, 
and it is expected to be smaller than the variance of the standard MLMC estimator thanks to the 
presence of the control variate. The second term represents the error due to the approximation of 
the mean of the smoothed quantity of interest via sparse grid Stochastic Collocation; the third 
one represents the mean of the finite element error of the unsmoothed quantity of interest. When 
$\epsilon$ goes to 0 the regularized input random field tends to the original one. Consequently the solution 
p tends to the solution p; this means that the variance associated to the estimator tends to 0. On 
the other hand, according to the previous considerations, an accurate approximation of the mean 
of the quantity of interest $E^{SC}[Q_{h_L}']$ by a Stochastic Collocation scheme becomes extremely costly.
and practically unfeasible for rough random fields. The parameter $\epsilon$ should therefore be chosen so as to have a good variance reduction while still keeping a manageable sparse grid approximation problem. The practical way in which we have chosen $\epsilon$ as well as the others parameters (finest level $L$, sparse grid level, sample sizes $\{M_l\}$) in our numerical experiments will be discussed in Section 5.3. How to optimally choose $\epsilon$ is still an open question and under investigation.

5.1 Sparse grid approximation of the mean of the Control Variate

In this section we review the Stochastic Collocation scheme used to compute the mean of the control variate. As mentioned before, the log-permeability field $\gamma^\epsilon$, and hence the pressure $p^\epsilon$, depend on a sequence of random variables $\{y_n\}_{n\in\mathbb{N}}$. First, we consider a truncated Karhunen-Loève expansion of the log-permeability, according to (7), with a possibly arbitrarily large $N$. Once the problem has been parametrized with a finite number $N$ of random variables $\{y_n\}_{n=1,...,N}$, we compute the sparse grid approximation of the pressure $p$ as in [3], namely

$$p_N^{\epsilon,w}(y_1,...,y_N) = \sum_{i\in\mathcal{I}(w)} \bigotimes_{n=1}^{N} \Delta_n^{m(i_n)}[p](y_1,...,y_N),$$

(15)

where $i = (i_1,...,i_N) \in \mathbb{N}^N$ denotes a multi-index, $\mathcal{I}(w)$ an index set and $w$ represents the polynomial level used for the construction of the index set $\mathcal{I}(w)$; $\Delta_n^{m(i_n)} = u_n^{m(i_n)} - u_n^{m(i_n-1)}$ represents the difference between two consecutive interpolants in the variable $y_n$ that use respectively $m(i_n)$ and $m(i_n-1)$ points. In particular we use Kronrod-Patterson-Normal knots (KPN), see [24, 25], which are numerically computed nested quadrature formulas with $m(i_n) = 1, 3, 9, 19, 35$ for $i_n = 1,...,5$ and maximal degree of exactness.

Following the strategy proposed in [3], we include in the index set $\mathcal{I}(w)$ only those indexes with the largest profit, i.e. the ratio between the error contribution associated to the multi-index $i$ and the corresponding work, defined as the number of sparse grid knots associated to the multi-index $i$. If $\{y_j\}_{j=1}^{M_{SC}}$ denotes the collection of points composing the sparse grid and $\{q_j\}_{j=1}^{M_{SC}}$ the corresponding weights in the quadrature formula, the final approximation of the mean of the control variate reads

$$\mathbb{E}^{SC}[Q^\epsilon] = \sum_{j=1}^{M_{SC}} Q(p_N^{\epsilon,w}(y_j))q_j.$$  

(16)

The numerical results presented in [3] (see also [15]) show that the convergence rate of this quasi-optimal sparse grid procedure does not really depend on the number of random variables used in the parametrization of the random field $\gamma^\epsilon$ (i.e. it holds also for $N \to \infty$). Moreover they show numerically an algebraic decay of the error that justifies our use of the error model $M_{SC}^\alpha$ to compute the optimal number of samples $\{M_l\}_{l=0}^\infty$ and $M_{SC}$ in the MLCV algorithm.

5.2 Error analysis of the MLCV method

In this section we study the statistical error of the MLCV estimator and give bounds on the variance terms $\text{Var}(Q_{h^N}^{CV} - Q_{h^{N-1}}^{CV})$ in the case of the Stochastic Darcy Problem (2) with log-normal permeability. This, in particular, implies the study of the discretization error $Q_{h^N}^{CV} - Q_{h^N}^{CV}$ as a function of both the mesh size $h$ and the regularization parameter $\epsilon$. The main result of this section is given in Theorem 5.1. Before proceeding with the analysis, we define the random variables

$$a^\epsilon_{\text{max}}(x,\omega) = \max_{x\in\overline{D}} a^\epsilon(x,\omega), \quad a^\epsilon_{\text{min}}(x,\omega) = \min_{x\in\overline{D}} a^\epsilon(x,\omega).$$

and restrict ourself, in this section, to the case of a fully homogeneous Dirichlet problem ($\Gamma_D = \partial D$, $g = 0$) defined on a convex bounded domain $D$. Moreover, we assume that the Gaussian random field $\gamma$ is defined in $\mathbb{R}^d$ and for technical reasons, we consider the following smoothed version $\gamma^\epsilon$, slightly different from the one given in (11). Let $D_\eta = \{x \in \mathbb{R}^d \text{ s.t. } \text{dist}(x,\overline{D}) \leq \eta\}$ and consider
a function $\varphi \in C^\infty(\mathbb{R}^d)$, $0 \leq \varphi \leq 1$, $\varphi = 1$ on $D_{n\epsilon}$ and $\varphi = 0$ on $D_1^c$ for some $n \in \mathbb{N}$ such that $n\epsilon < 1$. Then, we define the smoothed field $\gamma^\epsilon$ as

$$
\gamma^\epsilon(x) = (\tilde{\gamma} \ast \phi_\epsilon)(x), \quad \text{where } \tilde{\gamma}(x) = \varphi(x)\gamma(x) \quad \text{and} \quad \phi_\epsilon(x) = \frac{e^{-|x|^2}}{(2\pi \epsilon^2)^{d/2}}. \tag{17}
$$

Essentially, $D_{n\epsilon}$ represents the domain upon which the convolution integral involved in the definition (17) is computed up to an error that can be made arbitrarily small by increasing $n$. By taking $n > 3$ we will have $\gamma^\epsilon = \tilde{\gamma} \ast \phi_\epsilon \approx \gamma \ast \phi_\epsilon$ in $D$ up to a very small error. On the other hand, $\tilde{\gamma}$ has a compact support so that the quantities $\tilde{\gamma}_{\max}(\omega) = \max_{x \in \mathcal{D}} \tilde{\gamma}(x, \omega)$, $\tilde{\gamma}_{\min}(\omega) = \min_{x \in \mathcal{D}} \tilde{\gamma}(x, \omega)$, $\|\tilde{\gamma}(\cdot, \omega)\|_{C^0(\mathbb{R}^d)}$ are all $L^p_\varphi(\Omega)$ functions, $\forall q \in \mathbb{R}_+$ and can be bounded by the corresponding quantities on $\gamma$ evaluated in the extended domain $\overline{D}_1$. In particular, we have that $|\tilde{\gamma}|_{C^0(\mathbb{R}^d)} \leq \|\varphi\|_{C^0(\mathbb{R}^d)} \|\gamma\|_{C^0(\overline{D}_1)}$. We start with the following observation.

**Lemma 5.2.** Let $\gamma(x, \omega)$ be a Gaussian random field with realizations a.s. in $C^0(\overline{D}_1)$ and $\gamma^\epsilon(x, \omega)$ a smoothed version of $\gamma(x, \omega)$ as introduced in (17). Moreover set $a = e^\gamma$ and $a^\epsilon = e^{\gamma^\epsilon}$. For all $0 \leq \beta \leq \min(\alpha, 1)$ it holds:

$$
\|a(\cdot, \omega) - a^\epsilon(\cdot, \omega)\|_{C^0(\overline{D}_1)} \lesssim C_{5.2}(\omega, \alpha)e^{\min(\alpha-\beta, 2)}, \quad \text{a.s. in } \Omega,
$$

where

$$
C_{5.2}(\omega, \alpha) = a_{\max}(\omega) \left[1 + e^{(\gamma^\epsilon-\gamma)(\cdot, \omega)}\right]_{C^0(\overline{D}_1)} \left(1 + |\gamma(\cdot, \omega)|_{C^0(\alpha+1)(\overline{D}_1)}\right) \|\gamma(\cdot, \omega)\|_{C^0(\alpha+0.3)(\overline{D}_1)} \|\hat{\varphi}(\cdot, \omega)\|_{C^0(\alpha+0.3)(\overline{D}_1)}.
$$

Moreover, if $\alpha > 1$, it holds also the following bound for the standard $C^1$ norm

$$
\|a(\cdot, \omega) - a^\epsilon(\cdot, \omega)\|_{C^1(\overline{D}_1)} \lesssim \hat{C}_{5.2}(\omega, \alpha)e^{\min(\alpha-1, 2)}, \quad \text{a.s. in } \Omega,
$$

where

$$
\hat{C}_{5.2}(\omega, \alpha) = a_{\max}(\omega) \left[1 + e^{(\gamma^\epsilon-\gamma)(\cdot, \omega)}\right]_{C^0(\overline{D}_1)} \left(1 + |\gamma(\cdot, \omega)|_{C^1(\overline{D}_1)}\right) \|\gamma(\cdot, \omega)\|_{C^0(\alpha+0.3)(\overline{D}_1)} \|\hat{\varphi}(\cdot, \omega)\|_{C^0(\alpha+0.3)(\overline{D}_1)}.
$$

The constants $C_{5.2}(\omega, \alpha)$ and $\hat{C}_{5.2}(\omega, \alpha)$ are both $L^p_\varphi$ integrable $\forall q \in \mathbb{R}_+$.

**Proof.** See appendix A. 

Next we use this result to estimate how the distance between the solution of the original problem (3) and that of the auxiliary one with smoothed coefficient $a^\epsilon$ in a given Sobolev norm, namely $\|p-p^\epsilon\|_{H^{1+\beta}(D)}$, depends on the regularization parameter $\epsilon$. The following result holds:

**Lemma 5.3.** Let $a(x, \omega)$ and $a^\epsilon(x, \omega)$ be as in Lemma 5.2 and $f \in L^2(D)$. A.s. in $\Omega$ it holds:

$$
\|p(\cdot, \omega) - p^\epsilon(\cdot, \omega)\|_{H^{1+\beta}(D)} \lesssim \hat{C}_{5.2}(\omega, \alpha) \|f\|_{L^2(D)}e^{\min(\alpha, 2)},
$$

$$
\|p(\cdot, \omega) - p^\epsilon(\cdot, \omega)\|_{H^{1+\beta}(D)} \lesssim \frac{C_{5.2}(\omega, \alpha)}{\alpha_{\min}(\omega)\alpha_{\min}(\omega)} \|f\|_{L^2(D)} \inf_{0 \leq \beta < \min(\alpha, 1), 0 < \eta < \alpha} \min(\alpha-\beta-\eta, 2).
$$

where

$$
\hat{C}_{5.2}(\omega, \alpha) = \frac{C_{5.2}(\omega, \alpha)}{\alpha_{\min}(\omega)\alpha_{\min}(\omega)},
$$

$$
C_{5.2}(\omega, \alpha) = \begin{cases} 
C_{5.2}(\omega, \alpha)C_{3.1}(\omega, \alpha)C_{3.1}(\omega, \alpha) & \alpha \leq 1, \\
\hat{C}_{5.2}(\omega, \alpha)C_{3.1}(\omega, \alpha)C_{3.1}(\omega, \alpha) & \alpha > 1.
\end{cases}
$$
and \( C_3^* (\omega, \alpha) \) as in (4) with \( a \) replaced by \( a^\epsilon \). If the assumptions hold also for \( \alpha > 1 \) then it is also valid the bound
\[
\| p(\cdot, \omega) - p^\epsilon(\cdot, \omega) \|_{H^2(D)} \lesssim C_{5,3}(\omega, \alpha) \| f \|_{L^2(D)} \epsilon^{\min(\alpha - 1, 2)},
\]

Moreover, the constants \( \tilde{C}_{2,3}(\omega, \alpha) \) and \( C_{5,3}(\omega, \alpha) \) are \( L^q \) integrable \( \forall q \in \mathbb{R}_+ \).

**Proof.** We start by noticing that the original problem (2) satisfies the bound
\[
\| p \|_{H^3_0(D)} \leq \frac{\| f \|_{L^2(D)}}{a_{\min}}.
\]

By considering the difference between the original and the regularized problem we get:
\[
\int_D a^\epsilon \nabla (p - p^\epsilon) \nabla v dx = - \int_D (a - a^\epsilon) \nabla p \nabla v dx;
\]
then, in order to prove the first bound, by choosing \( v = p - p^\epsilon \) in (18), we directly get
\[
\| p - p^\epsilon \|_{H^3_0(D)} \leq \| a - a^\epsilon \|_{C^0(D)} \frac{\| p \|_{H^3_0(D)}}{a_{\min}},
\]
which, from Lemma 5.2 and the above bound on \( \| p \|_{H^3_0(D)} \), implies the desired result. In order to complete the proof we will use the result in Lemma B.1 in Appendix B that states that, \( \forall b \in C^\alpha(D) \), and \( \forall v \in H^\beta(D) \) for some \( 0 < \beta < \min(\alpha, 1) \), the following bound holds
\[
\| bv \|_{H^\beta(D)} \lesssim \frac{1}{\sqrt{\eta}} \| b \|_{C^{\beta+1}} \| v \|_{H^\beta(D)} \quad \forall \eta \leq \alpha - \beta.
\]
By integrating by parts (18) we obtain
\[
\int_D a^\epsilon \nabla (p - p^\epsilon) \nabla v dx = \int_D \text{div} ((a - a^\epsilon) \nabla p) v dx = \int_D \tilde{f} v dx.
\]
In order to use the result given in Lemma 3.1 we need to ensure that \( \tilde{f} \) is in \( H^{\beta - 1} \). Indeed
\[
\| \text{div} ((a - a^\epsilon) \nabla p) \|_{H^{\beta - 1}(D)} \lesssim \| (a - a^\epsilon) \nabla p \|_{H^\beta(D)}
\]
\[
\lesssim \frac{1}{\sqrt{\eta}} \| a - a^\epsilon \|_{C^{\beta+1}} \| p \|_{H^{\beta+1}(D)} \quad \forall \eta \leq \alpha - \beta.
\]
Hence for the difference \( p - p^\epsilon \) the following estimate holds
\[
\| p - p^\epsilon \|_{H^{\beta+1}(D)} \lesssim \frac{a_{\max}(\omega) \| a^\epsilon(\cdot, \omega) \|_{C^\beta(D)} \| \tilde{f}(\cdot, \omega) \|_{H^{\beta - 1}(D)}}{\alpha - \beta}
\]
\[
\lesssim \frac{1}{(\alpha - \beta)^2} \sqrt{\eta} a_{\max}(\omega) a_{\max}(\omega) \| a(\cdot, \omega) \|_{C^\infty(D)} C_{5,2}(\omega, \alpha) \| p \|_{H^{\beta+1}(D)} \epsilon^{\min(\alpha - \beta - \eta, 2)}
\]
\[
\lesssim \frac{a_{\max}(\omega) a^\epsilon(\cdot, \omega) a_{\max}(\omega) a(\cdot, \omega) \| a(\cdot, \omega) \|_{C^\infty(D)} C_{5,2}(\omega, \alpha) \| f \|_{H^{\beta - 1}(D)} \epsilon^{\min(\alpha - \beta - \eta, 2)}}{(\alpha - \beta)^2}.
\]
In the case \( \alpha > 1 \) we use again the result given in Lemma 3.1
\[
\| p(\cdot, \omega) \|_{H^2(D)} \lesssim \frac{a_{\max}(\omega) \| a(\cdot, \omega) \|_{C^1(D)} \| f(\cdot, \omega) \|_{L^2(D)}}{a_{\min}(\omega)^3}.
\]
analogously we need to ensure that \( \tilde{f} \) is in \( L^2(D) \). Indeed
\[
\| \text{div} ((a - a') \nabla p) \|_{L^2(D)} \leq \| \nabla (a - a') \cdot \nabla p \|_{L^2(D)} + \| (a - a') \\text{div} (\nabla p) \|_{L^2(D)} \\
\lesssim \| \nabla (a - a') \|_{C^0(\Omega)} \| \nabla p \|_{L^2(D)} + \| a - a' \|_{C^0(\Omega)} \| \nabla p \|_{L^2(D)} \lesssim \| a - a' \|_{C^1(\Omega)} \| p \|_{H^2}.
\]
Therefore it holds
\[
\| p - p' \|_{H^2(D)} \lesssim \frac{a_{\text{max}}(\omega) \| a' \|_{C^1(\Omega)}}{(a_{\text{min}})^{\beta}(\omega)} \frac{a_{\text{max}}(\omega) \| a' \|_{C^1(\Omega)}}{(a_{\text{min}})^{\beta}(\omega)} \tilde{C}_{5,2}(\omega, \alpha) \| f \|_{L^2(D)} \epsilon^{\min(\alpha - 1, 2)}.
\]

We finally investigate how the \( H^{1+\beta} \)-norm of the “double difference” \( p - p_h - (p' - p_h') \) depends on both the mesh parameter \( h \) and the regularization parameter \( \epsilon \).

**Lemma 5.4.** Let \( a(x, \omega) \) and \( a'(x, \omega) \) be as in Lemma 5.2 and \( f \in L^2(D) \). By using linear finite elements for the spatial discretization, a.s. in \( \Omega \) it holds:
\[
\| p(\cdot, \omega) - p_h(\cdot, \omega) - (p'(\cdot, \omega) - p_h'(\cdot, \omega)) \|_{H^1(D)} \lesssim C_{5,4}(\omega, \alpha) \| f \|_{L^2(D)} \inf_{0 \leq \beta \leq 1 \atop 0 < \eta + \beta \leq \alpha} \frac{h^{\beta \min(\alpha - \eta, 2)}}{\alpha^{-2} \sqrt{\eta}}
\]
where
\[
C_{5,4}(\omega, \alpha) = \begin{cases} 
\frac{1}{a_{\text{min}}} (C_{5,2}(\omega, \alpha) C_{3,2}(\omega, \alpha) + (a_{\text{min}} + a_{\text{max}})^2 C_{5,3}(\omega, \alpha)) & \alpha \leq 1, \\
\frac{1}{a_{\text{min}}} (C_{5,2}(\omega, \alpha) C_{3,2}(\omega, \alpha) + (a_{\text{min}} + a_{\text{max}})^2 C_{5,3}(\omega, \alpha)) & \alpha > 1.
\end{cases}
\]

If the assumptions hold also for \( \alpha > 1 \) then the following bound holds as well
\[
\| p(\cdot, \omega) - p_h(\cdot, \omega) - (p'(\cdot, \omega) - p_h'(\cdot, \omega)) \|_{H^1(D)} \lesssim C_{5,4}(\omega, \alpha) \| f \|_{L^2(D)} h^{\min(\alpha - 1, 2)}.
\]

**Proof.** Let us consider the difference between the original problem and the auxiliary one in the continuous and in the discretized case:
\[
\int_D a' \nabla (p - p') \nabla v dx = - \int_D (a - a') \nabla p \nabla v dx \quad \forall v \in H^1_0(D);
\]
\[
\int_D a' \nabla (p_h - p_h') \nabla v dx = - \int_D (a - a') \nabla p_h \nabla v dx \quad \forall v \in V_h,0
\]
By taking the difference between these two equations we get
\[
\int_D a' \nabla (p - p' - p_h + p_h') \nabla v dx = - \int_D (a - a') \nabla (p - p_h) \nabla v dx \quad \forall v \in V_h,0;
\]
by using this equality, \( \forall v_h \in V_{h,0} \), we can bound the term \( \| p_h^\epsilon - p_h - v_h \|_{H^1_0(D)} \) as
\[
\| p_h^\epsilon - p_h - v_h \|_{H^1_0(D)}^2 \leq \frac{1}{a_{\text{min}}^2} \int_D a' \nabla (p_h^\epsilon - p_h - v_h \pm (p^\epsilon - p)) \nabla (p_h^\epsilon - p_h - v_h) dx \\
= \frac{1}{a_{\text{min}}^2} \left( \int_D a' \nabla (p_h^\epsilon - p_h - (p^\epsilon - p)) \nabla (p_h^\epsilon - p_h - v_h) dx + \int_D a' \nabla (p^\epsilon - p - v_h) \nabla (p_h^\epsilon - p_h - v_h) dx \right) \\
\leq \frac{1}{a_{\text{min}}^2} \left( \int_D (a - a') \nabla \nabla (p_h^\epsilon - p_h - v_h) dx + \int_D a' \nabla (p^\epsilon - p - v_h) \nabla (p_h^\epsilon - p_h - v_h) dx \right) \\
\leq \frac{1}{a_{\text{min}}^2} \left( \| a - a' \|_{L^\infty(D)} \| p - p_h \|_{H^1_0(D)} + a_{\text{max}}^2 \| p - p' + v_h \|_{H^1_0(D)} \right) \| p_h^\epsilon - p_h - v_h \|_{H^1_0(D)};
\]
so we finally get
\[
\| p_h^\epsilon - p_h - v_h \|_{H^1_0(D)} \leq \frac{\| a - a' \|_{L^\infty(D)}}{a_{\text{min}}^2} \| p - p_h \|_{H^1_0(D)} + \frac{a_{\text{max}}}{a_{\text{min}}} \| p^\epsilon - p - v_h \|_{H^1_0(D)};
\]
using now the triangular inequality
\[\|p^r - p - (p_h^r - p_h)\|_{H^1_r(D)} \leq \|p_h^r - p_h - v_h\|_{H^1_r(D)} + \|p^r - p - v_h\|_{H^1_r(D)} \quad \forall v_h \in V_h,\]
and the arbitrariness of \(v_h\), for any \(0 \leq \beta < \min(\alpha, 1)\), \(0 < \eta + \beta \leq \alpha\), we obtain
\[\|p^r - p - (p_h^r - p_h)\|_{H^1_r(D)} \leq \frac{|a - a'|_{L^\infty(D)}}{a'_{\min}} \|p - p_h\|_{H^1_r(D)} + \left(1 + \frac{a'_{\max}}{a'_{\min}}\right) \inf_{v_h \in V_h} \|p^r - p - v_h\|_{H^1_r(D)} \leq \frac{\|f\|_{L^2(D)}}{(\alpha - \beta)a'_{\min}} C_{5.2}(\omega, \alpha)C_{3.2}(\omega, \alpha)\epsilon a' \beta + \|f\|_{L^2(D)} \left(1 + \frac{a'_{\max}}{a'_{\min}}\right) C_{5.3}(\omega, \alpha) h^{\beta \epsilon_{\min}(\alpha - \beta - \eta, 2)} \left(\frac{1}{(\alpha - \beta)^2 \sqrt{\eta}}\right), \]
\[= C_{5.4}(\omega, \alpha)\|f\|_{L^2(D)} \frac{h^{\beta \epsilon_{\min}(\alpha - \beta - \eta, 2)}}{(\alpha - \beta)^2 \sqrt{\eta}}.\]

By taking the infimum we get the desired result. If the assumptions hold also for \(\alpha > 1\) then it can be analogously shown that
\[\|p(\cdot, \omega) - p_h(\cdot, \omega) - (p^r(\cdot, \omega) - p_h^r(\cdot, \omega))\|_{H^1_r(D)} \lesssim C_{5.4}(\omega, \alpha)\|f\|_{L^2(D)} h^{\epsilon_{\min}(\alpha - 1, 2)}\]

The next theorem extends the previous result to a linear quantity of interest.

**Theorem 5.1.** Let \(a(x, \omega)\) and \(a'(x, \omega)\) be as in Lemma 5.2, \(f \in L^2(D)\) and let \(Q(\cdot)\) be a functional on \(H^{1-r}(D)\), i.e. \(Q \in H^{r-1}(D)\) with \(r = \min(\alpha, 1)\), representing our QoI. Then, by using linear finite elements for the spatial discretization, a.s. in \(\Omega\) it holds:
\[|Q(p - p_h)(\omega) - Q(p^r - p_h^r)(\omega)| \lesssim C_{5.1}(\omega, \alpha)\|f\|_{L^2(D)}\|Q\|_{H^{r-1}(D)} \inf_{0 \leq t < r} \frac{h^t}{\epsilon_{\alpha - t}} \inf_{0 \leq \beta < r} \frac{h^{\beta \epsilon_{\min}(\alpha - \beta - \eta)}}{(\alpha - \beta)^2 \sqrt{\eta}}\]
where
\[C_{5.1}(\omega, \alpha, \beta) = \begin{cases} C_{3.2}(\omega, \alpha)C_{5.2}(\omega, \alpha) + 2a'_{\max}(\omega)C_{5.4}(\omega, \alpha) & \alpha \leq 1, \\ C_{3.2}(\omega, \alpha) \left(C_{5.2}(\omega, \alpha) + 2a'_{\max}(\omega)C_{5.4}(\omega, \alpha)\right) & \alpha > 1. \end{cases}\]

If the assumptions hold also for \(\alpha > 1\) then, the following bound holds as well
\[|Q(p - p_h)(\omega) - Q(p^r - p_h^r)(\omega)| \lesssim C_{5.1}(\omega, \alpha)\|f\|_{L^2(D)}\|Q\|_{L^2(D)} h^{2 \epsilon_{\min}(\alpha - 1, 2)}.\]

**Proof.** Let us consider the adjoint problems related to the original and the auxiliary problems having \(Q(\cdot)\) as right hand side
\[\int_D a\nabla v \nabla \Phi dx = Q(v), \quad \int_D a'\nabla v \nabla \Phi^r dx = Q(v), \quad \forall v \in H^1_0(D)\]
where \(\Phi\) and \(\Phi^r\) are respectively the solutions of the two adjoint problems. Moreover, we denote by \(\Phi_h\) and \(\Phi_h^r\) their respective finite element approximation. By choosing \(v = p - p_h\) in the first problem and \(v = p^r - p_h^r\) in the second problem and by taking the difference we get:
\[Q(p - p_h) - Q(p^r - p_h^r) = \int_D a\nabla (p - p_h) \nabla \Phi dx - \int_D a'\nabla (p^r - p_h^r) \nabla \Phi^r dx.\]
Using the Galerkin orthogonality and adding and subtracting some mixed terms we get:

\[
Q(p - p_h) - Q(p^* - p^*_h) = \int_D a \nabla (p - p_h) \nabla (\Phi - \Phi_h) \, dx - \int_D a^* \nabla (p^* - p^*_h) \nabla (\Phi^* - \Phi^*_h) \, dx
\]
\[
\pm \int_D a^* \nabla (p - p_h) \nabla (\Phi - \Phi_h) \, dx \pm \int_D a^* \nabla (p - p_h) \nabla (\Phi^* - \Phi^*_h) \, dx;
\]

By properly grouping the terms above we obtain:

\[
|Q(p - p_h) - Q(p^* - p^*_h)| \leq \left| \int_D (a - a^*) \nabla (p - p_h) \nabla (\Phi - \Phi_h) \, dx \right|
\]
\[
+ \left| \int_D a^* \nabla (p - p_h) \nabla (\Phi - \Phi_h - (\Phi^* - \Phi^*_h)) \, dx \right|
\]
\[
\leq \|a - a^*\|_{L^\infty(D)} \|p - p_h\|_{H^3(D)} \|\Phi - \Phi_h\|_{H^3(D)}
\]
\[
+ \|a^*\|_{L^\infty(D)} \|p - p_h - (p^* - p^*_h)\|_{H^3(D)} \|\Phi^* - \Phi^*_h\|_{H^3(D)}.
\]

Since for the solutions of the adjoint problems we have identical error bounds as for the primal ones we obtain the bound

\[
|Q(p - p_h) - Q(p^* - p^*_h)| \lesssim C_{5.2}(\omega, \alpha) C_{5.2}^2(\omega, \alpha) \|f\|_{H^{\beta_2 - 1}(D)} \|Q\|_{H^{\beta_2 - 1}(D)} \frac{h^{\beta_1 + \beta_2 \min(\alpha, 2)}}{(\alpha - \beta_1)(\alpha - \beta_2)}
\]
\[
+ a^*_{\max}(\omega) C_{5.4}(\omega, \alpha) C_{5.4}(\omega, \alpha) \|f\|_{H^{\beta_2 - 1}(D)} \|Q\|_{H^{\beta_2 - 1}(D)} \frac{h^{\beta_3 + \beta_4 \min(\alpha - \beta_3 - \eta_2, 2)}}{(\alpha - \beta_3)(\alpha - \beta_4)}
\]
\[
+ a^*_{\max}(\omega) C_{5.4}(\omega, \alpha) C_{5.4}(\omega, \alpha) \|f\|_{H^{\beta_2 - 1}(D)} \|Q\|_{H^{\beta_2 - 1}(D)} \frac{h^{\beta_5 + \beta_6 \min(\alpha - \beta_5 - \eta_6, 2)}}{(\alpha - \beta_5)(\alpha - \beta_6)}
\]

where \(\beta_i, i = 1, \ldots, 6\) and \(\eta_j, j = 3, 6\) are the parameters coming from the bounds of the primal and adjoint problems. Since the bound is valid \(\forall \beta_i < \rho\), it is possible to choose \(\beta_1 = \beta_2 = \beta_4 = \beta_5 = \rho\); moreover the remaining part of the bound assumes its maximum value when \(\beta_3 = \beta_6 = \beta\) and \(\eta_3 = \eta_6 = \eta\); hence, \(\forall \theta < \beta < \rho\) and \(\alpha \geq 0\) such that \(\beta + \eta \leq \alpha\), the bound can be rewritten as

\[
|Q(p - p_h) - Q(p^* - p^*_h)| \lesssim C_{5.1}(\omega, \alpha) \|f\|_{L^2(D)} \|Q\|_{H^{\beta - 1}(D)} h^t \frac{h^{\beta \min(\alpha - \beta - \eta, 2)}}{(\alpha - \beta)^2 \sqrt{\eta}}.
\]

By taking the first infimum over \(t\) and the second infimum over \(\beta\) and \(\eta\) we obtain the desired result. If the assumptions hold also for \(\alpha > 1\) then it can be analogously shown that

\[
|Q(p - p_h)(\omega) - Q(p^* - p^*_h)(\omega)| \lesssim C_{5.1}(\omega, \alpha) \|f\|_{L^2(D)} \|Q\|_{L^2(D)} h^2 \frac{h^{\beta \min(\alpha - 1, 2)}}{(\alpha - \beta)^2 \sqrt{\eta}}.
\]

**Proposition 5.1.** Up to logarithmic terms, the infima in the previous estimates can be bound as follows:

\[
\inf_{0 \leq t \leq \min(\alpha, 1)} h^t \frac{h^t}{(\alpha - \beta)^2 \sqrt{\eta}} \lesssim h^{\min(\alpha, 1)} \quad \forall h \leq e^{-\frac{1}{\beta}}
\]
\[
\inf_{0 \leq \beta \leq \min(\alpha, 1)} h^{\beta \min(\alpha - \beta - \eta, 2)} \frac{h^{\beta \min(\alpha - \beta - \eta, 2)}}{(\alpha - \beta)^2 \sqrt{\eta}} \lesssim \begin{cases} h^{\min(\alpha, 1)} e^{\min(0, \alpha - 1, 2)}, & h \leq e^{-\frac{1}{\beta}} \\ h^{\max(0, \alpha - 2, 1)} e^{\min(\alpha, 2)}, & h \geq e^{-\frac{1}{\beta}} \end{cases}
\]
Theorem 5.1. The mean square error related to the estimator (13) can be bounded as

\[ |Q(p - p_h) - Q(p' - p_h')| \leq C_{5.1}(\omega, \alpha) \|f\|_{L^2(D)} \|Q\|_{L^2(D)} \left\{ \begin{array}{l}
\frac{h_0^{1/2} \min(\alpha, 1)}{\epsilon_{\min}(\max(0, \alpha - 1), 2)} \leq e^{-\frac{\epsilon}{\epsilon_0}} \\
\frac{h_0 \min(\alpha, 1) \min(\min(0, \alpha - 2), 0) \min(\alpha, 2)}{\epsilon_{\min}(\alpha, 2)} \leq e^{-\frac{\epsilon}{\epsilon_0}} \leq e^{-\frac{\epsilon}{\epsilon_0}.
\end{array} \right. \]

If we look at the bound given in Theorem 5.1, in light of the estimates presented in Proposition 5.1, we can see that the infimum is achieved for \( \beta, \eta \) close to 0 and \( t \) close to \( \min(\alpha, 1) \) when \( h \geq e^{-\frac{\epsilon}{\epsilon_0}} \) and for \( \beta, t \) close to \( \min(\alpha, 1) \) and \( \eta \) close to 0 when \( h \geq e^{-\frac{\epsilon}{\epsilon_0}} \). This means that, in practice, there are two convergence regimes: for values of \( \epsilon \) larger than \( e^{-\frac{\epsilon}{\epsilon_0}} \) we have a slower convergence rate with respect to \( h \) than the standard MLMC one, compensated however by the presence of an \( \epsilon \) term that makes the variance reduction with respect to the MLMC case significant; on the contrary when \( h \) gets smaller than \( e^{-\frac{\epsilon}{\epsilon_0}} \) we recover the same \( h \)-convergence rate of the standard MLMC case: in this regime we have a further variance reduction, given by the factor \( \epsilon_{\min}(\alpha, 2) \), only if the input random field is smooth enough (\( \alpha > 1 \)). In general we can state that we get always an overall variance reduction with respect to the standard MLMC case and that this variance reduction affects all the possible levels if the input random field is sufficiently smooth (\( \alpha > 1 \)) and only the levels for which \( h_t > e^{-\frac{\epsilon}{\epsilon_0}} \) otherwise.

In light of these results and considerations the mean square error associated to the MLCV estimator satisfies the following

**Theorem 5.2.** Let \( a(x, \omega) \) and \( a'(x, \omega) \) be as in Lemma 5.2, \( f \in L^2(D) \) and let \( Q \) and \( r \) be as in Theorem 5.1. The mean square error related to the estimator (13) can be bounded as

\[
e\left(\hat{Q}_{h_{1.1}}(M_t)\right)^2 \leq c_{5.1}(\alpha, 2) \|f\|_{L^2(D)}^2 \|Q\|_{L^2(D)}^2 \sum_{l=0}^{L} \left( \inf_{0 < \tau < r} \frac{h_1^\alpha}{\alpha - \eta} \inf_{0 < \beta < r} \frac{h_1^\beta \epsilon_{\min}(\alpha - \beta - \eta, 2)}{(\alpha - \beta)^2 \sqrt{\eta}} \right)
+ 2 \left[ E[Q_{h_{1.1}}] - E[$$SC$$[Q_{h_{1.1}}]]^2 + 2E[Q_{h_{1.1}} - Q]^2 \right]
\]

where \( c_{5.1}(\alpha, q) = ||C_{5.1}(\omega, \alpha)||_{L^q(\Omega)} \). If the assumptions hold also for \( \alpha > 1 \) then it is valid also the bound

\[
e\left(\hat{Q}_{h_{1.1}}(M_t)\right)^2 \leq c_{5.1}(\alpha, 2) \|f\|_{L^2(D)}^2 \|Q\|_{L^2(D)}^2 \sum_{l=0}^{L} \frac{h_1^1 \epsilon_{\min}(\alpha - 1, 2)}{M_t}
+ \left( E[Q_{h_{1.1}}] - E[$$SC$$[Q_{h_{1.1}}]]^2 + 2E[Q_{h_{1.1}} - Q]^2 \right)
\]

Proof. The formula of the mean square error related to the estimator (13) is

\[
e\left(\hat{Q}_{h_{1.1}}(M_t)\right)^2 \leq \sum_{l=0}^{L} \frac{\text{Var}(Q_{h_{1.1}} - Q_{h_{1.1-1}})}{M_t} + 2E[Q_{h_{1.1}} - Q_{h_{1.1}}^{SC}]^2 + 2E[Q_{h_{1.1}} - Q]^2.
\]

We get

\[
\text{Var}(Q_{h_{1.1}} - Q_{h_{1.1-1}}) \leq 2\text{Var}(Q_{h_{1.1}} - Q_{h_{1.1}}) + 2\text{Var}(Q_{h_{1.1-1}} - Q_{h_{1.1}})
\leq 2\|Q(p - p_{h_{1.1}}) - Q(p' - p_{h_{1.1}})\|_{L^2(D)}^2 + 2\|Q(p - p_{h_{1.1-1}}) - Q(p' - p_{h_{1.1-1}})\|_{L^2(D)}^2
\leq c_{5.1}(\alpha, 2) \|f\|_{L^2(D)}^2 \|Q\|_{L^2(D)}^2 \left( \min_{0 < \tau < r} \frac{h_1^\alpha}{\alpha - \eta} \inf_{0 < \beta < r} \frac{h_1^\beta \epsilon_{\min}(\alpha - \beta - \eta, 2)}{(\alpha - \beta)^2 \sqrt{\eta}} \right)^{2}.
\]

By replacing in the inequality of the mean square error we get the desired result. The result concerning the case \( \alpha > 1 \) can be shown analogously.

The complete result can be found in Appendix D.

**Corollary 5.1.** Up to logarithmic terms, the bound in Theorem 5.1 becomes

\[
|Q(p - p_h) - Q(p' - p_h')| \leq C_{5.1}(\omega, \alpha) \|f\|_{L^2(D)} \|Q\|_{L^2(D)} \left\{ \begin{array}{l}
\frac{h_0^{1/2} \min(\alpha, 1)}{\epsilon_{\min}(\max(0, \alpha - 1), 2)} \leq e^{-\frac{\epsilon}{\epsilon_0}} \\
\frac{h_0 \min(\alpha, 1) \min(\min(0, \alpha - 2), 0) \min(\alpha, 2)}{\epsilon_{\min}(\alpha, 2)} \leq e^{-\frac{\epsilon}{\epsilon_0}} \leq e^{-\frac{\epsilon}{\epsilon_0}.
\end{array} \right. \]
5.3 The MLCV Algorithm

In this section we present the algorithm used in order to guarantee a mean square error smaller than a prescribed tolerance tol. In order to be efficient, the method requires a strategy to select properly the number of levels L and the number of samples \( M_l \) to be taken on each level \( l = 0, 1, \ldots, L \) as well as the degree of approximation of the Stochastic Collocation Method in order to get a sufficiently accurate approximation of the mean of the control variate \( \mathbb{E}[Q(p')] \). Before going into the details let us start with this important consideration: depending on the smoothness of the input random field \( a \) two possible strategies can be followed, namely:

- **Strategy 1**: if the input random field is smooth enough, i.e. if \( \alpha > 1 \), then our theoretical results predict a variance reduction on each level; therefore \( \text{Var}(Q_{h_{l+1}}^{CV} - Q_{h_l}^{CV}) < \text{Var}(Q_{h_{l+1}} - Q_{h_l}) \forall l = 0, \ldots, L \) and it is advantageous to apply the MLCV scheme as presented in (13), keeping the control variate on each level;

- **Strategy 2**: if the random field is rough, i.e. if \( \alpha \leq 1 \), then our theoretical results predict a variance reduction only on the coarsest levels and more precisely for all the levels such that \( h_l < e^{-\frac{\alpha}{2}} \varepsilon \); therefore the most effective strategy consists in selecting as coarsest level the grid of mesh size \( h_0 \) such that \( h_0 \approx e^{-\frac{\alpha}{2}} \varepsilon \), keep the control variate only on this level and use a standard MLMC method on the subsequent levels; by doing this, we need to compute the approximate mean of the control variate on the coarsest mesh and not anymore on the finest one as in Strategy 1, namely:

\[
\hat{Q}_{\{h_i\},\{M_l\}}^{MLCV} = \frac{1}{M_{l_0}} \sum_{i=1}^{M_{l_0}} \left( Q_{h_{i}}^{CV} - Q_{h_{i}}^{TV} \right) + \sum_{l=l_0+1}^{L} \frac{1}{M_{l}} \sum_{i=1}^{M_{l}} \left( Q_{h_{i}}^{CV} - Q_{h_{j}}^{CV} \right) + \mathbb{E}^{SC}[Q_{h_{i+1}}]. \tag{22}
\]

The general algorithm used to properly choose the parameters \( \{M_l\}, L \) and the sparse grid level \( w \) is the following:

1. We run the deterministic problem for different mesh sizes, with a small number of samples, to have an estimate of the finite element error, or in other terms the weak error, from which we fit the constants \( c_w, r_w \in \mathbb{R}_+ \) of the error model \( |\mathbb{E}[Q_{h_2} - Q]| = c_w h_l^{r_w} \).

2. Given a prescribed tolerance tol we select the finest grid having mesh size \( h_L \) in such a way to guarantee the discretization error model, which does not depend on \( \epsilon \), smaller than tol.

3. We set \( h_0 = O(L_c) \) and evaluate, again by taking a few samples on each level, \( \text{Var}(Q_{h_{l+1}}^{CV} - Q_{h_{l}}^{CV}) \), \( \text{Var}(Q_{h_{l+1}} - Q_{h_{l}}) \) and \( \text{Var}(Q_{h_{l}}^{CV}) \) on the levels in which, according to the selected strategy, these quantities are needed. Based on the estimate (20) we fit the statistical error in two different regions, namely \( \forall \left( Q_{h_{l+1}}^{CV} - Q_{h_{l}}^{CV} \right) \approx c_{s_{l}} h_l^{r_{s_{l}}} \) for \( l = 0, \ldots, l^* \) and \( \forall \left( Q_{h_{l+1}}^{CV} - Q_{h_{l}}^{CV} \right) \approx c_{s_{l}} h_l^{r_{s_{l}}} \) for \( l = l^* + 1, \ldots, L \).

4. We run the sparse grid on increasing approximation levels to estimate the sparse grid error. In particular, we fit the constants \( c, \delta \in \mathbb{R}_+ \) of the error model \( |\mathbb{E}[Q'] - \mathbb{E}^{SC}[Q']| = c M_{SC}^{-\delta} \).

5. According to the selected strategy and the previously estimated convergence rates, we compute the number of samples \( M_l \) for \( l = 0, \ldots, L \) and the number of knots \( M_{SC} \) to be used in the sparse grid approximation of the expected value of the control variate by solving an optimization problem in such a way to have the sum between the sampling and the stochastic collocation error smaller than tol\( \delta \). This optimization is described in the next subsection.

6. Once all the parameters appearing in the equations have been estimated the method can be run.

We remark that this algorithm requires a certain number of samples per level to estimate all the parameters of the different error models. These extra samples might have actually an impact on the overall complexity of the algorithm. A more efficient way of fitting the error models in a standard MLMC algorithm has been proposed in [18]. Its extension to MLCV is under investigation.
5.3.1 Optimization Problem

Once the sequence of increasingly fine grids $T_{h_0}, ..., T_{h_L}$ has been determined, we solve an optimization problem to find the optimal number of samples $M_l$ for $l = 0, ..., L$ and the optimal number of knots $M_{SC}$ forming the sparse grid upon which the expected value of the control variate is computed. The optimization problem minimizes the computational cost needed to achieve a prescribed tolerance in the mean square error. The computational cost needed to solve a single deterministic problem of mesh size $h_l$ is assumed to be of the form $C_l = kh_l^{-d\rho}$, where $\rho$ is a factor typically larger than 1 and smaller than 3/2 for optimal solvers. The model for the computational cost associated to the MLCV estimator for the two strategies is:

- **strategy 1:**
  \[ C(M_l, M_{SC}) = 2M_0C_0 + 2 \sum_{l=1}^{L} M_l(C_l + C_{l-1}) + M_{SC}C_L, \]  \[ (23) \]

- **strategy 2:**
  \[ C(M_l, M_{SC}) = 2M_0C_0 + \sum_{l=l_0+1}^{L} M_l(C_l + C_{l-1}) + M_{SC}C_{l_0}, \]  \[ (24) \]

where the factor 2 in the above estimates comes from the fact that on each level on which the control variate is used, we have to solve both the original problem and the regularized one. The associated error, according to the selected strategy is:

- **strategy 1:**
  \[ e(M_l, M_{SC})^2 = \frac{c_1 \sum_{l=0}^{l^*} h_l^{r_1}}{M_l} + c_2 \sum_{l=l_0+1}^{L} h_l^{r_2} + cM_{SC}^{-\delta}, \] where $l^* \approx -\log_2(\epsilon)$

- **strategy 2:**
  \[ e(M_l, M_{SC})^2 = \sum_{l=l_0}^{L} \frac{c_1 h_l^{r_1}}{M_l} + cM_{SC}^{-\delta} \]

**Remark.** In the estimate of the $\mathbb{V} \left( Q_{h_l}^{CV} - Q_{h_{l-1}}^{CV} \right)$, according to the selected strategy, we have considered only the two extreme regimes $\beta = 0$, leading to $\mathbb{V} \mathbb{A}r \left( Q_{h_l}^{CV} - Q_{h_{l-1}}^{CV} \right) \sim O(h_l^{r_1})$, and $\beta = \min(\alpha, 1)$, leading to $\mathbb{V} \mathbb{A}r \left( Q_{h_l}^{CV} - Q_{h_{l-1}}^{CV} \right) \sim O(h_l^{r_2})$.

**Remark.** The parameters $c_{s_1}$ and $c_{s_2}$ strongly depend on the choice of $\epsilon$.

Once all the constants appearing in the previous inequalities have been estimated, according to the strategy selected, we perform a Lagrangian optimization by considering the Lagrange function

\[ L(M_l, M_{SC}, \lambda) = C(M_l, M_{SC}) + \lambda(e(M_l, M_{SC})^2 - \epsilon_l^2). \]

Here below we report the results of such optimization procedure in the case of Strategy 1, by assuming $h_l = 2^{-(1+l)}$:

- $M_0 = \epsilon_l^{-2} \sqrt{\lambda} \sqrt{\frac{c_1 h_l^{r_1}}{2C_0}}$
- $M_l = \epsilon_l^{-2} \sqrt{\lambda} \sqrt{\frac{c_1 h_l^{r_1}}{3C_l}}$ for $l = 1, ..., l^*$
- $M_l = \epsilon_l^{-2} \sqrt{\lambda} \sqrt{\frac{c_1 h_l^{r_2}}{3C_l}}$ for $l = l^* + 1, ..., L$
- $M_{SC} = \epsilon_l^{-2} \sqrt{\lambda} \lambda^{\frac{1}{1+r_1}} \left( \frac{\delta_{x_0} h_l}{\epsilon_l} \right)^{\frac{1}{1+r_2}}$

where $\lambda$ has to be computed from:

\[ \frac{1}{\sqrt{\lambda}} = \frac{1}{\sqrt{C_0(\sqrt{2v_0} + \sum_{l=1}^{L} \sqrt{3v_l}2^l)} + c(\frac{1}{\sqrt{\lambda}})^{\frac{1}{1+r_1}} (12^{L}s \frac{\epsilon}{\epsilon_0})^{\frac{1}{1+r_2}}}, \]

where $v_l$, $l = 0, ..., L$, are the fitted variances previously introduced.
Remark. By looking at these results it is important to notice that an optimal solution can be found only if \( \delta \geq 1 \); this means that using a stochastic collocation method in order to approximate the mean of the control variate brings some advantages only if the stochastic collocation converges at least like a Monte Carlo method.

6 Numerical Results

In this section we present some numerical results obtained using the proposed method. We underline that all the results presented hereafter are obtained in the case of a lognormally distributed random field \( a(x, \omega) \) such that \( \log(a(x, \omega)) \) has a covariance function belonging to the Matérn family (5). The sampling from the random field \( a(x, \omega) \) is done via FFT [20], e.g. by expanding the field on a Fourier basis. On the other hand, in order to compute the expected value of the control variate via Stochastic Collocation, we considered a KL expansion of the input random field on a Fourier basis. On the other hand, in order to compute the expected value of the control variate via Stochastic Collocation, we considered a KL expansion of the input random field as input, the variance reduction with respect to the standard MLMC case appears on each level, and, again, the more \( \epsilon \) gets smaller the more the variance reduction is significant.

In Figure 4 and Figure 5 we show convergence plots for the two other sources of errors, namely the Stochastic Collocation error committed when approximating the mean of the control variate on a sparse grid, and the error coming from the spatial discretization, which determines the finest mesh of our sequence of meshes.

![Figure 2: Variance of the difference of the QoI](image)

**Figure 2:** Variance of the difference of the QoI \( Q = \int_D u(x, \omega) \, dx \) between consecutive grids. \( Y_l = Q_l - Q_{l-1}, \nu = 0.5, L_c = 0.5, \sigma = 1, h_0 = 0.5 \).

Figure 2 shows the variance of \( Q_l \) as well as the variance of the difference \( Q_l - Q_{l-1} \) for the standard MLMC approach and the MLCV, in the case of rough fields (\( \nu = 1/2 \)). As predicted by the theory, the variance reduction in MLCV appears only on the coarsest levels and, starting from a certain level \( l^* = - \log_2 \epsilon \) for which \( h_{l^*}, \epsilon \) the variance of the difference of the QoI between consecutive grids of the MLCV and MLMC methods are identical.

The second comparison, shown in Figure 3, demonstrates that, by considering a smoother random field as input, the variance reduction with respect to the standard MLMC case appears on each level, and, again, the more \( \epsilon \) gets smaller the more the variance reduction is significant.
Concerning the Stochastic Collocation error we see that the fitted error model $cM_{SC}^{-\delta}$, actually describes well the decay of the error; moreover, the convergence rate of the square of the error remains larger than one, which guarantees the existence of an optimal number of sample points $M_l$ for each level and an optimal number of sparse grids knots $M_{SC}$, as mentioned before.

Concerning the discretization error we see on Figure 5 that the weak error presents different slopes depending on the smoothness of the input random field: in particular when $a$ is rough (in this case $\nu = 0.5$) the convergence rate is close to 1; on the other hand when the random field $a$ has smooth realizations (in this case $\nu = 2.5$ so the realizations are twice differentiable) the convergence rate is close to 2.

To conclude the presentation of the numerical results we show a plot of the overall error; since the finite element error is the same (up to a constant) in the mean square error associated to the MLMC and MLCV estimators, in order to make the comparison between the two methods as clear as possible, we select the finest mesh size $h_L$ in such a way to have the two finite element errors comparable, i.e. a fraction of a prescribed tolerance $\text{tol}^2$. Then we compare the other terms coming from the mean square error associated to the MLMC and MLCV estimators. Of course, other choices are possible concerning the algorithm (see e.g. [18, 19]) which will not be discussed here. Hence, the error obtained with our model after having optimized all the parameters, thought as sum of the Stochastic Collocation error and the statistical error, is shown against the estimated CPU time, according to the computational cost model defined in (23) and (24).
Figure 5: Discretization error computed as $E[(Q_{h_L} - Q_{h_U})^2]$. LC = 0.5, $\sigma = 1$.

Figure 6 shows a remarkable improvement in terms of mean square error with respect to the case of the standard MLMC method. In order to achieve the same accuracy of the MLMC method, roughly speaking, the proposed MLCV method presents a gain in terms of computational time of about one order of magnitude in the rough case and about two orders of magnitude in the smooth case.

Figure 6: Error vs Computational cost. Error = SC error + Statistical error.

7 Conclusions and future work

In this work we have proposed a new Multi Level Monte Carlo algorithm with Control Variate and applied it to solve elliptic partial differential equation with log-normal coefficients with covariance function from the Matérn family, with particular focus on the case of rough coefficients. The control variate is obtained by solving an auxiliary problem with a regularized coefficient and its mean can be effectively computed by a Stochastic Collocation method.

The proposed strategy considerably improves the performance of the standard MLMC method in terms of error versus computational cost, in both cases of rough and smooth coefficients, where we have always observed a gain with respect to the standard MLMC method.

The choice of the regularization parameter $\epsilon$ is rather delicate in the case of rough coefficients, as it should properly balance the variance reduction achievable in MLMC and the performance of
the stochastic collocation.

So far this choice has been done heuristically; more analysis is needed to derive optimal values of the regularization parameter.

We are also exploring the possibility of taking a level dependent $\epsilon$, possibly in combination with the general idea of Multi Index Monte Carlo introduced in [19]. Results will be reported in a forthcoming work.

A Proof of Lemma 5.2

We consider a fixed $\omega \in \Omega$ and we will not specify the dependence on $\omega$ in the proof. In order to prove Lemma 5.2 we will need the following three preliminary lemmas.

**Lemma A.1.** Let $\gamma(x)$ be a deterministic function in $C^\alpha(\mathbb{R}^d)$ and, $\forall h \in \mathbb{R}^d$, let us define $D_{h,\beta}\gamma(x)$ as

$$D_{h,\beta}\gamma(x) = \frac{\gamma(x + h) - \gamma(x)}{|h|^\beta}.$$  

Then, $\forall 0 < \beta \leq \min(1, \alpha)$ it holds

$$\|D_{h,\beta}\gamma\|_{C^{\alpha-\beta}(\mathbb{R}^d)} \leq (1 + 2\sqrt{d})\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)},$$

and in particular

$$|D_{h,\beta}\gamma|_{C^{\alpha-\beta}(\mathbb{R}^d)} \leq 2\sqrt{d}\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)}.$$

**Proof.** Let us denote $\alpha = A + s$, with $A \in \mathbb{N}$ and $s \in (0, 1]$.

- We first consider the case $0 \leq \beta \leq \alpha - 1$ so that $A = 0$ and $s = \alpha$. The norm we want to bound can be written as

$$\|D_{h,\beta}\gamma\|_{C^{\alpha-\beta}(\mathbb{R}^d)} = \|D_{h,\beta}\gamma\|_{C^{\alpha}(\mathbb{R}^d)} + |D_{h,\beta}\gamma|_{C^{\alpha-\beta}(\mathbb{R}^d)} =$$

$$= \|D_{h,\beta}\gamma\|_{C^{\alpha}(\mathbb{R}^d)} + \sup_{x,t \in \mathbb{R}^d} \left( \frac{\|D_{h,\beta}\gamma\|_{C^{\alpha}(\mathbb{R}^d)}(x + t) - (D_{h,\beta}\gamma)(x)}{|t|^{\alpha-\beta}} \right).$$

The first term can be bounded as

$$(i) = \sup_{x \in \mathbb{R}^d} \left( \frac{\|\gamma(x + h) - \gamma(x)\|}{|h|^\beta} \right) \leq \sup_{x \in \mathbb{R}^d} \max \left\{ \sup_{|h| \geq 1} \left( \frac{\|\gamma(x + h) - \gamma(x)\|}{|h|^\beta} \right), \sup_{|h| \leq 1} \left( \frac{\|\gamma(x + h) - \gamma(x)\|}{|h|^\beta} \right) \right\}$$

$$\leq \sup_{x \in \mathbb{R}^d} \left( \left( \|\gamma(x + h)\| + \|\gamma(x)\| \right), \sup_{|h| \leq 1} \left( \frac{\|\gamma(x + h) - \gamma(x)\|}{|h|^\alpha} \right) \right) \leq 2\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)} + |\gamma|_{C^{\alpha}(\mathbb{R}^d)}.$$

The second term can be bounded as

$$(ii) = \max \left\{ \sup_{x,t \in \mathbb{R}^d, |h| \geq |h|} \left( \frac{\|\gamma(x + t + h) - \gamma(x + t) - \gamma(x + h) + \gamma(x)\|}{|h|^\beta|t|^{\alpha-\beta}} \right), \sup_{x,t \in \mathbb{R}^d, |h| \leq |h|} \left( \frac{\|\gamma(x + t + h) - \gamma(x + h) - \gamma(x + t) + \gamma(x)\|}{|h|^\beta|t|^{\alpha-\beta}} \right) \right\}$$

$$\leq \max \left\{ \sup_{x,t \in \mathbb{R}^d, |h| \geq |h|} \left( \frac{\|\gamma(x + t + h) - \gamma(x + t) + \gamma(x + h) - \gamma(x)\|}{|h|^\beta|t|^{\alpha-\beta}} \right), \sup_{x,t \in \mathbb{R}^d, |h| \leq |h|} \left( \frac{\|\gamma(x + t + h) - \gamma(x + h) + \gamma(x + t) - \gamma(x)\|}{|t|^\beta|t|^{\alpha-\beta}} \right) \right\}$$

$$\leq 2\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)}.$$

Hence we get $\|D_{h,\beta}\gamma\|_{C^{\alpha-\beta}(\mathbb{R}^d)} \leq 3\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)}$ and $|D_{h,\beta}\gamma|_{C^{\alpha-\beta}(\mathbb{R}^d)} \leq 2\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)}$.

- Let us consider now the case $0 < \beta < 1 < \alpha$ so that $\alpha = A + s$ with $A \geq 1$. The proof can be
further divided in two parts: $s > \beta$ and $s < \beta$ since for $s = \beta$ the result is obvious. We start with the case $s > \beta$. The norm that we want to bound can be written as

\[
\|D_{h,\beta}\gamma\|_{C_0^\beta(R^d)} = \|D_{h,\beta}\gamma\|_{C_0^\beta} + \sum_{k=1}^A |D_{h,\beta}\gamma|_{C^k} + |D_{h,\beta}\gamma|_{C_0^{\beta}}
\]

\[
= \|D_{h,\beta}\gamma\|_{C_0^\beta} + \sum_{k=1}^A \max_{|i|=k} \|D^i(D_{h,\beta}\gamma)\|_{C_0^\beta} + \max_{|i|=\lambda} \{ \frac{|D^i(D_{h,\beta}\gamma)(x + t) - D^i(D_{h,\beta}\gamma)(x)|}{|t|^{s-\beta}} \}. \tag{ii}
\]

In what follows, we denote $\xi^y_x$ a point of the segment $\overline{xy}$, i.d. $\xi^y_x = \theta x + (1 - \theta)y$ for some $\theta \in [0, 1]$. The first term (i) can be bounded as

\[
(i) = \sup_{x \in R^d} \frac{\gamma(x + h) - \gamma(x)}{|h|^\beta} \leq \sup_{x \in R^d} \max_{|h| \geq 1} \left\{ \sup_{|h| \leq 1} \frac{\gamma(x + h) - \gamma(x)}{|h|^\beta}, \sup_{|h| \leq 1} |\nabla \gamma(\xi^x_x + h)\cdot h| \right\} \leq 2\|\gamma\|_{C_0^\beta} + \sqrt{d} \|\gamma\|_{C^1(R^d)}.
\]

Each term of (ii), for $k = 1, \ldots, A - 1$, can be bounded as

\[
\max_{|i|=k} \left\{ \sup_{x \in R^d} \frac{|D^i\gamma(x + h) - D^i\gamma(x)|}{|h|^\beta} \right\} \leq \max_{|i|=k} \left\{ \sup_{x \in R^d} \left( \sup_{|h| \geq 1} |D^i\gamma(x + h)| + |D^i\gamma(x)| \right), \sup_{|h| \leq 1} \frac{|\nabla D^i\gamma(\xi^x_x + h)\cdot h|}{|h|^\beta} \right\} \leq 2\|\gamma\|_{C_0^\beta} + \sqrt{d} \|\gamma\|_{C^1(R^d)}.
\]

The last term of (ii) for $k = A$, analogously to what we did in the case $0 < \beta \leq \alpha \leq 1$, can be bounded as

\[
|D_{h,\beta}\gamma|_{C^A(R^d)} \leq 2|\gamma|_{C^A(R^d)} + |\gamma|_{C_0^\beta(R^d)}.
\]

Hence the term (ii) can be bounded as

\[
(ii) \leq 2\|\gamma\|_{C^1(R^d)} + (2 + \sqrt{d}) \sum_{k=2}^A |\gamma|_{C^k(R^d)} + |\gamma|_{C_0^\beta(R^d)}.
\]

The last term (iii) can be bounded as

\[
(iii) \leq \max_{|i|=A} \left\{ \max_{x,t \in R^d} \sup_{|h| \geq |t|} \left( \sup_{|h| \leq |t|} \frac{|D^i\gamma(x + h + t) - D^i\gamma(x + t) - D^i\gamma(x)|}{|h|^\beta |t|^{s-\beta}} \right) \right\} \leq 2\|\gamma\|_{C_0^\beta(R^d)}.
\]

So the norm of $\|D_{h,\beta}\gamma\|_{C_0^\beta}$ can be bounded as

\[
\|D_{h,\beta}\gamma\|_{C_0^\beta} \leq (i) + (ii) + (iii) \leq 2\|\gamma\|_{C_0^\beta} + (2 + \sqrt{d}) \sum_{k=1}^A |\gamma|_{C^k(R^d)} + 3|\gamma|_{C_0^\beta(R^d)} \leq (2 + \sqrt{d}) \|\gamma\|_{C_0^\beta(R^d)}
\]

and $\|D_{h,\beta}\gamma\|_{C_0^\beta} \leq 2\|\gamma\|_{C_0^\beta}$. 

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• Let us consider now the case \( s < \beta \). The quantity we want to bound becomes

\[
\|D_{h,\beta}\gamma\|_{C^{\alpha-\beta}(\mathbb{R}^d)} = \|D_{h,\beta}\gamma\|_{C^0(\mathbb{R}^d)} + \sum_{k=1}^{A-1} |D_{h,\beta}\gamma|_{C^k(\mathbb{R}^d)} + |D_{h,\beta}\gamma|_{C^{\alpha-\beta}(\mathbb{R}^d)}
\]

\[
= \|D_{h,\beta}\gamma\|_{C^0(\mathbb{R}^d)} + \sum_{k=1}^{A-1} \max_{|i|=k} \|D^k(D_{h,\beta}\gamma)\|_{C^0(\mathbb{R}^d)} + \max_{|i|=A-1} \sup_{x,t} \left\{ \frac{|D^k(D_{h,\beta}\gamma)(x+t) - D^k(D_{h,\beta}\gamma)(x)|}{|t|^{1+s-\beta}} \right\}
\]

We have already derived a bound for the terms (i) and (ii). The term (iii) can be bounded as follows:

\[
(iii) = \max_{|i|=A-1} \sup_{x,t\in\mathbb{R}^d} \left\{ \frac{|D^k(D_{h,\beta}\gamma)(x+t) - D^k(D_{h,\beta}\gamma)(x)|}{|t|^{1+s-\beta}} \right\}
\]

By bounding separately the two terms we get

\[
I_i = \sup_{x,t\in\mathbb{R}^d, |t|\geq|h|} \frac{|D^i\gamma(x+t+h) - D^i\gamma(x+t) - D^i\gamma(x+h) + D^i\gamma(x)|}{|h|^\beta |t|^{1+s-\beta}}
\]

\[
= \sup_{x,t\in\mathbb{R}^d, |t|\geq|h|} \frac{|(\nabla D^i\gamma(x) + \cdot h) - (\nabla D^i\gamma(x+h) + \cdot h)|}{|h|^\beta |t|^{1+s-\beta}}
\]

\[
\leq \sup_{x,t\in\mathbb{R}^d, |t|\geq|h|} \max_{j=1,...,d} \frac{\partial x_j(D^i\gamma(x+h+t)) - \partial x_j(D^i\gamma(x))}{|\xi_{i,x+h+t} - \xi_{i,x}|^s} \frac{|(\nabla D^i\gamma(x) + \cdot h) - (\nabla D^i\gamma(x+h) + \cdot h)|}{|h|^\beta |t|^{1+s-\beta}}
\]

\[
\leq \sqrt{d}\gamma|_{C^0(\mathbb{R}^d)} \sup_{x,t\in\mathbb{R}^d, |t|\geq|h|} \frac{|h|^{1-\beta}(|h|^s + |t|^s)}{|t|^{1+s-\beta}} \leq 2\sqrt{d}\gamma|_{C^0(\mathbb{R}^d)}.
\]

Similarly for the term \( II_i \), we have:

\[
II_i = \sup_{x,t\in\mathbb{R}^d, |t|\leq|h|} \frac{|D^i\gamma(x+t+h) - D^i\gamma(x+h) - D^i\gamma(x+t) + D^i\gamma(x)|}{|h|^\beta |t|^{1+s-\beta}}
\]

\[
= \sup_{x,t\in\mathbb{R}^d, |t|\leq|h|} \frac{|(\nabla D^i\gamma(x) + \cdot h) - (\nabla D^i\gamma(x+h) + \cdot h)|}{|h|^\beta |t|^{1+s-\beta}}
\]

\[
\leq \sup_{x,t\in\mathbb{R}^d, |t|\leq|h|} \max_{j=1,...,d} \frac{\partial x_j(D^i\gamma(x+h+t)) - \partial x_j(D^i\gamma(x))}{|\xi_{i,x+h+t} - \xi_{i,x}|^s} \frac{|(\nabla D^i\gamma(x) + \cdot h) - (\nabla D^i\gamma(x+h) + \cdot h)|}{|h|^\beta |t|^{1+s-\beta}}
\]

\[
\leq \sqrt{d}\gamma|_{C^0(\mathbb{R}^d)} \sup_{x,t\in\mathbb{R}^d, |t|\leq|h|} \frac{|h|^{1-\beta}(|h|^s + |t|^s)}{|h|^\beta} \leq 2\sqrt{d}\gamma|_{C^0(\mathbb{R}^d)}.
\]

and then the term (iii) can be bounded as (iii) \( \leq 2\sqrt{d}\gamma|_{C^0(\mathbb{R}^d)} \). Finally the norm of \( \|D_{h,\beta}\gamma\|_{C^{\alpha-\beta}(\mathbb{R}^d)} \) can be bounded as

\[
\|D_{h,\beta}\gamma\|_{C^{\alpha-\beta}(\mathbb{R}^d)} \leq (i)+(ii)+(iii) \leq 2\|\gamma\|_{C^0(\mathbb{R}^d)} + (2\sqrt{d}) \sum_{k=1}^{A-1} |a|_{C^k(\mathbb{R}^d)} + \sqrt{d}\gamma|_{C^A(\mathbb{R}^d)} + (1+2\sqrt{d})\gamma|_{C^0(\mathbb{R}^d)}.
\]
By comparing this expression with the one obtained in the previous case it is possible to conclude that \( \forall h \in \mathbb{R}^d, 0 < \beta \leq \min\{\alpha, 1\} \) it holds

\[
\|D_{h, \beta} \gamma\|_{C^{\alpha-s}(\mathbb{R}^d)} \leq (1 + 2\sqrt{d})\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)}, \quad |D_{h, \beta} \gamma|_{C^{\alpha-s}(\mathbb{R}^d)} \leq 2\sqrt{d}\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)}.
\]

Lemma A.2. Let \( \gamma(x) \in C^\alpha(\mathbb{R}^d) \) be a deterministic function as in Lemma A.1, and let \( \gamma'(x) \) be a smoothed version of \( \gamma(x) \) as in (11). It holds:

\[
\|\gamma - \gamma'\|_{C^0(\mathbb{R}^d)} \leq C(\alpha, d)\|\gamma\|_{C^{\min\{\alpha, 2\}}(\mathbb{R}^d)} e^{\min\{\alpha, 2\}},
\]

where \( C(\alpha, d) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}^d} |y|^\alpha e^{-\|x\|^2} \, dy \).

Proof. By definition we have

\[
\|(\gamma - \gamma')(x)\| = \left\| \int_{\mathbb{R}^d} (\gamma(x + y) - \gamma(x)) \phi_\epsilon(y) \, dy \right\| \quad \forall x \in \mathbb{R}^d.
\]

- Let us start with the case \( 0 < \alpha \leq 1 \): if \( \gamma(x) \in C^\alpha(\mathbb{R}^d) \) then we obtain

\[
\|(\gamma - \gamma')(x)\| \leq \int_{\mathbb{R}^d} \left| \frac{\gamma(x + y) - \gamma(x)}{|y|^\alpha} \right| |y|^\alpha \phi_\epsilon(y) \, dy \leq \|\gamma\|_{C^\alpha(\mathbb{R}^d)} \int_{\mathbb{R}^d} |y|^\alpha \phi_\epsilon(y) \, dy \leq C(\alpha, d)\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)} e^\alpha.
\]

- If \( 1 < \alpha \leq 2 \) we consider a Taylor expansion of \( \gamma(x + y) \) around \( x \) and set \( \alpha = 1 + s \) with \( s \in (0, 1] \). Since odd moments of a normal distribution vanish, we get:

\[
\|(\gamma - \gamma')(x)\| = \left\| \int_{\mathbb{R}^d} \left( \nabla \gamma(x) \cdot y + (\nabla \gamma(\xi x^+ y) - \nabla \gamma(x)) \cdot y \right) \phi_\epsilon(y) \, dy \right\|
\]

\[
\int_{\mathbb{R}^d} \max_{|\xi| = 1} \left| \frac{D^\alpha(\xi x^+ y) - D^\alpha(\gamma(x))}{\xi x^+ y - y} \right| \sqrt{d} |y|^{1+s} \phi_\epsilon(y) \, dy \leq C(\alpha, d)\sqrt{d}\|\gamma\|_{C^{\alpha}(\mathbb{R}^d)} e^\alpha.
\]

- Finally by considering \( 2 < \alpha \) and by expanding further the function \( \gamma \), since the second moment of a normal distribution does not vanish, we get:

\[
\|(\gamma - \gamma')(x)\| = \left\| \int_{\mathbb{R}^d} \left( \nabla \gamma(x) \cdot y + \sum_{j,k=1}^d \frac{\partial^2 \gamma}{\partial x_j \partial x_k}(\xi x^+ y) y_j y_k \right) \phi_\epsilon(y) \, dy \right\|
\]

\[
\leq C(\alpha, d)\|\gamma\|_{C^2(\mathbb{R}^d)} e^2.
\]

Lemma A.3. Let \( \gamma(x) \in C^\alpha(\overline{T}) \) and \( \gamma'(x) \in C^\alpha(\overline{T}) \) be two deterministic functions and let \( a(x) = e^{\gamma(x)} \) and \( a'(x) = e^{\gamma'(x)} \). For any \( 0 < \beta \leq \min\{1, \alpha\} \) it holds

\[
\|a - a'\|_{C^\beta(\overline{T})} \leq \|a\|_{C^0(\overline{T})} \|1 + \frac{a'}{a}\|_{C^0(\overline{T})} \left( 1 + \|\gamma\|_{C^\alpha(\overline{T})} \right) \|\gamma - \gamma'\|_{C^\beta(\overline{T})}.
\]

Proof. We bound separately the terms coming from the definition of the \( C^\beta \) norm, namely \( \|a - a'\|_{C^\beta(\overline{T})} = \|a - a'\|_{C^0(\overline{T})} + |a - a'|_{C^\alpha(\overline{T})} \). For the first one we simply observe that

\[
\|a - a'\|_{C^0(\overline{T})} \leq \|e^\gamma + e^{\gamma'}\|_{C^0(\overline{T})} \|\gamma - \gamma'\|_{C^\alpha(\overline{T})}.
\]

For the second term we start by considering the inequality

\[
|a - a'|_{C^\beta(\overline{T})} \leq \|e^\gamma\|_{C^0(\overline{T})} \left( 1 - e^{\gamma} \right)_{C^\beta(\overline{T})} + \|e^{\gamma'}\|_{C^\alpha(\overline{T})} \left( 1 - e^{\gamma} \right)_{C^\beta(\overline{T})}.
\]
The terms in the above equation can be bounded as follows:

\[(i) \leq \|e^{\gamma^* - \gamma}\|_{C^\alpha(\bar{D})} \|\gamma^* - \gamma\|_{C^{\beta}(\bar{D})},\]

\[(ii) \leq \|e^{\gamma}\|_{C^\alpha(\bar{D})} \|\gamma\|_{C^{\beta}(\bar{D})},\]

\[(iii) \leq \left(1 + e^{\gamma^* - \gamma}\right) \|\gamma^* - \gamma\|_{C^\alpha(\bar{D})}.\]

By putting everything together we obtain

\[
\|a - a^\alpha\|_{C^\alpha(\bar{D})} \leq \left(\|e^{\gamma} + e^{\gamma^*}\|_{C^\alpha(\bar{D})} + \|e^{\gamma}\|_{C^\alpha(\bar{D})} \|\gamma\|_{C^{\beta}(\bar{D})}\right) \left(1 + e^{\gamma^* - \gamma}\right) \|\gamma^* - \gamma\|_{C^\alpha(\bar{D})}

+ \|e^{\gamma}\|_{C^\alpha(\bar{D})} \|e^{\gamma^* - \gamma}\|_{C^\alpha(\bar{D})} \|\gamma^* - \gamma\|_{C^{\beta}(\bar{D})}

\leq \|e^{\gamma}\|_{C^\alpha(\bar{D})} \|1 + e^{\gamma^* - \gamma}\|_{C^\alpha(\bar{D})} (1 + \|\gamma\|_{C^{\beta}(\bar{D})}) \|\gamma^* - \gamma\|_{C^{\beta}(\bar{D})}

\]

which is the desired result.

Thanks to these results we can prove Lemma 5.2.

\[\text{Proof. (of Lemma 5.2.) From lemma A.1 we have that } \hat{\gamma} \in C^\alpha(\mathbb{R}^d) \text{ implies } D_{h, \beta} \hat{\gamma} \in C^{\alpha-\beta}(\mathbb{R}^d) \forall \beta \leq \min(\alpha, 1). \text{ By using the definitions given in (17), thanks to Lemmas A.2 and A.1 we get}

\[
\|D_{h, \beta} \hat{\gamma} - (D_{h, \beta} \hat{\gamma})^*\|_{C^\alpha(\mathbb{R}^d)} \leq |D_{h, \beta} \hat{\gamma}|_{C^{\min(\alpha-\beta, 2)}(\mathbb{R}^d)} \epsilon^{\min(\alpha-\beta, 2)}

\leq |\hat{\gamma}|_{C^{\min(\alpha-2+\beta)}(\mathbb{R}^d)} \epsilon^{\min(\alpha-\beta, 2)}

\]

Since \(D_{h, \beta} \gamma^* = (D_{h, \beta} \hat{\gamma})^*\) and thanks to the fact that the previous estimate is valid uniformly in \(h\), we can take the supremum of \(\|D_{h, \beta} \gamma - (D_{h, \beta} \gamma)^*\|_{C^0(\mathbb{R}^d)}\) with respect to \(h\). By doing this we get

\[|\hat{\gamma} - \gamma^*|_{C^\beta(\mathbb{R}^d)} \leq \sup_{h \in \mathbb{R}^d} \|D_{h, \beta} \gamma - (D_{h, \beta} \gamma)^*\|_{C^0(\mathbb{R}^d)} \leq |\hat{\gamma}|_{C^{\min(\alpha, 2+\beta)}(\mathbb{R}^d)} \epsilon^{\min(\alpha-\beta, 2)}.

\]

Now we get the desired result by observing that \(|\hat{\gamma}|_{C^\alpha(\mathbb{R}^d)} \leq \|\varphi\|_{C^\alpha(D_1)} \|\gamma\|_{C^\alpha(D_1)}\). In fact, since \(\varphi\) vanishes on \(D_1^c\), we obtain

\[|\hat{\gamma}|_{C^\alpha(\mathbb{R}^d)} = \max \left\{\sup_{x \in D_1, y \in \mathbb{R}^d} |\gamma(x)(\varphi(x) - \varphi(y)) + \varphi(y)(\gamma(x) - \gamma(y))|, \sup_{y \in D_1, x \in \mathbb{R}^d} |\gamma(y)(\varphi(y) - \varphi(x)) + \varphi(x)(\gamma(y) - \gamma(x))| \right\}

\leq \max \left\{\|\gamma\|_{C^\alpha(D_1)} \|\varphi\|_{C^\alpha(\mathbb{R}^d)} + \sup_{x \in D_1} \frac{|\varphi(y)(\gamma(x) - \gamma(y))|}{|x - y|^\alpha}, \|\gamma\|_{C^\alpha(D_1)} \|\varphi\|_{C^\alpha(\mathbb{R}^d)} + \sup_{y \in D_1} \frac{|\varphi(x)(\gamma(y) - \gamma(x))|}{|x - y|^\alpha} \right\}

\leq \|\gamma\|_{C^\alpha(D_1)} \|\varphi\|_{C^\alpha(\mathbb{R}^d)} + \|\gamma\|_{C^\alpha(D_1)} \|\gamma\|_{C^\alpha(D_1)} = \|\gamma\|_{C^\alpha(D_1)} \|\varphi\|_{C^\alpha(D_1)} + \|\gamma\|_{C^\alpha(D_1)} \|\varphi\|_{C^{\min(\alpha, 2+\beta)}(\mathbb{R}^d)} \|\gamma\|_{C^{\alpha-\beta}(\mathbb{R}^d)} \leq \|\varphi\|_{C^\alpha(D_1)} \|\gamma\|_{C^\alpha(D_1)}.

Hence, by considering the inequality given in Lemma A.3:

\[\|a - a^\alpha\|_{C^\alpha(\bar{D})} \leq \|a\|_{C^0(\bar{D})} \|1 + \frac{a^\alpha}{a}\|_{C^\alpha(\bar{D})} \|1 + \log(a)\|_{C^\alpha(\bar{D})} \|\gamma - \gamma^*\|_{C^\alpha(\bar{D})} \text{ a.s. in } \Omega;

\]

since in \(D\) it holds \(\gamma = \hat{\gamma}\) we get \(\|\gamma - \gamma^*\|_{C^\alpha(\bar{D})} = \|\hat{\gamma} - \gamma^*\|_{C^\alpha(\bar{D})} \leq \|\hat{\gamma} - \gamma^*\|_{C^\alpha(\mathbb{R}^d)}\) and we can conclude that

\[
\|a - a^\alpha\|_{C^\alpha(\bar{D})} \leq \|a\|_{C^0(\bar{D})} \left(1 + \frac{a^\alpha}{a}\right) \|1 + \frac{a^\alpha}{a}\|_{C^\alpha(\bar{D})} \|1 + \log(a)\|_{C^\alpha(\bar{D})} \|\gamma - \gamma^*\|_{C^{\min(\alpha, 2+\beta)}(\mathbb{R}^d)} \|\gamma\|_{C^{\min(\alpha, 2+\beta)}(\mathbb{R}^d)} \epsilon^{\min(\alpha-\beta, 2)}

\leq C_{5,2}(\omega, \alpha) \epsilon^{\min(\alpha-\beta, 2)}.

\]
To prove the second bound concerning the $C^1$ norm when $\alpha > 1$ we start again from the definition:

$$\|a - a^\prime\|_{C^1(\Omega)} = \|a - a^\prime\|_{C^0(\Omega)} + \max_{|I| = 1} \|D^i(a - a^\prime)\|_{C^0(\Omega)}.$$ 

The first term, thanks to Lemma A.2, can be bounded as

$$\|a - a^\prime\|_{C^0(\Omega)} \leq \max_{|I| = 1} \|1 + e^\gamma - \gamma\|_{C^0(\Omega)} \|\gamma - \gamma^\prime\|_{C^0(\Omega)} \leq \max_{|I| = 1} \|1 + e^\gamma - \gamma\|_{C^0(\Omega)} \|\varphi\|_{C^{\min(\alpha, 2)}(\Omega)} \|\gamma\|_{C^{\min(\alpha, 2)}(\Omega)} \|\epsilon\|_{C^{\min(\alpha, 2)}(\Omega)}^{\min(\alpha, 2)}.$$ 

For the second term, since the derivatives and the convolution commute, we obtain

$$D^\prime \left(e^\gamma \left(1 - e^\gamma\right)\right) \leq |e^\gamma D^\prime\gamma(1 - e^\gamma) + e^\gamma e^\gamma D^\prime\gamma(\epsilon\gamma - \gamma)| \leq e^\gamma \left(1 + e^\gamma\right) \left(\|D^\prime\gamma\|_{\gamma^\prime - \gamma} + \|D^\prime\gamma - (D^\prime\gamma)\|\right)$$ 

therefore we get

$$\|D^i(a - a^\prime)\|_{C^0(\Omega)} \leq \max_{|I| = 1} \left[1 + e^\gamma - \gamma\right] \left(\|D^\prime\gamma\|_{C^0(\Omega)} \|\gamma - \gamma^\prime\|_{C^0(\Omega)} + \|D^\prime\gamma - (D^\prime\gamma)\|_{C^0(\Omega)}\right)$$ 

$$\leq \max_{|I| = 1} \left[1 + e^\gamma - \gamma\right] \left(\|D^\prime\gamma\|_{C^0(\Omega)} \|\gamma\|_{C^{\min(\alpha, 2)}(\Omega)} + \|\gamma\|_{C^{\min(\alpha, 2)}(\Omega)} \|\epsilon\|_{C^{\min(\alpha, 2)}(\Omega)}^{\min(\alpha, 2)}\right)$$ 

which implies

$$\max_{|I| = 1} \|D^i(a - a^\prime)\|_{C^0(\Omega)} \leq \max_{|I| = 1} \left[1 + e^\gamma - \gamma\right] \left(\|\gamma\|_{C^1(\Omega)} \|\gamma\|_{C^{\min(\alpha, 2)}(\Omega)} \|\epsilon\|_{C^{\min(\alpha, 2)}(\Omega)}^{\min(\alpha, 2)} + \|\gamma\|_{C^{\min(\alpha, 2)}(\Omega)} \|\epsilon\|_{C^{\min(\alpha, 2)}(\Omega)}^{\min(\alpha, 2)}\right).$$ 

Finally, by putting everything together, and by recalling that $|\gamma|_{C^\beta(\Omega)} \leq \|\varphi\|_{C^\beta(\Omega)} \|\gamma\|_{C^\beta(\Omega)}$ for all $\beta \in \mathbb{R}_+$, we get the desired result:

$$\|a - a^\prime\|_{C^1(\Omega)} \leq \max_{|I| = 1} \left[1 + e^\gamma - \gamma\right] \left(1 + |\gamma|_{C^1(\Omega)} \right) \|\gamma\|_{C^{\min(\alpha, 3)}(\Omega)} \|\varphi\|_{C^{\min(\alpha, 3)}(\Omega)}^{\min(\alpha, 2)} \|\epsilon\|_{C^{\min(\alpha, 2)}(\Omega)}^{\min(\alpha, 2)}, \text{ a.s. in } \Omega.$$ 

\[\square\]

### B Products of Hölder and Sobolev functions

**Lemma B.1.** Let $b \in C^\alpha(\Omega)$ and let $v$ be a function in $H^\beta(D)$ for some $0 < \beta < \alpha \leq 1$. It holds

$$\|bv\|_{H^\beta(D)} \leq \frac{1}{\sqrt{\eta}} \|b\|_{C^{\beta+\eta}} \|v\|_{H^\beta(D)} \quad \forall 0 < \eta \leq \alpha - \beta.$$

**Proof.** By definition the $H^\beta$ norm of the function $bv$ is

$$\|bv\|_{H^\beta(D)}^2 = \|bv\|_{L^2(D)}^2 + \|v\|_{H^\beta(D)}^2 = \|bv\|_{L^2(D)}^2 + \int_{D \times D} \frac{\|b(x)v(x) - b(y)v(y)\|^2}{|x - y|^{d+2\beta}} dx dy.$$ 

The first term can be easily bounded as $\|bv\|_{L^2(D)}^2 \leq \|b\|_{C^0(\Omega)}^2 \|v\|_{L^2(D)}^2$. For the second term we obtain

$$\int_{D \times D} \frac{\|b(x)v(x) - b(y)v(y)\|^2}{|x - y|^{d+2\beta}} dx dy \leq 2\|b\|_{C^0(\Omega)}^2 \|v\|_{H^\beta(D)}^2 + 2 \int_{D \times D} \frac{\|b(x) - b(y)\|^2}{|x - y|^{2(|\beta+\eta|)}} \|v\|_2^2 dx dy$$ 

$$\leq 2\|b\|_{C^0(\Omega)}^2 \|v\|_{H^\beta(D)}^2 + 2 \|b\|_{C^{\beta+\eta}(\Omega)}^2 \int_{D \times D} \frac{\|v\|_2^2}{|x - y|^{d-2\eta}} dx dy.$$ 

If we extend $v$ by 0 in $\mathbb{R}^d \setminus D$, and denote $\hat{v}$ this extension and $\rho = \max_{x \in D} |x|$, the integral appearing in the right hand side of the above inequality can be bounded as

$$\int_{D \times D} \frac{\|v\|_2^2}{|x - y|^{d-2\eta}} dx dy \leq \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{\hat{v}(y)^2}{|x - y|^{d-2\eta}} 1_{\{|x - y| \leq 2\rho\}} dx dy \leq \|\hat{v}\|_{L^1(\mathbb{R}^d)}^2 \|1_{\{|x| \leq 2\rho\}}\|_{L^1(\mathbb{R}^d)} \leq \frac{\rho^{2\eta}}{\eta} \|v\|_{L^2(D)}^2.$$
By putting everything together we obtain
\[ \|bv\|_{H^\beta(D)} \lesssim \frac{1}{\sqrt{h}} \|b\|_{C^{\beta+n}(\overline{D})} \|v\|_{H^\beta(D)}, \]
which is the desired result. \(\square\)

C  Regularity of Gaussian random fields with Matérn Covariance

**Lemma C.1.** Let \(\widetilde{\text{cov}}_\gamma(|x - y|)\) be a covariance function belonging to the Matérn family defined in (5) on an open bounded convex domain \(D\). Then, if \(\nu\) is not an integer, \(\widetilde{\text{cov}}_\gamma \in C^{2\nu}(\overline{D} \times \overline{D})\), otherwise \(\widetilde{\text{cov}}_\gamma \in C^\nu(\overline{D} \times \overline{D})\) for any \(\alpha < 2\nu\) if \(\nu \in \mathbb{N}_+\).

**Proof.** By definition we have
\[
\text{cov}_\gamma(x_1, x_2) = \widetilde{\text{cov}}_\gamma(|x_1 - x_2|) = \frac{\sigma^2}{\Gamma(\nu)2^{\nu-1}} \left( \sqrt{2\nu} \frac{|x_1 - x_2|}{L_c} \right)^\nu K_\nu \left( \sqrt{2\nu} \frac{|x_1 - x_2|}{L_c} \right);
\]

where
\[ K_\nu : \mathbb{R}_+ \to \mathbb{R}_+ \text{ is given by } K_\nu(\rho) = \frac{\pi^{\frac{\nu}{2}}}{\Gamma(\nu)} (I_{-\nu}(\rho) - I_\nu(\rho)) \text{ where } I_\alpha(\rho) = \sum_{m=0}^{\infty} \frac{\rho^m}{m! \Gamma(m+\alpha)} \left( \frac{\rho}{2} \right)^{2m+\alpha}. \]

This formula is valid when \(\nu\) is not an integer, i.e. \(\nu = n + s\) with \(n \in \mathbb{N}\) and \(s \in (0,1)\). Since \(\forall \epsilon > 0\) the function \(K_\nu \in C^{\infty}([\epsilon, +\infty)\), and consequently \(\widetilde{\text{cov}}_\gamma\) as well, in order to prove the result we focus on the asymptotic behavior of the function \(\widetilde{\text{cov}}_\gamma(|x - y|)\) in a neighborhood of \(|x - y| = 0\).

By denoting \(\lambda_\nu = \frac{\sqrt{2\nu}}{L_c}\) and by recalling that, for any \(x \in \mathbb{R} \setminus \mathbb{Z}\) it holds \(\Gamma(-x) = \frac{\pi}{\sin \pi x} \Gamma(x+1)\), it is possible to obtain
\[
\widetilde{\text{cov}}_\gamma(|x_1 - x_2|) = \sigma^2 \frac{\sqrt{2\nu}}{\Gamma(\nu) \sin \pi \nu} \left( \sum_{m=0}^{\infty} \frac{\lambda_\nu^{2m} |x_1 - x_2|^{2m}}{m! \Gamma(m - \nu + 1)} - \sum_{m=0}^{\infty} \frac{\lambda_\nu^{2(m+\nu)} |x_1 - x_2|^{2(m+\nu)}}{m! \Gamma(m + \nu + 1)} \right)\]
\[= \sigma^2 \left( \sum_{m=0}^{n} \frac{(-1)^m \Gamma(\nu - m) \lambda_\nu^{2m} |x_1 - x_2|^{2m}}{m! \Gamma(\nu)} - \frac{\lambda_\nu^{2\nu} |x_1 - x_2|^{2\nu}}{\Gamma(\nu) \Gamma(\nu + 1) \sin(\pi \nu)} \right)\]
\[+ \frac{\sigma^2}{\Gamma(\nu) \sin \pi \nu} \left( \sum_{m=0}^{\infty} \frac{\lambda_\nu^{2(m+n)} |x_1 - x_2|^{2(m+n)}}{(m+n)! \Gamma(m + n - \nu + 1)} - \frac{\lambda_\nu^{2(m+\nu)} |x_1 - x_2|^{2(m+\nu)}}{m! \Gamma(m + \nu + 1)} \right).\]

Hence, the asymptotic behavior is
\[ \widetilde{\text{cov}}_\gamma(|x_1 - x_2|) \sim \sigma^2 \left\{ \sum_{m=0}^{n} \left( \frac{(-1)^m \Gamma(\nu - m) \lambda_\nu^{2m} |x_1 - x_2|^{2m}}{m! \Gamma(\nu)} - \frac{\lambda_\nu^{2\nu} |x_1 - x_2|^{2\nu}}{\Gamma(\nu) \Gamma(\nu + 1) \sin(\pi \nu)} \right) \right\}.\]

(25)

Since the function \(f(z) = |z|^{2\nu} : \mathbb{R}^d \to \mathbb{R}\) belongs to the space \(C^{2\nu}(\overline{D})\) we can conclude that \(\widetilde{\text{cov}}_\gamma \in C^{2\nu}(\overline{D} \times \overline{D})\).

When \(\nu = n \in \mathbb{N}_+\) the previous definition gives removable indeterminate values of the form \(\frac{0}{0}\); in this case the Bessel function \(K_\nu\) can be defined through the limit \(K_\nu(\rho) = \lim_{\nu \to n} K_\nu(\rho)\). The
covariance function becomes:
\[
\tilde{\text{cov}}_\gamma(|x_1 - x_2|) = \lim_{\nu \to \infty} \frac{\sigma^2 \pi}{\Gamma(\nu) \sin \nu \pi} \left( \sum_{m=0}^{\infty} \frac{\lambda^2_{\nu} |x_1 - x_2|^{2m}}{m! \Gamma(m - \nu + 1)} - \sum_{m=0}^{\infty} \frac{\lambda^2_{\nu} |x_1 - x_2|^{2(m+\nu)}}{m! \Gamma(m + \nu + 1)} \right)
\]
\[
= \sigma^2 \sum_{m=0}^{\infty} \frac{(-1)^m (n - m - 1)! \lambda^2_{\nu}}{m! |x_1 - x_2|^{2m}}
+ \lim_{\nu \to \infty} \frac{\sigma^2}{\Gamma(\nu) \sin \nu \pi} \left( \sum_{m=0}^{\infty} \frac{\lambda^2_{\nu} |x_1 - x_2|^{2(m+n)}}{(m+n)! \Gamma(m+n-\nu+1) \Gamma(m+n+\nu+1)} \left( m! (\Gamma(m+n+1) - \Gamma(m+n+1)) \right) \right)
\]
\[
= \sigma^2 \sum_{m=0}^{\infty} \frac{(-1)^m (n - m - 1)! \lambda^2_{\nu}}{m! |x_1 - x_2|^{2m}}
+ \frac{(-1)^{n+1} \sigma^2}{(n-1)!} \sum_{m=0}^{\infty} \frac{\lambda^2_{\nu} |x_1 - x_2|^{2m+2n}}{(m+n)! \Gamma(m+n+1) \Gamma(m+n-\nu+1) \Gamma(m+n+\nu+1)} \left( m! (\Gamma(m+n+1) - \Gamma(m+n+1)) \right)
\]
Again we focus on the asymptotic behavior of the function \(\tilde{\text{cov}}_\gamma(|x_1 - x_2|)\) in a neighborhood of \(|x_1 - x_2| = 0\). We obtain
\[
\tilde{\text{cov}}_\gamma(|x_1 - x_2|) \sim \sigma^2 \left\{ \sum_{m=0}^{\infty} \frac{(-1)^m (n - m - 1)! \lambda^2_{\nu}}{m! |x_1 - x_2|^{2m}} - \frac{(-1)^n 2 \lambda^2_{\nu}}{n! |x_1 - x_2|^{2n} \log (\lambda_n |x_1 - x_2|)} \right\}
\]
Since the function \(f(z) = |z|^{2n} \log(|z|) : \mathbb{R}^d \to \mathbb{R}\) belongs to the space \(C^\alpha(\hat{D})\) for any \(\alpha < 2\nu\) we can conclude that \(\tilde{\text{cov}}_\gamma \in C^\alpha(\hat{D} \times \hat{D})\) for any \(\alpha < 2\nu\).

**Remark.** Let \(\text{cov}_\gamma(|x - y|)\) be a covariance function belonging to the Matérn family defined in (5) and let \(\gamma(x, \omega)\) be a centered Gaussian random field defined on \(\hat{D}\). Denote \(\nu = n + \alpha\) with \(n \in \mathbb{N}\) and \(\alpha \in (0, 1)\). Then, for any multi-index \(i \in \mathbb{N}^d\) such that \(|i| \leq n\), it holds:
\[
\mathbb{E}[D^i \gamma(x, \cdot) D^i \gamma(y, \cdot)] = \frac{\partial^{2|i|}}{\partial x_1^{i_1} \cdots \partial x_d^{i_d} \partial y_1^{i_1} \cdots \partial y_d^{i_d}} \text{cov}_\gamma(|x - y|).
\]

**Lemma C.2.** Let \(\gamma(x, \omega)\) be a centered Gaussian random field with covariance function \(\tilde{\text{cov}}_\gamma\) as in Lemma C.1. Then \(\gamma\) admits a version with trajectories a.s. in \(C^{\alpha}\) form any \(0 < \alpha < \nu\).

**Proof.** Let us start with the case in which \(\nu\) is not an integer. Lemma C.1 tells us that \(\tilde{\text{cov}}_\gamma \in C^{2\nu}(\hat{D})\). Therefore, thanks to (26), by writing \(\nu = n + s\) with \(n \in \mathbb{N}\) and \(s \in (0, 1)\), for any multi-index \(i \in \mathbb{N}^d\) such that \(|i| = n\), we obtain
\[
\mathbb{E}[(D^i \gamma(x, \cdot) - D^i \gamma(y, \cdot))^2] = \mathbb{E}[(D^i \gamma(x, \cdot))^2] + \mathbb{E}[(D^i \gamma(y, \cdot))^2] - 2 \mathbb{E}[D^i \gamma(x, \cdot) D^i \gamma(y, \cdot)] = \frac{\partial^{2|i|}}{\partial x_1^{i_1} \cdots \partial x_d^{i_d} \partial y_1^{i_1} \cdots \partial y_d^{i_d}} \text{cov}_\gamma(|x - y|) \leq C(\nu)|x - y|^{2s},
\]
where the last inequality comes from the fact that the coefficients appearing in the covariance function decay sufficiently fast. Since for any positive integer \( p \) it holds \( \mathbb{E}[(\partial^2 \gamma(x, \cdot) - \partial^2 \gamma(y, \cdot))^2] \leq c_p \mathbb{E}[(\partial^2 \gamma(x, \cdot) - \partial^2 \gamma(y, \cdot))^2] \) with \( c_p = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} x^{2p} e^{-\frac{x^2}{2}} \, dx \) we have

\[
\mathbb{E}[(\partial^2 \gamma(x, \cdot) - \partial^2 \gamma(y, \cdot))^2] \leq c_p C(\nu) \mathbb{E}|x - y|^{2p}.
\]

Thanks to the Kolmogorov continuity theorem (see e.g., [27]) we can deduce that there exists a version of \( \partial^2 \gamma \) which belongs to \( C^\alpha(\bar{D}) \) for any \( a < \frac{2p-\beta}{2p} \); by taking the limit for \( p \to +\infty \) we can conclude that there exist a version of \( \partial^2 \gamma \) which belongs to \( C^\alpha(\bar{D}) \) for any \( a \) strictly smaller than \( s \). Consequently, since this reasoning can be repeated for every \( k < n, k \in \mathbb{N} \), by picking 1 instead of \( s \), we deduce that there exist a version of \( \gamma \) which belongs to \( C^\alpha(\bar{D}) \) for any \( \alpha \) strictly smaller than \( \nu \). The proof in the case \( \nu \in \mathbb{N} \) is similar. By writing \( \nu = n + 1 \) in this case, thanks to (26), for any \( \epsilon > 0 \) and for any multi-index \( i \in \mathbb{N}^d \) such that \( |i|_1 = n \) we obtain

\[
\mathbb{E}[(\partial^2 \gamma(x, \cdot) - \partial^2 \gamma(y, \cdot))^2] \leq \bar{C}(\nu) \mathbb{E}|x - y|^{2}\epsilon.
\]

Again, thanks to the Kolmogorov continuity theorem we can deduce that there exists a version of \( \partial^2 \gamma \) which belongs to \( C^\alpha(\bar{D}) \) for any \( a < \frac{\beta}{2p} - \frac{\beta}{2p} \); thanks to the arbitrariness of \( \epsilon \) by taking the limit for \( p \to +\infty \) we can conclude that there exist a version of \( \partial^2 \gamma \) which belongs to \( C^\alpha(\bar{D}) \) for any \( a \) strictly smaller than 1. Consequently we deduce that there exist a version of \( \gamma \) which belongs to \( C^\alpha(\bar{D}) \) for any \( \alpha \) strictly smaller than \( \nu \). \( \square \)

### D Optimal rates in Theorem 5.1

Here we present a sharper bound for the infimum \( \inf_{0 \leq \beta \leq \min(a, 1)} \frac{h^{\beta \min(\alpha - \beta - \eta, 2)}}{(\alpha - \beta)^2 \sqrt{\eta}} \) than the one presented in Proposition 5.1 that can be obtained with very tedious calculations.

**Lemma D.1.** Let \( \epsilon \leq e^{-\frac{\alpha}{2}} \); the following bounds hold:

- \( 1/2 \leq \alpha \leq 1 \):

  \[
  \inf_{0 \leq \beta \leq \alpha} \frac{h^{\beta \alpha - \beta - \eta}}{(\alpha - \beta)^2 \sqrt{\eta}} \lesssim \begin{cases}
  h^{\alpha} |\log h|^2, & h \geq e^\epsilon, \\
  h^{\alpha} |\log h|^2, & h \leq e^{-\frac{2}{5}} \epsilon, \\
  e^{\alpha} |\log \epsilon|^2, & h \geq e^{-\frac{2}{5}} \epsilon.
  \end{cases}
  \]

- \( 1 < \alpha \leq 2 \):

  \[
  \inf_{0 \leq \beta \leq 1} \frac{h^{\beta \alpha - \beta - \eta}}{(\alpha - \beta)^2 \sqrt{\eta}} \lesssim \begin{cases}
  h^{\alpha - 1} |\log h|^2, & h \leq \min(e^{-\frac{3}{10}} \epsilon, e^{-\frac{2}{5}} \epsilon), \\
  h^{\alpha} |\log h|^2, & \min(e^{-\frac{3}{10}} \epsilon, e^{-\frac{2}{5}} \epsilon) \leq h \leq e^{-\frac{2}{5}} \epsilon, \\
  h^{\alpha} |\log h|^2, & h \leq e^{-\frac{2}{5}} \epsilon, \\
  h^{\alpha} |\log h|^2, & h \geq e^\epsilon, \\
  h^{\alpha} |\log h|^2, & h \leq e^{-\frac{2}{5}} \epsilon, \\
  h^{\alpha} |\log h|^2, & h \geq e^\epsilon, \\
  e^{\alpha} |\log \epsilon|^2, & h \geq e^{-\frac{2}{5}} \epsilon.
  \end{cases}
  \]
$2 < \alpha \leq 3$: 

\[
\inf_{0 \leq \beta \leq 1} \frac{h^\beta e^{\alpha-\beta-\eta}}{(\alpha-\beta)^2 \sqrt{\eta}} \lesssim \begin{cases} 
  h^\alpha |\log h|^{\frac{3}{2}}, & h \leq \min(e^{\frac{1}{\alpha-1}}, e^{-\frac{\alpha}{2\epsilon}}), \\
  h^\alpha |\log h|^{\frac{3}{2}}, & \min(e^{\frac{1}{\alpha-1}}, e^{-\frac{\alpha}{2\epsilon}}) \leq h \leq e^{-\frac{\alpha}{2\epsilon}}, \\
  h^\alpha \left|\log \frac{h}{\epsilon}\right|^2 \left|\log \epsilon\right|^{\frac{1}{2}}, & h \geq e^{\frac{1}{2}}, \
  h^\alpha \left|\log \frac{h}{\epsilon}\right|^2 \left|\log \epsilon\right|^{\frac{1}{2}}, & \text{if } e^{-\frac{\alpha}{2\epsilon}} \leq h \leq e^{-\frac{\alpha}{2\epsilon}}, \\
  e^\alpha |\log \epsilon|^{\frac{3}{2}}, & \text{if } \epsilon \geq e^{-\frac{1}{\alpha-1}}, \\
  h^{\alpha-2}\epsilon^2 |\log \epsilon|^{\frac{3}{2}}, & \text{if } \epsilon \leq e^{-\frac{1}{\alpha-1}}, \quad h \geq e^{-\frac{\alpha}{2} \epsilon}.
\end{cases}
\]

\[
\alpha > 3: 
\] 

\[
\inf_{0 \leq \beta \leq 1} \frac{h^\beta e^{\alpha-\beta-\eta}}{(\alpha-\beta)^2 \sqrt{\eta}} \lesssim h^2.
\]

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