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Jocelyne Erhel, Zoubida Mghazli, Mestapha Oumouni

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Abstract

In this work, we present a numerical analysis of a probabilistic approach to quantify the migration of a contaminant, under the presence of uncertainty on the permeability of the porous medium. More precisely, we consider the flow problem in a random porous medium coupled with the advection-diffusion equation and we are interested in the approximation of the mean spread and the mean dispersion of the solute. The conductivity field is represented by a Karhunen-Loève (K-L) decomposition of its logarithm. The flow model is solved using a mixed finite element method in the physical space. The advection-diffusion equation is computed thanks to a probabilistic particular method, where the concentration of the solute is the density function of a stochastic process. This process is solution of a stochastic differential equation (SDE), which is discretized using an Euler scheme. Then, the mean of the spread and of the dispersion are expressed as functions of the approximate stochastic process. A priori error estimates are established on the mean of the spread and of the dispersion. Numerical examples show the effectiveness of the approach.

key words: Elliptic and parabolic PDE with random coefficients, Karhunen-Loève expansion, Monte-Carlo method, Stochastic differential equation, Euler scheme.

Introduction

Mathematical modeling and numerical simulation are important tools in the prediction of pollutant transport in groundwater. In order to take into account the limited knowledge of the geological characteristics, the uncertainty and the lack of measures, the permeability coefficient is modeled as a random field. Then, a stochastic model allows to obtain numerical predictions describing closely the behavior of the real system.

Numerical models with random input data have been extensively studied recently. Classical Monte Carlo methods converge very slowly in general. Stochastic Galerkin methods as well as a stochastic collocation methods (see [1, 2, 12, 20, 26, 32, 33]) based on sparse tensor products have gained much attention since they are very effective and accurate for computing statistics from solutions of PDEs with random input data. In most of these methods, the conductivity field is first discretized in the probability space, usually with a truncated Karhunen-Loève (K-L) expansion to deal with finite dimension and a classical approximation in the physical space. However,

these approaches suffer from a curse of dimensionality, especially when the number of variables in the (K-L) expansion (stochastic dimension) is very large. Recently, a similar approach using a Quasi Monte Carlo method to solve a flow problem was proposed in [21, 25]. This method converges with the order $O(\frac{\log(M)^r}{M})$, where M is the number of simulations and the coefficient $r > 0$ increases with the dimension [31]. It seems theoretically that Quasi Monte Carlo also suffers from a curse of dimensionality, in particular for large scale problem.

Our objective is to study and to quantify the migration of a contaminant, by computing statistics of interest which are mean values of physical quantities [3, 4, 10, 9]. The stochastic model includes a flow problem coupled with an advection-diffusion equation. A log-normal random conductivity field a with a smooth correlation function is considered: $a = e^G$, where G is a Gaussian random field with a piecewise smooth covariance function.

The physical space is first discretized, then a discrete random conductivity field is generated as a piecewise and finite random variables (see [3, 4, 34, 35, 21, 13]). In [3, 4, 10, 9], a standard finite element method is used for the flow equation, yielding the random velocity field required in the transport model. The transport equation describes the concentration of the solute, and can be seen as a Fokker-Planck equation if the domain is infinite. It is related to a stochastic process which admits the concentration as a density function. This process is simulated with a random walk, which approximates the trajectories of particles thanks to a time discretization using an Euler scheme. The first quantity of interest here is the spreading, which is a function of the stochastic process. The second quantity of interest is the macro dispersion, defined as the temporal derivative of the spreading. Thanks to Itô's formula, the macro dispersion is also a function of the stochastic process [33, 7]. A classical Monte Carlo method is then used to estimate the mean values of the spreading and the macro dispersion.

Convergence of numerical results is analyzed in [3, 4, 9], showing the efficiency of the approach. A numerical analysis of this numerical model is proposed in [6] and [7], giving error bounds for the mean values of the quantities of interest.

In this paper, we also derive error bounds for the velocity field and for the mean values of quantities of interest, but with a different numerical model. In order to work with a velocity having regular trajectories, we choose to discretize the permeability field in the stochastic space through a truncated Karhunen-Loève (K-L) expansion. We then discretize the flow equation with a mixed finite element method rather than a classical finite element method, because it is well suited to flow equations thanks to nice properties. Indeed, it approximates both head and velocity with the same accuracy, and it ensures a local and a global mass conservation [23]. Error bounds are also studied for the flow equation with a log-normal random permeability field and a mixed finite element method in [22], but without a truncated (K-L) expansion.

In this paper, the transport equation is still solved with a random walk. Thanks to the regular trajectories of the velocity field, we obtain an accurate approximation of the stochastic transport process with respect to time discretization. Mean values of the spreading and the macro dispersion are still estimated by a classical Monte Carlo method.

As in [6] and [7], we propose a numerical analysis of this model with a (K-L)

expansion and a mixed finite element method. In order to establish error bound of the quantities of interest, we consider general test functions, namely the functions having a polynomial growth with its derivatives.

The paper is organized as follows. In section 1, we describe the physical model and the main quantities of interest. In section 2, the different steps of the numerical model are explained: the Karhunen-Loève (K-L) truncation of the permeability parameter, the mixed finite element method and the probabilistic particular method (random walk). In section 3, an error analysis of the approach is established. The first estimate gives error bounds for the outputs of the model, due to the (K-L) truncation. The second estimate gives a weak error for the random walk simulating the transport stochastic process, taking into account the time and space steps. Then the total error on the quantities of interest is established, taking into account all the numerical parameters, namely the time and space steps, the order of truncation of the permeability, the total number of simulations and the number of particles in the random walk. Finally, in section 4, we present a numerical bi-dimensional example, where the log-permeability has an exponential covariance in a square domain. Results illustrate the convergence and the efficiency of the approach.

1 Problem setting

1.1 Steady flow equation

The porous medium is assumed isotropic and the porosity is supposed constant, equal to 1. The Domain D is a bounded box in $\mathbb{R}^d$, $(d = 1, 2, 3)$. The permeability field a is modeled as a stochastic function to take into account the heterogeneity of the medium and the lack of data. Let $(\Omega, \mathcal{F}, dP)$ be a complete probability space. We consider the steady flow in a porous medium without source:

$$\begin{cases} v(\omega, x) = -a(\omega, x)\nabla p(\omega, x), & \text{in } \Omega \times D, \\ \text{div}(v)(\omega, x) = 0 & \text{in } \Omega \times D, \\ \text{Boundary conditions}, \end{cases} \tag{1}$$

where v is the velocity and p is the hydraulic head, both on $\Omega \times D$. The boundary conditions can be for example mixed or periodic boundary conditions, and imposed for almost all ω. The permeability field a follows a log-normal law and is given by the following transformation:

$$a(\omega, x) = e^{G(\omega,x)} \text{ on } \Omega \times D, \tag{2}$$

where G is a Gaussian field characterized by its covariance function

$$\text{cov}[G](x, y) = \sigma^2 \exp\left\{-\left(\frac{|x - y|}{l_c}\right)^{\delta}\right\},$$

where $|.|$ denotes the euclidian norm, $\delta > 0$, σ^2 is the variance of G and l_c is the correlation length. The field G is an infinite dimensional noise, hence for a numerical approximation, we choose a Karhunen-Loève (K-L) truncation to represent a in a finite dimensional space with regular trajectories.

1.2 Transport equation

An inert solute is injected into the porous medium. The migration of the solute is governed by convection, molecular diffusion and kinematic dispersion. Here, kinematic dispersion is neglected, molecular diffusion is assumed homogeneous and isotropic. Then, the migration of the solute is described by the following advection-diffusion equation:

$$\begin{cases} \partial_t c(\omega,t,x) + v(\omega,x)\nabla c(\omega,t,x) - D_m \triangle c(\omega,t,x) = 0 \quad \text{in } \Omega \times [0,T] \times D, \\ c(\omega,0,x) = c_0(x) \quad x \in D, \\ \text{Boundary conditions,} \end{cases} \tag{3}$$

where c is the concentration of the solute, D_m is the diffusion coefficient and c_0 is the initial condition at $t = 0$. For an injection of the solute, $c_0 = \frac{\mathbb{1}_B}{|B|}$ where B is a box with volume $|B|$ included in D. Equation (3) can be completed with Dirichlet, mixed or periodic boundary conditions on ∂D.

1.3 Quantities of interest

The main objective of our study is to compute the mean of the spread $\mathcal{S}(t)$ and the mean of the dispersion coefficient $\mathcal{D}_t$ (see [19]). First, let $\Gamma(\omega,t) = \int_D c(\omega,t,x)x dx$ be the center of mass of the solute distribution. Then we define $S(\omega,t)$ the spread of the solute around Γ and $D(\omega,t)$ the dispersion coefficient as:

$$S(\omega,t) = \int_D c(\omega,t,x)|x - \Gamma(\omega,t)|^2 dx \quad \text{and} \quad D(\omega,t) = \frac{1}{2}\frac{d}{dt}S(\omega,t). \tag{4}$$

Then we are interested by the mean of the quantities (4):

$$\mathcal{S}(t) = \mathbb{E}_\omega[S(\cdot,t)] \quad \text{and} \quad \mathcal{D}(t) = \mathbb{E}_\omega[D(\cdot,t)]. \tag{5}$$

In practice, the domain D is chosen very big versus the box of injection $\mathbf{B}$ and a very small amount of the solute gets at the boundary $\partial D (c_{\partial D} = 0)$. It is harmless to replace (3) by:

$$\begin{cases} \partial_t c(\omega,t,x) + v(\omega,x)\nabla c(\omega,t,x) - D_m \triangle c(\omega,t,x) = 0 \quad \text{in } \Omega \times [0,T] \times \mathbb{R}^d \\ c(\omega,0,x) = c_0(x) \quad x \in \mathbb{R}^d, \end{cases} \tag{6}$$

where the velocity v is extended continuously by zero outside a neighborhood of the domain D where the extension is smooth. We can also extend equation (3) on $\mathbb{R}^d$ when the boundary conditions are periodic and we have $\text{div}(v) = 0$ on $\mathbb{R}^d$.

The quantities of interest (4, 5) are given by an integral of c. Hence a probabilistic particle method is preferred to a deterministic method because it avoids to approximate the concentration c at each point in D. The method consists in simulating a cloud of particles throughout the physical domain. In equation (6), the concentration c is a law of a stochastic process which describes the movement of the particles. Another reason to choose a probabilistic particle approach is to avoid numerical diffusion [37].

In order to describe the probabilistic particular method, we introduce another probability space $(\Theta, \mathfrak{A}, \mathcal{P})$ which is independent of $(\Omega, \mathcal{F}, \mathcal{P})$. We consider a d-dimensional Brownian Motion $(W_t)_{t\geq 0}$ on Θ and a random variable ζ which is W_t-independent and admits c_0 as a density.

For each $\omega \in \Omega$, the function $c(\omega, \cdot, \cdot)$ is the unique solution of (6) as a probability function of $X_t(\omega, \cdot)$ solution of the following SDE (see [17]):

$$\begin{cases} dX_t(\omega, \theta) = v(\omega, X_t)dt + \sqrt{2D_m}dW_t(\theta) \\ X_0 = \zeta(\theta). \end{cases} \tag{7}$$

Not that because the drift v is not Lipschitz continuous (see [6]), the SDE (7) has not strong uniqueness, but only weak uniqueness, i.e the law of each solution X_t is unique. Since we are interested in quantities given by a functional of c, only weak uniqueness of (7) is needed. Therefore, the mean spread can be given by a variance of X_t as follows:

$$\mathcal{S}(t) = \mathbb{E}_\omega\left[\mathbb{E}_\theta\left[|X_t - \mathbb{E}_\theta[X_t]|^2\right]\right]. \tag{8}$$

The dispersion $\mathcal{D}(t)$ as a derivative of $\mathcal{S}(t)$ is estimated by Finite differences approximation in [6, 10, 18, 29], the result is very sensitive to the step taken [6]. Here we propose as in [7, 33] an explicit formula using Itô's formula:

$$\mathcal{D}(t) = \mathbb{E}_\omega\left[\mathbb{E}_\theta[< X_t, v(X_t) >] - < \mathbb{E}_\theta[X_t], \mathbb{E}_\theta[v(X_t)] >\right] + \text{trace}(D_m). \tag{9}$$

where we note by $< ., . >$, the scalar product in $\mathbb{R}^d$.

The quantities of interest studied here are the mean of the spread and the macro spreading given in (5). It follows that these quantities are given as the mean of some functions of the process X_t. Thus, for some vector valued and measurable functions f and g, we define the following quantity of interest

$$\mathcal{Q}(t) := \mathbb{E}_\omega\left[f\left(\mathbb{E}_\theta[g(X_t)]\right)\right]. \tag{10}$$

In practice, we are interested by the asymptotic behavior of the quantity (10). Therefore, we describe a numerical approach to approximate (10) and we establish an a priori error estimate on the proposed approximation at the final time.

2 Numerical approach

2.1 Stochastic approximation of the permeability

The spread $S(.,.)$ and dispersion $D(.,.)$ defined in (4) are both an infinite dimensional noise, since they depend on v which depends on the field G which is infinite dimensional noise. The first step consists of choosing a suitable discretization for G. The most widely used representation of a second order random field $G(\cdot, \cdot)$ is the Karhunen-Loève expansion (K-L) [27, 1, 11]. This decomposition is truncated up to an order N, to deal with a finite dimensional noise parameterized by N random

variables. The K-L expansion consists at decomposing G in the series of products of deterministic functions and random variables as follows:

$$G(\omega, x) = \mathbb{E}_\omega[G(\cdot, x)] + \sum_{n=1}^{\infty} \sqrt{\lambda_n} b_n(x) Y_n(\omega), \tag{11}$$

where $\lambda_1 \geq \lambda_2, \ldots > 0$ and $\{b_n\}_{n=1}^{\infty}$ are respectively the eigenvalues and the eigenfunctions solutions of the following eigenvalue problem:

$$\int_D \mathrm{cov}[G](x, y) b(y) dy = \lambda b(x), \tag{12}$$

where the random variables $\{Y_n\}_{n=1}^{\infty}$ are determined by:

$$Y_n(\omega) = \frac{1}{\sqrt{\lambda_n}} \int_D (G(\omega, x) - \mathbb{E}_\omega[G(\cdot, x)]) b_n(x) dx.$$

Since, the permeability field follows a log-normal law, G is a Gaussian field, hence the set of the random variables $\{Y_n\}_{n=1}^{N}$ are independent Gaussian random variables with mean zero and unit variance.

In general, the eigenvalue problem (12) for the (K-L) expansion has to be solved numerically, but in some particular cases, it can be solved analytically for a square or cubic box as the tensor product of one dimensional analytic solution.

For each $N > 1$, we assume that the eigenvalues $(\lambda_n)_{n\geq 1}^{N}$ and eigenfunctions $(b_n)_{n\geq 1}^{N}$ satisfy the following assumptions:

Assumptions 2.1

- *The eigenfunctions $(b_n)_{n=1}^{N}$ are twice continuously differentiable.*
- *The series $\sum_{n\geq 1}^{N} \lambda_n \|b_n\|_\infty^2$ is convergent.*

Not that such assumptions are fulfilled in the case $\delta = 1$ for an exponential covariance on a square or cubic domain or $\delta = 2$ for a Gaussian covariance, and more generally if the covariance function is an analytic function on $D \times D$ (see [1, 11]).

The first assumption is usually verified by a continuous covariance function and implies that the trajectories of a are sufficiently smooth. The second assumption is verified by a piecewise analytic covariance function and is necessary for the convergence truncated head p_N solution of (15) to a continuous head p (see [8]).

We define the truncated Karhunen-Loève expansion G_N as a truncation of the series (11) up to a suitable order N:

$$G_N(\omega, x) = \mathbb{E}_\omega[G(\cdot, x)] + \sum_{n=1}^{N} \sqrt{\lambda_n} b_n(x) Y_n(\omega) \tag{13}$$

The decomposition given in (13) is an optimal decomposition of G, with respect to the norm of $L^2(\Omega; L^2(D))$. We then approximate the permeability field a by a_N:

$$a_N(\omega, x) := e^{G_N(\omega, x)} = \exp\left(\mathbb{E}_\omega[G(\cdot, x)] + \sum_{n=1}^{N} \sqrt{\lambda_n} b_n(x) Y_n(\omega) \right). \tag{14}$$

Then, we replace the flow equation (1) by one associated with a_N:

$$\begin{cases} v_N(\omega,x) = -a_N(\omega,x)\nabla p_N(\omega,x), & \text{in } \Omega\times D,\\ \operatorname{div}(v_N)(\omega,x) = 0 & \text{in } \Omega\times D,\\ \text{Boundary conditions.} \end{cases} \tag{15}$$

The transport equation with a velocity field v_N of finite dimensional noise is given by:

$$\begin{cases} \partial_t c_N(\omega,t,x) + v_N(\omega,x)\nabla c_N(\omega,t,x) - D_m \triangle c_N(\omega,t,x) = 0 \quad \text{in } \Omega\times[0,T]\times\mathbb{R}^d,\\ c_N(\omega,0,x) = c_0(x) \quad x\in\mathbb{R}^d, \end{cases} \tag{16}$$

where v_N is extended to $\mathbb{R}^d$ as the velocity v. With periodic boundary conditions, $\operatorname{div}(v_N) = 0$ in $\mathbb{R}^d$.

The concentration c_N solution of (16) is an approximation of the concentration c solution of (6). For each $\omega\in\Omega$, $c_N(\omega,\cdot,\cdot)$ is the probability density of the process $X_N(\omega,\cdot,\cdot)$, solution of the following SDE on Θ:

$$\begin{cases} dX_N(\omega,t,\cdot) = v_N(\omega, X_N(\omega,t,\cdot))dt + \sqrt{2D_m}dW_t,\\ X_N(\omega,0,\cdot) = \zeta. \end{cases} \tag{17}$$

Note that since the trajectories of the drift v_N are Lipschitz continuous, the SDE (17) has a strong uniqueness.

Using the law of $X_N(\omega,t,\cdot)$ (a.e) for each $\omega\in\Omega$, we can approximate (10) by:

$$\mathcal{Q}_N(t) := \mathbb{E}_\omega\left[f\left(\mathbb{E}_\theta[g(X_N(t))]\right)\right]. \tag{18}$$

2.2 Monte-Carlo simulations

Monte-Carlo sampling is used to approximate the mean on Ω of the quantities of interest. We consider M realizations of the parameter $a_N(\omega_1,\cdot),\ldots,a_N(\omega_M,\cdot)$ of the permeability field. For each realization ω_i, we solve the flow equation (15) and the SDE (17). We approximate the quantity $\mathcal{Q}_N(t)$ in (18) by:

$$\mathcal{Q}_N(t) \approx \frac{1}{M}\sum_{i=1}^{M} Q_N(\omega_i,t),$$

where each realization of the quantity $Q_N(\omega_i,t)$ is computed by

$$Q_N(\omega_i,t) = f\left(\mathbb{E}_\theta[g(X_N(\omega_i,t))]\right). \tag{19}$$

2.3 Space discretization of the flow problem

For each realization ω_i, we have to solve the flow problem (15). We propose to use a mixed finite element method, which has several nice properties. Indeed, it approximates both p_N and v_N with the same accuracy and ensures local and global mass conservation.

With both Dirichlet and Neumann boundary conditions, the solution is not regular at the points where the Dirichlet and Neumann boundaries meet. These difficulties can be avoided by regularizing the solution at the critical points. The solution is regular with periodic or non-homogeneous Dirichlet regular boundary conditions. Here, to simplify the presentation, we consider a non-homogeneous Dirichlet boundary condition γ and assumed to be smooth on ∂D.

For (a.e) each $\omega_i \in \Omega$, a mixed formulation of (15) is given by the weak formulation (20):

Find $(p_N(\omega_i,.), v_N(\omega_i,.)) \in L^2(D) \times H(\mathrm{div}, D)$ such that

$$\begin{cases} \displaystyle\int_D a_N^{-1} v_N w dx - \int_D p_N \ \mathrm{div}(w) dx = -\int_{\partial D} \gamma w.\vec{n} dl & \forall w \in H(\mathrm{div}, D), \\ \displaystyle\int_D \mathrm{div}(v_N)\mu dx = 0 & \forall \mu \in L^2(D). \end{cases} \tag{20}$$

We consider $\{\mathcal{T}_h\}_{h>0}$, a regular triangulation of the domain D. Let $\mathcal{M}_h$ be the subspace of piecewise constants in $L^2(\Omega)$ and $RT_0(\mathcal{T}_h)$ be the 0-order Raviart-Thomas subspace in $H(div, D)$. For each ω_i, we define the approximate problem (21):

Find $(p_{N,h}(\omega_i,.), v_{N,h}(\omega_i,.)) \in \mathcal{M}_h \times RT_0(\mathcal{T}_h)$ such that

$$\begin{cases} \displaystyle\int_D a_N^{-1} v_{N,h} w_h dx - \int_D p_{N,h} \mathrm{div}(w_h) = -\int_{\partial D} \gamma w_h.\vec{n} dl & \forall w_h \in RT_0(\mathcal{T}_h) \\ \displaystyle\int_D \mathrm{div}(v_{N,h})\mu_h = 0, & \forall \mu_h \in \mathcal{M}_h. \end{cases} \tag{21}$$

Problem (21) is well-posed [5] for each (a.s) $\omega_i \in \Omega$ and $v_{N,h} \in L^p(\Omega; L^\infty(D))$. In the reference [22], an error analysis of the Mixed finite element is presented where the parameter a is not truncated. Thanks to the truncated K-L expansion, the solution (p_N, v_N) is smooth with respect to x. By using the error estimate for lowest order Raviart-Thomas interpolation [5, 22], there exists a constant C independent of h, v_N and p_N, such that

$$\|p_N - p_{N,h}\|_{L^p(\Omega;L^2(D))} + \|v_N - v_{N,h}\|_{L^p(\Omega;H(div,D))} \leq Ch\Big(\|v_N\|_{L^p(\Omega;H^1(D))} + \|p_N\|_{L^p(\Omega;H^1(D))} \Big). \tag{22}$$

2.4 Discrete transport equation

In order to discretize the advection-diffusion equation (16), we use a probabilistic particle method to avoid numerical diffusion. For each realization ω_i, $v_{N,h}(\omega_i,.)$ is the solution of (21) obtained with $a_N(\omega_i,.)$. We use an Euler scheme to discretize the equation (17) where v_N is replaced by $v_{N,h}$. For each $i = 1, \ldots, M$ the approximation $X_{N,\eta,h}(\omega_i, t, \theta)$ is given by the following scheme:

$$\begin{cases} X_{N,\eta,h}(\omega_i, t_{l+1}, \theta) = X_{N,\eta,h}(\omega_i, t_l, \theta) + v_{N,h}(\omega_i, X_{N,\eta,h}(t_l, \omega_i, \theta))dt + \sqrt{2D_m dt}\xi_{l+1}(\theta) \\ X_{N,\eta,h}(\omega_i, 0, \theta) = \zeta(\theta), \end{cases} \tag{23}$$

where $dt = \frac{T}{\eta}$ is a uniform step, $t_l = ldt$, $l = 0, \ldots, \eta$ and $\{\xi_l\}_{l=1}^{\eta}$ is a sequence of independent gaussian variables with zero mean and unit variance. We choose P realizations $\{X_{N,\eta,h}^{i,j}\}_{j=1}^{P}$

(the index i refers to the dependence of $X_{N,\eta,h}$ on ω_i and j refers to the dependance on θ_j). For each ω_i we approximate $Q_N(\omega_i, t)$ given in (19) by:

$$Q^P_{N,\eta,h}(\omega_i, t) = f\bigg(\frac{1}{P}\sum_{j=1}^{P} g(X^{i,j}_{N,\eta,h}(t))\bigg).$$

Thus, the quantity of interest $\mathcal{Q}_N(t)$ is approximated by $\mathcal{Q}^{M,P}_{N,\eta,h}$ given by:

$$\mathcal{Q}^{M,P}_{N,\eta,h}(t) := \frac{1}{M}\sum_{i=1}^{M} f\bigg(\frac{1}{P}\sum_{j=1}^{P} g(X^{i,j}_{N,\eta,h}(t))\bigg). \tag{24}$$

In the next section, we give an error analysis of the above algorithm, where we estimate the total weak error $|\mathcal{Q}(T) - \mathcal{Q}^{M,P}_{N,\eta,h}(T)|$.

3 Error analysis of the approach

In this section we derive the error estimates of the approach. It includes all the numerical parameters, namely the truncation error, temporal and spatial error and the statistical one. In what follows, we consider $\mathcal{C}^r_{pol}(\mathbb{R}^d)$ the space of functions which have a polynomial growth with their derivatives up to r and $\mathcal{C}^r_b(\mathbb{R}^d)$ the space of bounded functions and all their derivatives up to r are bounded. We note that when we deal with a realization of the random fields, the dependence with ω is noted once time and and omitted in the rest as in the notation of the random fields.

3.1 Truncation error

3.1.1 Convergence of a_N to a

Here we give a bound of the truncation error resulting from the truncation of the parameter $a \approx a_N$, where a_N is given by a suitable order N in the (K-L) expansion as in (14). The truncation error $v - v_N$ is nonzero and contributes to the total error on the quantities of interest. Then, it is necessary to study and take account this truncation error, to increase the reliability of the approximations.

Now we establish the convergence of a_N to a with respect to the norm of $L^q(\Omega, L^2(D))$, for $q \geq 1$. We define (a.e) the following bounds of a as given in [2, 8]:

$$a_{max}(\omega) = \max_{x\in\bar{D}} a(\omega, x) \;\text{ and }\; a_{min}(\omega) = \min_{x\in\bar{D}} a(\omega, x), \tag{25}$$

Under assumption 2.1, $a_{min} \in L^q(\Omega)$ and $a_{max} \in L^q(\Omega)$. In [8], a bound of the error $a - a_N$ is given in the space $L^q(\Omega; \mathcal{C}^0(\bar{D}))$, which depends on $\|b_n\|_\infty$, thus generally on λ_n. The following proposition concerns a bound of the error $\|a - a_N\|_{L^q(\Omega;L^2(D))}$.

Proposition 3.1 *There exists a constant $K > 0$ independent of N such that:*

$$\|a - a_N\|_{L^q(\Omega;L^2(D))} \leq K\sqrt{\sum_{n=N+1}^{\infty} \lambda_n}. \tag{26}$$

Proof: Thanks to the differentiability and the growth of the exponential function, the following inequality holds

$$|e^x - e^y| \leq \max(e^x, e^y)|x - y| \quad \forall x, y \in \mathbb{R}.$$

Applying this latter inequality with $x = G$ and $y = G_N$, we have

$$\begin{aligned}\|a(\omega,.) - a_N(\omega,.)\|_{L^2(D)} &\leq \|\max(e^{G(\omega,.)}, e^{G_N(\omega,.)})\|_{L^\infty(D)}\|G(\omega,.) - G_N(\omega,.))\|_{L^2(D)} \\ &\leq \|\max(e^{G(\omega,.)}, e^{G_N(\omega,.)})\|_{L^\infty(D)}\|G(\omega,.) - G_N(\omega,.))\|_{L^2(D)} \\ &\leq a_{max}(\omega)\sqrt{\sum_{n=N+1}^{\infty}\lambda_n Y_n(\omega)^2}.\end{aligned}$$

Taking the norm in $L^q(\Omega)$ and applying Cauchy-Schwarz inequality, we get

$$\|a - a_N\|_{L^q(\Omega;L^2(D))} \leq \|a_{max}\|_{L^{2q}(\Omega)}\left(\mathbb{E}\left[\left(\sum_{n=N+1}^{\infty}\lambda_n Y_n^2\right)^q\right]\right)^{\frac{1}{2q}}. \tag{27}$$

We define $\nu := \sum_{n=N+1}^{J}\lambda_n > 0$, with $J > N+1$. We have by the convexity of the function t^q,

$$\left(\sum_{n=N+1}^{J}\lambda_n Y_n^2\right)^q \leq \nu^{q-1}\sum_{n=N+1}^{J}\lambda_n|Y_n|^{2q}.$$

Let $m_q = \mathbb{E}[|Y_1|^{2q}]$, which is finite. We take the expectation of this latter inequality to obtain

$$\mathbb{E}\left[\left(\sum_{n=N+1}^{J}\lambda_n Y_n^2\right)^q\right] \leq m_q\left(\sum_{n=N+1}^{J}\lambda_n\right)^q. \tag{28}$$

When J tends to infinity in (28) we get by combining with the bound (27), the error bound of the proposition, where the constant K is given by $K = m_q^{\frac{1}{2q}}\|a_{max}\|_{L^{2q}(\Omega)}$ ■

Combining the bound (26) with the equality $\sum_{n=1}^{\infty}\lambda_n = |D|\sigma^2$, where $|D|$ is the measure of the physical domain D, allows for determining the appropriate number of random dimension N. For example, with $\delta \approx 1$,

$$\sum_{n=1}^{N+1}\lambda_n = \delta|D|\sigma^2. \tag{29}$$

In general, the stochastic dimension N depends on the regularity of the covariance function (see [1, 15]) and the correlation length l_c with respect to $|D|$.

3.1.2 Convergence of p_N to p and v_N to v

First, we recall the regularity properties of a and a_N. Let $q \geq 1$, $0 < \alpha < \frac{1}{2}$ and $\mathcal{C}^{0,\alpha}(D)$ the space of Hölder-Continuous functions.

Proposition 3.2 *The trajectories of a are in $\mathcal{C}^{0,\alpha}(D)$ and those of a_N are in $\mathcal{C}^2(D)$. The random variables a_{max}, $\frac{1}{a_{min}}$ are $L^q(\Omega)-$integrable, $a \in L^q(\Omega;\mathcal{C}^{0,\alpha}(D))$ and $a_N \in L^q(\Omega;\mathcal{C}^2(D))$.*

Proof: The regularity of the trajectories of a_N is satisfied by assumption 2.1. That of the trajectories of a is shown in [8]. ■

We recall regularity properties of problems (1) and (15). Thanks to the truncated K-L expansion, problem (15) has more regularity than problem (1).

Proposition 3.3 *Problem (1) is well posed, with* $p \in L^q(\Omega; \mathcal{C}^{1,\alpha}(D))$ *and* $v \in L^q(\Omega; \mathcal{C}^{0,\alpha}(D))$. *Problem (15) is well posed, with* $p_N \in L^q(\Omega; \mathcal{C}^3(D))$ *and* $v_N \in L^q(\Omega; \mathcal{C}^2(D))$.

Proof: The regularity of the trajectories of p_N and v_N is given by the elliptic regularity. That of v and p is given in [8].■

The convergence of p_N to p and v_N to v is given by the following proposition which shows that the truncation errors $\|p - p_N\|_{L^q(\Omega;H^1(D))}$, and $\|v - v_N\|_{L^q(\Omega;L^2(D))}$ are linked to the error on the permeability $\|a - a_N\|_{L^q(\Omega;L^2(D))}$.

Proposition 3.4 *There exist positive constants* K_1 *and* K_2, *independent of* N, *such that:*

$$\|p - p_N\|_{L^q(\Omega;H^1(D))} \leq K_1 \|a - a_N\|_{L^{2q}(\Omega;L^2(D))}, \tag{30}$$

$$\|v - v_N\|_{L^q(\Omega;L^2(D))} \leq K_2 \|a - a_N\|_{L^{2q}(\Omega;L^2(D))}. \tag{31}$$

Proof: For each $\omega \in \Omega$ (a.e) and $\mu \in H_0^1(D)$, p and p_N satisfy:

$$\int_D a \nabla p \nabla \mu dx = \int_D a_N \nabla p_N \nabla \mu dx = 0,$$

therefore, we get

$$\begin{aligned} \int_D a_N \nabla(p - p_N) \nabla \mu dx &= \int_D (a_N - a) \nabla p \nabla \mu dx + \int_D a \nabla p \nabla \mu dx - \int_D a_N \nabla p_N \nabla \mu dx \\ &\leq \|p\|_{\mathcal{C}^1(\bar{D})} \|a - a_N\|_{L^2(D)} \|\nabla \mu\|_{L^2(D)}. \end{aligned}$$

Let $a_{N,min}(\omega) = \min_{x \in \bar{D}} a_N(\omega)$ and taking $\mu = p - p_N$, we get

$$\|p - p_N\|_{H_0^1(D)} \leq \frac{\|p\|_{\mathcal{C}^1(\bar{D})}}{a_{N,min}} \|a - a_N\|_{L^2(D)}. \tag{32}$$

Taking the norm in $L^q(\Omega)$, we obtain

$$\begin{aligned} \|p - p_N\|_{L^q(\Omega;H_0^1(D))} &\leq \left(\mathbb{E}_\omega \left[\frac{\|p\|_{\mathcal{C}^1(\bar{D})}}{a_{N,min}} \|a - a_N\|_{L^2(D)} \right]^q \right)^{\frac{1}{q}} \\ &\leq \| \frac{\|p\|_{\mathcal{C}^1(\bar{D})}}{a_{N,min}} \|_{L^{2q}(\Omega)} \|a - a_N\|_{L^{2q}(\Omega;L^2(D))} \\ &\leq K_1 \|a - a_N\|_{L^{2q}(\Omega;L^2(D))} \end{aligned}$$

Where $K_1 = \|p\|_{L^{4q}(\Omega;\mathcal{C}^1(\bar{D}))} \left\| \frac{1}{a_{N,min}} \right\|_{L^{4q}(\Omega)}$.

Also, we have for each $\omega \in \Omega$ (a.e),

$$\begin{aligned} \|v - v_N\|_{L^2(D)} &\leq \| - a \nabla p + a_N \nabla p_N \|_{L^2(D)} \\ &\leq \|(a_N - a) \nabla p\|_{L^2(D)} + \|a_N \nabla (p_N - p)\|_{L^2(D)} \\ &\leq \|a_N - a\|_{L^2(D)} \|p\|_{\mathcal{C}^1(\bar{D})} + a_{max} \|\nabla (p_N - p)\|_{L^2(D)} \\ \text{(using (32))} &\leq \left(1 + \frac{a_{max}}{a_{N,min}}\right) \|p\|_{\mathcal{C}^1(\bar{D})} \|a - a_N\|_{L^2(D)}. \end{aligned}$$

Taking the norm in $L^q(\Omega)$, we get

$$\|v - v_N\|_{L^q(\Omega;L^2(D))} \leq K_2 \|a - a_N\|_{L^{2q}(\Omega;L^2(D))},$$

where $K_2 = \|p\|_{L^{4q}(\Omega;\mathcal{C}^1(\bar{D}))} \left\| 1 + \frac{a_{max}}{a_{N,min}} \right\|_{L^{4q}(\Omega)}$ ■

3.1.3 Convergence of c_N to c

We suppose that the initial condition c_0 of (16) and (6) is in $L^2(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$, with $\int_{\mathbb{R}^d} c_0(t,x)dx = 1$ and X_0 admits c_0 as a probability density.

Proposition 3.5

Equation (6) has unique solution c in $L^q(\Omega; \mathcal{C}^1(]0,T]; \mathcal{C}^2(\mathbb{R}^d)) \cap \mathcal{C}^0([0,T]; L^2(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)))$. Equation (16) has unique solution c_N in $L^q(\Omega; \mathcal{C}^1(]0,T], \mathcal{C}^4(\mathbb{R}^d) \cap \mathcal{C}^0([0,T], L^2(\mathbb{R}^d)) \cap L^\infty(\mathbb{R}^d)))$. For each $\omega \in \Omega$, $c(\omega,t,\cdot)$ is the density of $X_t(\omega,.)$ and $c_N(\omega,t,\cdot)$ is the density of $X_N(\omega,t,.)$

Proof: For each $\omega \in \Omega$, see [17] e.g. for the link with the SDE and for the regularity of the trajectories of c and c_N see [28]. The $L^q(\Omega)$ integrability of c and c_N is satisfied since v and v_N are $L^q(\Omega)$ integrable ■

The proposition which follows gives the convergence of c_N to c.

Proposition 3.6 *There exists a positive constant K_3 independent of N such that:*

$$\|c - c_N\|_{L^q(\Omega;\mathcal{C}^0([0,T];L^2(\mathbb{R}^d)))} \leq K_3 \|v - v_N\|_{L^{2q}(\Omega;L^2(\mathbb{R}))}. \tag{33}$$

Proof: With periodic boundary conditions, $\mathrm{div}(v) = \mathrm{div}(v_N) = 0$ on $\mathbb{R}^d$. Let us first consider this case. Setting $\psi(\omega,t,x) = c_N(\omega,t,x) - c(\omega,t,x)$, the function ψ is solution of the following parabolic problem:

$$\begin{cases} \partial_t \psi + v_N.\nabla\psi - D_m \triangle\psi = (v - v_N).\nabla c \quad \text{in } \Omega \times [0,T] \times \mathbb{R}^d \\ \psi(\omega,0,x) = 0 \quad \forall (\omega,x) \in \Omega \times \mathbb{R}^d. \end{cases} \tag{34}$$

Multiplying this equation by ψ and integrate over $\mathbb{R}^d$ to obtain:

$$\int_{\mathbb{R}^d} \psi \partial_t \psi \, dx + \int_{\mathbb{R}^d} v_N.\nabla\psi\psi \, dx + D_m \int_{\mathbb{R}^d} |\nabla\psi|^2 \, dx = \int_{\mathbb{R}^d} \psi (v - v_N).\nabla c \, dx, \tag{35}$$

since $\mathrm{div}(v_N) = 0$, we have $\int_{\mathbb{R}^d} v_N.\nabla\psi\psi dx = 0$. Using the integration by parts and the inequality $2ab \leq a^2 + b^2$, we obtain

$$\begin{aligned} \int_{\mathbb{R}^d} (v - v_N).\nabla c\psi dx &= \int_{\mathbb{R}^d} c(v_N - v).\nabla\psi dx \\ &\leq \frac{1}{2} \| \frac{c}{\sqrt{2D_m}} (v - v_N) \|^2_{L^2(\mathbb{R}^d)} + D_m \|\nabla\psi\|^2_{L^2(\mathbb{R}^d)} \\ &\leq \frac{1}{4D_m} \|c\|^2_{L^\infty(\mathbb{R}^d)} \|(v - v_N)\|^2_{L^2(\mathbb{R}^d)} + D_m \|\nabla\psi\|^2_{L^2(\mathbb{R}^d)} \end{aligned} \tag{36}$$

Furthermore we have $\int_{\mathbb{R}^d} \psi \partial_t \psi dx = \frac{1}{2} \partial_t \|\psi\|^2_{L^2(\mathbb{R}^d)}$, the bound (36) with equation (35) yields:

$$\partial_t \|\psi\|^2_{L^2(\mathbb{R}^d)} \leq \frac{1}{8D_m} \|c\|^2_{L^\infty(\mathbb{R}^d)} \|v - v_N\|^2_{L^2(\mathbb{R}^d)}.$$

We integrate in time and use $\psi(\omega,0,x) = 0$ to obtain

$$\sup_{0 \leq t \leq T} \|\psi\|_{L^2(\mathbb{R}^d)} \leq \sqrt{\frac{T}{8D_m}} \|c\|_{L^\infty([0,T]\times\mathbb{R}^d)} \|v - v_N\|_{L^2(\mathbb{R}^d)}.$$

Taking the norm in $L^q(\Omega)$, we conclude the estimation

$$\|c - c_N\|_{L^q(\Omega;\mathcal{C}^0([0,T],L^2(\mathbb{R}^d)))} \leq \sqrt{\frac{T}{8D_m}} \|c\|_{L^{2q}(\Omega;L^\infty([0,T]\times\mathbb{R}^d))} \|v - v_N\|_{L^{2q}(\Omega;L^2(\mathbb{R}^d))}.$$

With other boundary conditions, we extended v and v_N continuously by zeros on $\mathbb{R}^d$. Then, $\mathrm{div}(v) \neq 0$ and $\mathrm{div}(v_N) \neq 0$ on a small box $O \setminus D$ and the term $\|\mathrm{div}(v_N)\|_{L^\infty(O\setminus D)}$, which is finite, can be put in the constant K_3. ■

3.1.4 Weak convergence of $X_N(t)$ to X_t

The next result concerns the convergence in the law of the process $X_N(t)$ to X_t. Let $p, q, r \geq 1$, and $k \geq 2$. In what follows, we consider the functions test f in $\mathcal{C}^r_{pol}(\mathbb{R}^d)$ and g in $L^p(\Omega; \mathcal{C}^k_{pol}(\mathbb{R}^d))$.

The following bound is useful, it shows that the mean of any function of X_t with polynomial growth is finite.

Lemma 3.1 *There exists $C_{p,q,T} > 0$ such that:*

$$\mathbb{E}_\omega[|\mathbb{E}_\theta[|X_t|^p]|^q] \leq C_{p,q,T}\mathbb{E}_\theta[|X_0|^p] \tag{37}$$

Proof: it is straightforward, since $X_t = X_0 + \int_0^t v(., X_s)ds + \sqrt{2D_m}W_t$, and $v \in L^q(\Omega; L^\infty(\mathbb{R}^d))$. A similar bound holds for the process X_N and its approximation $X_{N,\eta,h}$ given in (23) regardless of N, h and η.■

The following result provides an estimate of the truncation error on the quantities of interest.

Theorem 3.1 *There exists $C > 0$, independent of N such that:*

$$\mathbb{E}_\omega\left[\mathbb{E}_\theta[g(X_T) - g(X_N(T)))]\right] \leq C\|v - v_N\|_{L^2(\Omega; L^2(\mathbb{R}^d))}. \tag{38}$$

Proof: For each $\omega \in \Omega$ (a.e), let u be the solution of the Kolmogorov backward equation associated to (17):

$$\begin{cases} \partial_t u(\omega, t, x) + v_N(\omega, x).\nabla u(\omega, t, x) + D_m \triangle u(\omega, t, x) = 0 \quad 0 \leq t < T, \\ u(\omega, T, x) = g(\omega, x). \end{cases} \tag{39}$$

Since the trajectories of v_N and g are given in $\mathcal{C}^2_{pol}(\mathbb{R}^d)$, the trajectories of u belong to $\mathcal{C}^1([0, T[, \mathcal{C}^4_{pol}(\mathbb{R}^d)) \cap \mathcal{C}^1([0, T], \mathcal{C}^2_{pol}(\mathbb{R}^d))$ [28] and are given by (Feynman-Kac formula, [24])

$$u(t, x) = \mathbb{E}_\theta[g(X_N(T))|X_N(t) = x].$$

In particular $u(0, X_N(0)) = u(0, X_0) = \mathbb{E}_\theta[g(X_N(T))]$. We define the following weak error:

$$e_T = \mathbb{E}_\theta[g(X_T)] - \mathbb{E}_\theta[g(X_N(T))] = \mathbb{E}_\theta[u(T, X_T)] - \mathbb{E}_\theta[u(0, X_0)].$$

The Itô's formula applied to $u(t, X_t)$ gives

$$du(s, X_s) = \partial_t u(s, X_s)ds + \nabla u(s, X_s)dX_s + D_m \triangle u(s, X_s)ds$$

where X_t is given by (7). Integrate this from 0 to T, we get

$$u(T, X_T) - u(0, X_0) = \int_0^T \left(\partial_t u + v(X_s).\nabla u + D_m \triangle u\right)(s, X_s)ds + \int_0^T \sqrt{2D_m}\nabla u(s, X_s)dWs,$$

Using the equation (39) at (s, X_s) and Taking the expectation on Θ, we obtain:

$$\begin{aligned} e_T &= \int_0^T \mathbb{E}_\theta\Big[\Big(v(X_s) - v_N(X_s))\Big).\nabla u(s, X_s)\Big]ds \\ &\leq \sup_{0 \leq t \leq T} \|\nabla u(t, X_t)\|_{L^2(\theta)} \int_0^T \|v(X_s) - v_N(X_s)\|_{L^2(\theta)}ds. \end{aligned} \tag{40}$$

For each $\omega \in \Omega$, the solution $c(\omega, t, .)$ of (6) is the probability density of the process $X_t(\omega, .)$ on Θ, therefore:

$$\begin{aligned} \|v_N(X_s) - v(X_s)\|^2_{L^2(\Theta)} &= \int_{\mathbb{R}^d} |v(x) - v_N(x)|^2 c(\cdot, t, x) dx \\ &\leq \sup_{0\leq t\leq T} \sup_{x\in\mathbb{R}^d} c(\cdot, t, x) \|v - v_N\|^2_{L^2(\mathbb{R}^d)} \end{aligned}$$

combining this latter bound with (40), we obtain:

$$e_T \leq T \sup_{0\leq t\leq T} \|\nabla u(t, X_t)\|_{L^2(\Theta)} \sup_{0\leq t\leq T,\, x\in\mathbb{R}^d} \sqrt{c(\cdot, t, x)} \|v - v_N\|_{L^2(\mathbb{R}^d)}. \tag{41}$$

Taking the expectation on Ω and using the Hölder inequality, we get:

$$\mathbb{E}_\omega[e_T] \leq TC_1 \|v - v_N\|_{L^2(\Omega, L^2(\mathbb{R}^d))},$$

where we set $C_1 = \| \sup_{0\leq t\leq T} \nabla u(t, Y_t)\|_{L^4(\Omega, L^2(\Theta))} \| \sup_{0\leq t\leq T,\, x\in\mathbb{R}^d} \sqrt{c(\cdot, t, x)}\|_{L^4(\Omega)}$. Using (37), the constant $\| \sup_{0\leq t\leq T} \|\nabla u(t, Y_t)\|_{L^2(\Theta)}\|_{L^4(\Omega; L^2(\Theta))}$ is finite. Also, since $c \in L^q(\Omega; L^\infty([0, T] \times \mathbb{R}^d))$, $\| \sup_{0\leq t\leq T, x\in\mathbb{R}^d} \sqrt{c(\cdot, t, x)}\|_{L^4(\Omega)}$ is finite. Thus C_1 is finite.■

3.2 Temporal and spatial discretization error

Here, we give a bound of the weak error $\mathbb{E}_\omega[\mathbb{E}_\theta[g(X_N(T))] - \mathbb{E}_\theta[g(X_{N,\eta,h}(T))]]$. It can be divided into tow terms. The first one, related to time discretization, is classical when the drift is $\mathcal{C}^2$ [30]. The second term concerns the space error and we show that it is of order h. Let $X_{N,\eta}(t)$ be an approximation by Euler scheme of the process $X_N(t)$ and $X_{N,\eta,h}(t)$ its perturbation as given in (23). The following proposition shows a bound of this error.

Proposition 3.7 *There exists a constant $C(T, g) > 0$ independent of dt and h such that:*

$$\mathbb{E}_\omega[\mathbb{E}_\theta[g(X_N(T))] - \mathbb{E}_\theta[g(X_{N,\eta,h}(T))]] \leq C(T, g)\,(dt + h)\,.$$

Proof: Let u solution of (39), then:

$$\mathbb{E}_\omega[\mathbb{E}_\theta[g(X_{N,\eta,h}(T))] - \mathbb{E}_\theta[g(X_N(T))]] = \mathbb{E}_\omega[\mathbb{E}_\theta[u(T, X_{N,\eta,h}(T)) - u(0, X_0)]] = \sum_{l=1}^{\eta} \mathbb{E}_\omega[\mathbb{E}_\theta[e_l]],$$

where we set $e_l = u(t_{l+1}, X_{N,\eta,h}(t_{l+1})) - u(t_l, X_{N,\eta,h}(t_l))$. Using Itô's formula, we have:

$$e_l = \int_{t_l}^{t_{l+1}} (\partial_t u + v_{N,h}(X_{N,\eta,h}(t_l))\nabla u + D_m \triangle u)\,(s, X_{N,\eta,h}(s)) ds + \int_{t_l}^{t_{l+1}} \sqrt{2D_m} \nabla u(s, X_{N,\eta,h}(s)) dW s,$$

we conclude that, $\mathbb{E}_\theta[e_l] = \int_{t_l}^{t_{l+1}} \mathbb{E}_\theta\left[(\partial_t u + v_{N,h}(X_{N,\eta,h}(t_l))\nabla u + D_m \triangle u)\,(s, X_{N,\eta,h})\right] ds.$

Using (39) at point $(s, X_{N,\eta,h}(s))$ and then taking the mean on Ω, we obtain:

$$\begin{aligned} \mathbb{E}_\omega[\mathbb{E}_\theta[e_l]] &= \int_{t_l}^{t_{l+1}} \mathbb{E}_\theta\left[\left(v_{N,h}(X_{N,\eta,h}(t_l)) - v_N(X_{N,\eta,h}(s))\right)\nabla u(s, X_{N,\eta,h}(s))\right] ds \\ &= \mathbb{E}_\omega[J_1] + \mathbb{E}_\omega[J_2], \end{aligned}$$

where we define $J_1 := \int_{t_l}^{t_{l+1}} \mathbb{E}_\theta\Big[\Big(v_{N,h}(X_{N,\eta,h}(t_l)) - v_N(X_{N,\eta,h}(t_l))\Big)\nabla u(s, X_{N,\eta,h}(s))\Big]ds$ and $J_2 := \int_{t_l}^{t_{l+1}} \mathbb{E}_\theta\Big[\Big(v_N(X_{N,\eta,h}(t_l)) - v_N(X_{N,\eta,h}(s))\Big)\nabla u(s, X_{N,\eta,h}(s))\Big]ds$.

For each $l = 2, \ldots, \eta$, Let $c_{\eta,h}(\omega, t_l, x)$ the density of $X_{N,\eta,h}(\omega, t_l, .)$. It belongs to $\mathcal{C}_0^\infty(\mathbb{R}^d)$, since it is given by the convolution of the density of the variable $X_{N,\eta,h}(\omega, t_l, .) + v_h(X_{N,\eta,h}(\omega, t_l, .)dt$ with the density of $\sqrt{2D_m dt}\xi_{l+1}$, and by induction we get:

$$c_{n,h}(\omega, t_l, x) \leq \tilde{K}\|c_0\|_\infty(1 + \|v\|_\infty l dt), \tag{42}$$

where $\tilde{K} > 0$ and independent of h and η. The term J_1 satisfies:

$$\begin{aligned} J_1 &\leq \int_{t_l}^{t_{l+1}} \|v_{N,h}(X_{N,\eta,h}(t_l)) - v_N(X_{N,\eta,h}(t_l))\|_{L^2(\Theta)}\|\nabla u(s, X_{N,\eta,h}(s))\|_{L^2(\Theta)}ds \\ &\leq \int_{t_l}^{t_{l+1}} \|\nabla u(s, X_{N,\eta,h}(s))\|_{L^2(\Theta)}ds\Big(\int_{\mathbb{R}^d} |v_{N,h}(x) - v_N(x)|^2 c_{\eta,h}(t_l, x)dx\Big)^{\frac{1}{2}} \\ &\leq dt \sup_{x\in\mathbb{R}^d}\sup_{l\leq\eta+1}\sqrt{c_{n,h}(t_l, x)}\sup_{t\leq T}\|\nabla u(t, X_{\eta,h}(t))\|_{L^2(\Theta)}\|v_N - v_{N,h}\|_{L^2(\mathbb{R}^d)} \end{aligned}$$

Taking the mean on Ω, we get:

$$\mathbb{E}_\omega[J_1] \leq C_1(dt)\|v_N - v_{N,h}\|_{L^2(\Omega;L^2(\mathbb{R}^d))}, \tag{43}$$

where $C_1 = \tilde{K}\|c_0\|_\infty(1 + T\|v\|_\infty)\sup_{t\leq T}\|\nabla u(t, X_{N,\eta,h}(t))\|_{L^2(\Theta)}\|_{L^2(\Omega)}$, which is finite thanks to Lemma 3.1. To bound $\mathbb{E}_\omega[J_2]$, let $\chi(s, x) = (v_N(X_{N,\eta,h}(t_l)) - v_N(x))\nabla u(s, x)$. Since $v_N \in \mathcal{C}_b^2(\mathbb{R}^d)$ and $u \in \mathcal{C}_{pol}^{1,4}([0, T[\times\mathbb{R}^d)$, $\chi \in \mathcal{C}_{pol}^{1,2}([0, T[\times\mathbb{R}^d)$. By Itô's formula, the derivative of $\varphi(s) := \mathbb{E}_\theta[\chi(s, X_{N,\eta,h}(s))]$ in $(t_l; t_{l+1}[$ is given by:

$$\frac{d\varphi}{ds}(s) = \mathbb{E}_\theta[\partial_s\chi(s, X_{N,\eta,h}(s)) + v_N(X_{N,\eta,h}(t_l))\nabla\chi(s, X_{N,\eta,h}(s)) + D_m\triangle\chi(s, X_{N,\eta,h}(s))].$$

Thanks to Lemma 3.1 the term $\mathbb{E}_\omega[\frac{d\varphi}{ds}]$ is bounded in $]t_l; t_{l+1}[$. Moreover, $\varphi(t_l) = 0$, then, there exists $C_2 > 0$ such that $\mathbb{E}_\omega[\varphi(s)] \leq C_2(s - t_l)$, for $t_l < s < t_{l+1}$. Then, since $\mathbb{E}_\omega[J_2] = \int_{t_l}^{t_{l+1}} \mathbb{E}_\omega[\varphi(s)]ds$, we get:

$$\mathbb{E}_\omega[J_2] \leq \frac{C_2}{2}dt^2. \tag{44}$$

We obtain a bound of $\mathbb{E}_\omega[\mathbb{E}_\theta[e_l]]$ by combining (43) with (44), and the total error by taking the sum over l. ■

3.3 Global error on the mean spread and the mean dispersion

Here we give the total weak error of the process X_t on $\Omega \times \Theta$, where the mean on Ω and Θ is computed by a Monte-Carlo sampling. This weak error is defined by the error at time T of the quantity of interest (10) approximated by (24):

$$\mathcal{E}r(T) := \mathcal{Q}(T) - \mathcal{Q}_{N,\eta,h}^{M,P}(T).$$

Theorem 3.2 *There exists a constant C, independent of M, N, h and the time step dt such that the following estimation holds:*

$$|\mathcal{E}r(T)| \leq C(f, g)\Big(\|v - v_N\|_{L^2(\Omega;L^2(\mathbb{R}^d))} + dt + h + \frac{1}{\sqrt{M}} + \frac{1}{\sqrt{P}}\Big).$$

Proof: We split naturally this error into four terms $|\mathcal{E}r(T)| \leq |\mathcal{E}r_1| + |\mathcal{E}r2| + |\mathcal{E}r3| + |\mathcal{E}r4|$, where we define:

$$\begin{aligned}
\mathcal{E}r_1 &= \mathcal{Q}(T) - \mathbb{E}_\omega\left[f\left(\mathbb{E}_\theta[g(X_N(T))]\right)\right], \\
\mathcal{E}r_2 &= \mathbb{E}_\omega\left[f\left(\mathbb{E}_\theta[g(X_N(T))]\right)\right] - \mathbb{E}_\omega\left[f\left(\mathbb{E}_\theta[g(X_{N,\eta,h}(T)]\right)\right], \\
\mathcal{E}r_3 &= \mathbb{E}_\omega\left[f\left(\mathbb{E}_\theta[g(X_{N,\eta,h}(T)]\right)\right] - \mathbb{E}_\omega\left[f\left(\frac{1}{P}\sum_{j=1}^{P} g(X_{N,\eta,h}(\theta_j,T)\right)\right], \\
\mathcal{E}r_4 &= \mathbb{E}_\omega\left[f\left(\frac{1}{P}\sum_{j=1}^{P} g(X_{N,\eta,h}(\theta_j,T)\right)\right] - \mathcal{Q}^{M,P}_{N,n,h}(T).
\end{aligned}$$

Using Taylor's formula together with Cauchy-Schwarz inequality we have:

$$|\mathcal{E}r_1| \leq \|\mathcal{D}f(Y)\|_{L^2(\Omega)}\|\mathbb{E}_\theta[g(X_N(T))] - \mathbb{E}_\theta[g(X_{N,\eta,h}(,T))]\|_{L^2(\Omega)}$$

where $Y = s\mathbb{E}_\theta[g(X_N(T))] + (1-s)\mathbb{E}_\theta[g(X_N(T))]$ with $0 < s < 1$. Therefore by Theorem 3.1 and the bound (37) the first error satisfies

$$|\mathcal{E}r_1| \leq C_1\|v - v_N\|_{L^2(\Omega;L^2(D))}.$$

Similarly, by Taylor's formula together with Cauchy-Schwarz inequality,

$$|\mathcal{E}r_2| \leq \|\mathcal{D}f(Z)\|_{L^2(\Omega)}\|\mathbb{E}_\theta[g(X_N(T))] - \mathbb{E}_\theta[g(X_{N,\eta,h}(T))]\|_{L^2(\Omega)}$$

such that $Z = s\mathbb{E}_\theta[g(X_N(T))] + (1-s)\mathbb{E}_\theta[g(X_{N,\eta,h}(T))]$ with $0 < s < 1$. Hence, using Proposition 3.7, knowing that $\|X_N(T)\|_{L^q(\Omega\times\Theta)} < \infty$ independently with N as in (37), we obtain a bound of the second term:

$$|\mathcal{E}r_2| \leq C_2(dt + h).$$

For each $\omega \in \Omega$, the set of the random variables $\{g(X_{N,\eta,h}(\omega,\theta_j,T))\}_{j=1}^P$ being independent, identically distributed in Θ. Then, using the law of large numbers and Taylor's formula, the third term satisfies:

$$|\mathcal{E}r_3| \leq C_3\frac{1}{\sqrt{P}},$$

where the constant C_3 depends on the variance of $g(X_{N,\eta,h})$ which is finite and can be bounded independently with N, n and h.

The forth term $\mathcal{E}r_4$ can be bounded by a similar way, let ψ defined by

$$\psi(\omega) = f\left(\frac{1}{P}\sum_{j=1}^{P} g(X_{N,\eta,h}(\omega,\theta_j,T))\right).$$

Since ϕ is a borelian function, the set $\left\{\psi(\omega_i) = f(\frac{1}{P}\sum_{j=1}^{P} g(X^{i,j}_{N,\eta,h}))\right\}_{i=1}^{M}$ being independent, identically distributed in Ω. By the law of large numbers the forth term satisfies:

$$|\mathcal{E}r_4| \leq C_4\frac{1}{\sqrt{M}}.$$

we conclude the total error of the theorem by combining the estimate of all partial errors. ■

Corollary 3.1 *There exists a constant $K_4 > 0$ independent of N such that:*

$$\|v - v_N\|_{L^2(\Omega;L^2(\mathbb{R}^d))} \leq K_4 \sqrt{\sum_{n=N+1}^{\infty} \lambda_n}. \tag{45}$$

Proof: By combining the bound (26) with (31) the estimate is given in $L^2(\Omega; L^2(D))$. In the case of periodic boundary conditions, we concluded by periodicity. With other boundary conditions, both v and v_N can be extended with the same manner outside of D. Thus, $v - v_N = 0$ outside of D ■

The spread and the dispersion coefficients are expressed as a function of the process X_t. Therefore, with a suitable choice of functions f and g, it is possible to apply Theorem 3.2. We define $\mathcal{S}^{M,P}_{N,\eta,h}(t)$ and $\mathcal{D}^{M,P}_{N,\eta,h}(t)$ respectively the approximation of $\mathcal{S}(t)$ and $\mathcal{D}(t)$:

$$\mathcal{S}^{M,P}_{N,h}(t) = \frac{1}{M}\sum_{i=1}^{M}\left(\frac{1}{P}\sum_{j=1}^{P}|X^{i,j}_{N,\eta,h}(t)|^2 - \left|\frac{1}{P}\sum_{j=1}^{P}X^{i,j}_{N,\eta,h}(t)\right|^2\right),$$

$$\begin{aligned}\mathcal{D}^{M,P}_{N,h}(t) \;=\; \frac{1}{M}\sum_{i=1}^{M}\Bigg(\frac{1}{P}\sum_{j=1}^{P} < X^{i,j}_{N,\eta,h}(t), v^i_{N,h}(X^{i,j}_{N,\eta,h}(t)) > - \frac{1}{P^2}\sum_{j,l=1}^{P} < X^{i,j}_{N,\eta,h}(t), v^i_{N,h}(X^{i,l}_{N,\eta,h}(t)) > \Bigg)\\ +\mathrm{trace}(D_m).\end{aligned}$$

Proposition 3.8 *There exists a constant $C_1 > 0$ and $C_2 > 0$, independent of M, h and the time step dt such that the following estimation holds:*

$$\begin{aligned}\left|\mathcal{S}(T) - \mathcal{S}^{M,P}_{N,h}(T)\right| &\leq C_1\left(\sqrt{\sum_{n=N+1}^{\infty}\lambda_n} + dt + h + \frac{1}{\sqrt{M}} + \frac{1}{\sqrt{P}}\right)\\ \left|\mathcal{D}(T) - \mathcal{D}^{M,P}_{N,h}(T)\right| &\leq C_2\left(\sqrt{\sum_{n=N+1}^{\infty}\lambda_n} + dt + h + \frac{1}{\sqrt{M}} + \frac{1}{\sqrt{P}}\right)\end{aligned}$$

Proof: The error at the final time of the spread can be easily concluded using the estimate of Theorem 3.2 and Corollary 3.1 by taking $g(.,x) = |x|^2$ with $f = x$, and $g(.,x) = x$ with $f(x) = |x|^2$.

To bound the error at time T of the dispersion, let define:

$$\begin{aligned}E_I &= \mathbb{E}_\omega\left[\mathbb{E}_\theta[< X_T, v_N(., X_T) >]\right] - \frac{1}{MP}\sum_{i=1}^{M}\sum_{j=1}^{P} < X^{i,j}_{N,\eta,h}(T), v_{N,h}(\omega_i, X^{i,j}_{N,\eta,h}(T)) >\\ E_{II} &= \mathbb{E}_\omega\left[< \mathbb{E}_\theta[X_T], \mathbb{E}_\theta[v_N(., X_T)] >]\right] - \frac{1}{MP^2}\sum_{i=1}^{M} < \sum_{j=1}^{P} X^{i,j}_{N,\eta,h}(T), \sum_{j=1}^{P} v_{N,h}(\omega_i, X^{i,j}_{N,\eta,h}(T)) >\end{aligned}$$

The first term is split into two errors: $E_I \leq e_1 + e_2$, where

$$\begin{aligned}e_1 &= \mathbb{E}_\omega\left[\mathbb{E}_\theta[< X_T, v_N(X_T) >]\right] - \frac{1}{MP}\sum_{i=1}^{M}\sum_{j=1}^{P} < X^{i,j}_{N,\eta,h}(T), v_N(\omega_i, X^{i,j}_{N,\eta,h}(T)) >,\\ e_2 &= \frac{1}{MP}\sum_{i=1}^{M}\sum_{j=1}^{P} < X^{i,j}_{N,\eta,h}(T), (v_N - v_{N,h})(\omega_i, X^{i,j}_{N,\eta,h}(T)) > .\end{aligned}$$

The error e_1 can be bounded using the estimate of Theorem 3.2 and Corollary 3.1 by choosing $f(x) = x$ and $g(.,x) = v_N(.,x)$, we get:

$$e_1 \leq C\Big(\sqrt{\sum_{n=N+1}^{\infty} \lambda_n} + dt + h + \frac{1}{\sqrt{M}} + \frac{1}{\sqrt{P}}\Big).$$

The second error e_2 is equivalent to $e_3 = \mathbb{E}_\omega\Big[\mathbb{E}_\theta[< X_{N,\eta,h}(T), (v_N - v_{N,h})(X_{N,\eta,h}) >]\Big]$ up to the Monte Carlo error $\mathrm{O}\Big(\frac{1}{\sqrt{M}} + \frac{1}{\sqrt{N}}\Big)$. Let $c_{N,\eta,h}(\omega, T, x)$ be the law of the process $X_{N,\eta,h}(\omega, T)$. We have:

$$\begin{aligned} e_3 &\leq \mathbb{E}_\omega\Big[\|X_{N,\eta,h}\|_{L^2(\Theta)}\|v_N(X_{N,\eta,h}) - v_{N,h}(X_{N,\eta,h})\|_{L^2(\Theta)}\Big] \\ &\leq \mathbb{E}_\omega\Big[\|X_{N,\eta,h}\|_{L^2(\Theta)} \sup_{x\in\mathbb{R}^d} \sqrt{c_{N,\eta,h}(\omega,T,x)}\|v_N - v_{N,h}\|_{L^2(\mathbb{R}^d)}\Big] \\ &\leq \|\|X_{N,\eta,h}\|_{L^2(\Theta)} \sup_{x\in\mathbb{R}^d} \sqrt{c_{N,\eta,h}(T,x)}\|_{L^2(\Omega)}\|v_N - v_{N,h}\|_{L^2(\Omega,L^2(\mathbb{R}^d))} \leq \tilde{C}h \end{aligned}$$

where $\tilde{C} = O(\|X_{N,\eta,h}\|_{L^4(\Omega)\otimes L^2(\Theta)}\|\sqrt{c_{N,\eta,h}(T,x)}\|_{L^4(\Omega)})$, which is finite and can be chosen independently of N, η, h, by using (42) and Lemma 3.1. Therefore we deduce that E_I satisfies:

$$E_I = O\Big(\sqrt{\sum_{n=N+1}^{\infty} \lambda_n} + dt + h + \frac{1}{\sqrt{M}} + \frac{1}{\sqrt{P}}\Big).$$

The second term E_{II} can be easily bounded in a similar way, side by side in the scalar product, to obtain:

$$E_{II} = O\Big(\sqrt{\sum_{n=N+1}^{\infty} \lambda_n} + dt + h + \frac{1}{\sqrt{M}} + \frac{1}{\sqrt{P}}\Big).$$

We conclude the error on the final time of the mean dispersion since

$$\Big|\mathcal{D}(T) - \mathcal{D}^{M,P}_{N,\eta,h}(T)\Big| \leq |E_I| + |E_{II}|.$$

■

4 Numerical experiments

4.1 Test cases

This section illustrates the convergence of the proposed method to compute the quantities of interest (5). In our example, the bi-dimensional domain is given by the box $D := [0, L]^2$. The conductivity is given by a random field a, which follows a log-normal probability distribution $G = log(a)$, where G is characterised by its mean $\mathbb{E}_\omega[G]$ and its exponential covariance function:

$$Cov(x, y) = \sigma^2 \exp(-\frac{|x - y|}{l_c}), \quad \forall x, y \in D^2, \tag{46}$$

where σ^2 is the variance, l_c is the correlation length.

In our experiments, $L = 10$, $l_c = \frac{L}{10} = 1$, $\sigma^2 = 1, 2$, or 3 and $\mathbb{E}_\omega[G] = 0$.

In the flow problem (1), boundary conditions are homogeneous Neumann on upper and lower sides of the domain D, Dirichlet $p = 4$ on the left side, Dirichlet $p = 0$ on the right.

The transport equation (3) is completed by boundary conditions which are homogeneous Neumann conditions on upper and lower sides and Dirichlet conditions $c = 0$ on the left and right sides. The diffusion coefficient is fixed as $D_m = 0.1$ and the initial condition at $t = 0$ is given by the window $\frac{\mathbb{1}_B}{|B|}$ where $B = [2.85, 3] \times [5, 5.15]$. The final time is $T = 5$.

We use a uniform triangular mesh of D, with $h = \frac{L}{50} = 0.2$. In the random walker, we use a time step, $dt = \frac{T}{50} = 0.1$.

With the covariance function (46), the Fredholm integral equation (12) can be solved analytically [20, 36] using a simple one dimensional problem. We consider the characteristic equation $(l_c^2 w^2 - 1)\sin(Lw) - 2l_c w \cos(Lw) = 0$ and we denote by $(w_k)_{k\geq 1}$ its increasing positive roots. Then, the one dimensional eigenpairs are, $\lambda_k = \frac{2l_c\sigma^2}{l_c^2 w_k^2 + 1}$ and $b_k(x_1) = \beta_k(\sin(w_k x_1) + l_c w_k \cos(w_k x_1))$, where $\beta_k = \dfrac{1}{\sqrt{(l_c^2 w_k.^2 + 1)L/2 + l_c}}$. Therefore, the eigenpairs $(\boldsymbol{b}_n, \boldsymbol{\lambda}_n)$ of the Fredholm integral (12) are given by the tensor product:

$$\boldsymbol{\lambda}_n = \lambda_{k_1}\lambda_{k_2} \quad \text{and} \quad \mathbf{b}_n(x) = b_{k_1}(x_1)b_{k_2}(x_2),\ k_1, k_2 \geq 1, \quad \text{with} \quad x = (x_1, x_2).$$

and ordered in decreasing order. We developed a Matlab software to compute these eigenpairs.

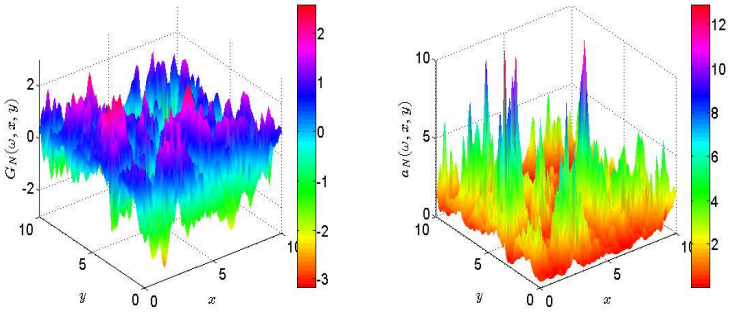

Figure 1: A realization of the random field for $\sigma = 1$. Left: G_N, right: a_N.

We use the bound (29) to truncate the field in the series (13). we get $N = 2336$ for $\sigma = 1$, $N = 3531$ for $\sigma = 2$ and $N = 5231$ for $\sigma = 3$.

In Figure 1, we plot one realisation of the field G_N (on the left) and the field $a_N = e^{G_N}$ (on the right) with $\sigma = 1$.

We use the Freefem++ software [16] to solve the flow equation with the mixed finite element method defined in section 3. The discrete linear flow system is solved with the direct algorithm implemented in the software UMFPACK. We implemented, also with Freefem++ framework, the random walk of the transport equation.

4.2 Convergence analysis of the spread and dispersion

In Figures 2, 3, 4, we plot the approximation of the mean spread $\mathcal{S}(t)$ (left) and the mean dispersion $\mathcal{D}(t)$ (right), using different numbers M of MC simulations in Ω and the variance $\sigma = 1, 2, 3$. We fix $P = 50000$ and plot four approximations with $M = 50, 300, 600, 1000$.

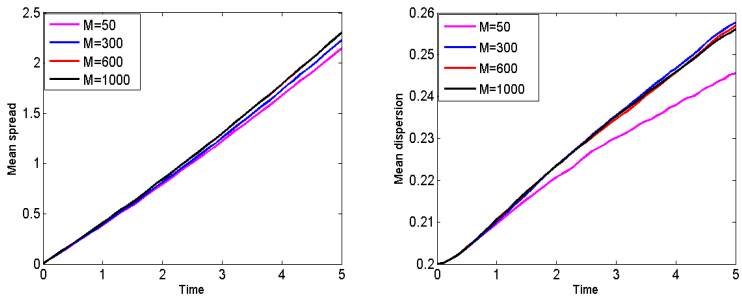

Figure 2: The mean spread and dispersion computed for various numbers of MC simulations M and with fixed $P = 50000$ particles and a variance $\sigma = 1$.

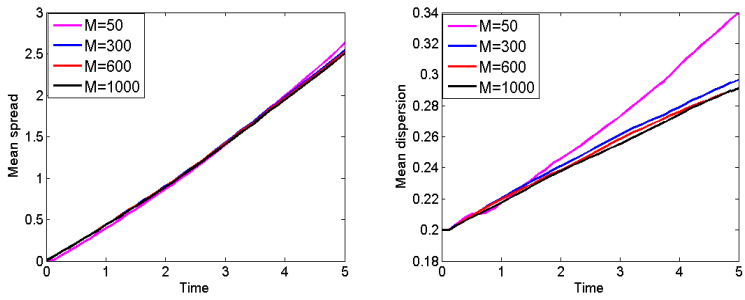

Figure 3: The mean spread and dispersion computed for various numbers of MC simulations M and with fixed $P = 50000$ particles and a variance $\sigma = 2$.

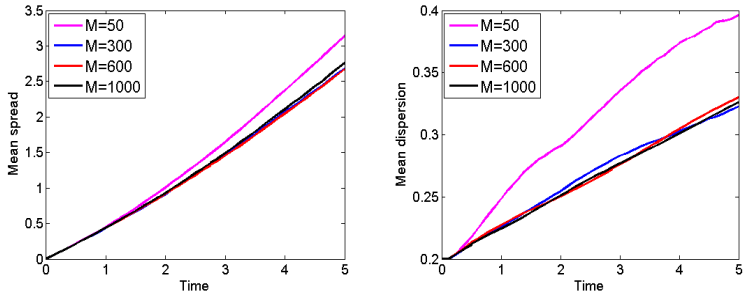

Figure 4: The mean spread and dispersion computed for various numbers of MC simulations M and with fixed $P = 50000$ particles and a variance $\sigma = 3$.

We observe that when we fix a large number of particles, both the mean of the spread and the mean of the dispersion converge rapidly with respect to the number of the simulations

M in the probability set Ω. We also observe that the convergence rate depends slightly on σ of the field G. In all cases, with $M = 600$ we get a smooth spread and dispersion.

We assume that this efficiency is related to the small variance of $S(.,t)$ and $D(.,t)$ as a random function in Ω, since the Monte Carlo error is given by $\frac{\tilde{\sigma}}{\sqrt{M}}$, where $\tilde{\sigma}^2$ is the variance of $S(.,t)$ or $D(.,t)$.

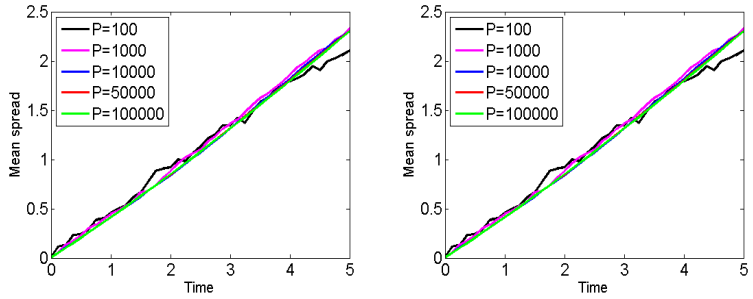

Figure 5: The mean spread and mean dispersion computed for various numbers particles P and with fixed $M = 600$ MC simulations and a variance $\sigma = 1$.

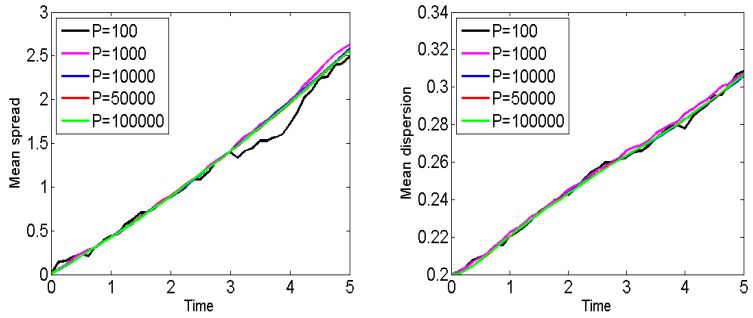

Figure 6: The mean spread and mean dispersion computed for various numbers particles P and with fixed $M = 600$ MC simulations and a variance $\sigma = 2$.

In Figures 5, 6, 7, we plot the approximation of $\mathcal{S}(t)$ (left) and $\mathcal{D}(t)$ (right), with different numbers of particles P and variance $\sigma = 1, 2, 3$. We fix $M = 600$ and plot five approximations with $P = 100, 1000, 10000, 50000, 100000$.

The result of the simulation shows that the convergence with respect to the number of particles is done with a large P compared with M the number of simulations. We observe the presence of oscillations with small P ($P = 100$ or $P = 1000$) for both the mean spread and dispersion, these oscillations are removed with a large P such that $P = 50000$.

In Figure 8 we plot the computed $\mathcal{S}(T)$ and $\mathcal{D}(T)$ at the final time T versus P the number of particles with various MC simulation. In Figure 9 we plot the computed $\mathcal{S}(T)$ and $\mathcal{D}(T)$ at the final time T versus M the number of MC simulations with various number

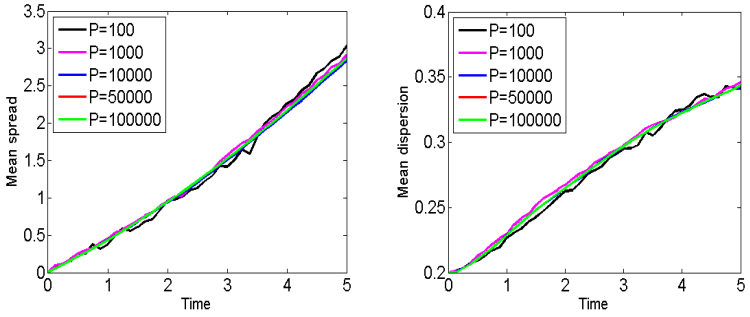

Figure 7: The mean spread and mean dispersion computed for various numbers particles P and with fixed $M = 600$ MC simulations and a variance $\sigma = 3$.

P of particles. We observe that the convergence quite rapidly when we increase the number of simulations $M \approx 600$, provided that the number of particles is large enough $P \approx 50000$.

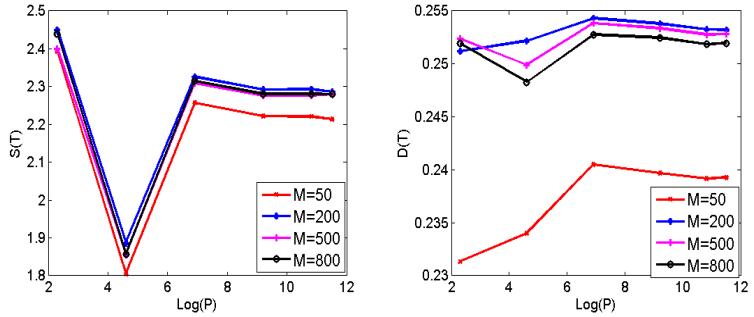

Figure 8: The mean spread and mean dispersion at the final time T versus the number of particles P and computed with various MC simulations, in the case $\sigma = 1$.

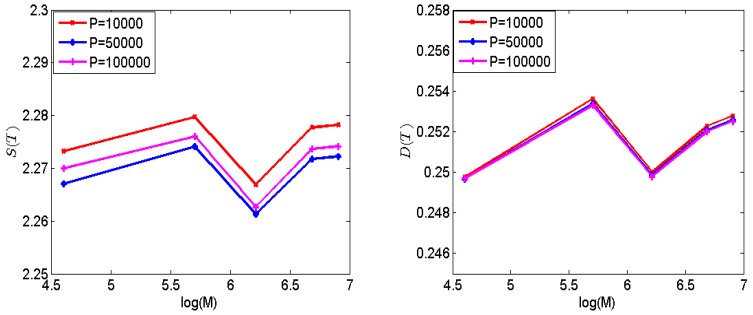

Figure 9: The mean spread and mean dispersion at the final time T versus M the numbers of MC simulations and computed with various particles P, in the case $\sigma = 1$.

4.3 Error analysis of the spread and dispersion

The trajectories of the truncated parameter a_N have at least $\mathcal{C}^2$ regularity. Therefore, the space discretization error on the approximation of the quantities (24) is driven by the order $O(h)$, and the time discretization error is driven by the order $O(dt)$, as shown in Proposition 4.5. These orders of the convergence are checked by taking various approximations of $\mathcal{S}(t)$ and $\mathcal{D}(t)$ with different space steps h and different time steps dt, with fixed numbers $M = 500$ MC simulations and $P = 50000$ particles.

We define a reference solution $\tilde{\mathcal{S}}(t)$ of the spread and $\tilde{\mathcal{D}}(t)$ of the dispersion with a space step $h = \frac{L}{60}$ and a time step $dt = \frac{T}{60}$.

We fix $dt = \frac{T}{60}$ and we vary the step h, by choosing $h = \frac{L}{n_h}$ with $n_h = 8, 16, 24, 32, 50, 60$. For each value of h, we define the relative errors $e_{\mathcal{S}}(h)$ and $e_{\mathcal{D}}(h)$ using the reference solution at the final time T:

$e_{\mathcal{S}}(h) = \frac{|\tilde{\mathcal{S}}(T) - \mathcal{S}_h(T)|}{|\tilde{\mathcal{S}}(T)|}$ and $e_{\mathcal{D}}(h) = \frac{|\tilde{\mathcal{D}}(T) - \mathcal{D}_h(T)|}{|\tilde{\mathcal{D}}(T)|}$.

Then , we fix the step $h = \frac{L}{60}$ and vary the time step , by choosing $\delta t = \frac{T}{n_t}$ with $n_t = 5, 10, 20, 30, 40, 50, 60$. For each value of dt, we define the relative errors $e_{\mathcal{S}}(dt)$ and $e_{\mathcal{D}}(dt)$ using the reference solution at the final time T. We observe that the two errors have a linear behavior as in Proposition 4.5.

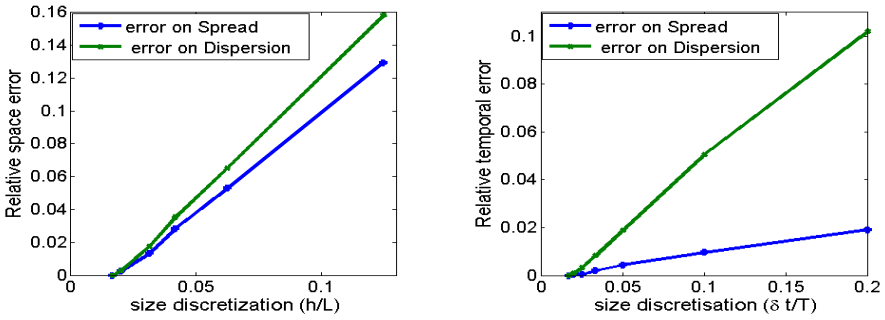

Figure 10: Left: Relative errors $e_{\mathcal{S}}(h)$, $e_{\mathcal{D}}(h)$ of space discretization at $T = 5$. Right: Relative errors $e_{\mathcal{S}}(dt)$ and $e_{\mathcal{D}}(dt)$ of temporal discretization at $T = 5$.

4.4 Comparison with approximation by difference of the dispersion

The method proposed in [9] consists in using an approximation by finite differences to compute the mean of dispersion. Another time step ds is introduced to compute $\mathcal{D}(t)$ by the following approximation:

$$\mathcal{D}(t) = \frac{d\mathcal{S}(t)}{2dt} \approx \frac{\mathcal{S}(t + ds) - \mathcal{S}(t)}{2ds}. \tag{47}$$

With a finite element method, it leads under additional assumptions at the following error bound (see [6] for more details),

$$\mathcal{E}r(T) = O\left(dt + ds + h|\ln h| + \frac{1}{\sqrt{M}} + \frac{1}{\sqrt{Pds}}\right). \tag{48}$$

In order to compare the explicit formulation (9) with the approximation (47), we run test cases , where we choose $M = 200$, $h = \frac{L}{20}$. For the explicit formulation, we choose $P = 10^5$ particles and the time step $dt = \frac{T}{50}$. For the approximation (47), we vary the numbers of particles P and the time step $dt = ds$. Results are given in Figure 11.

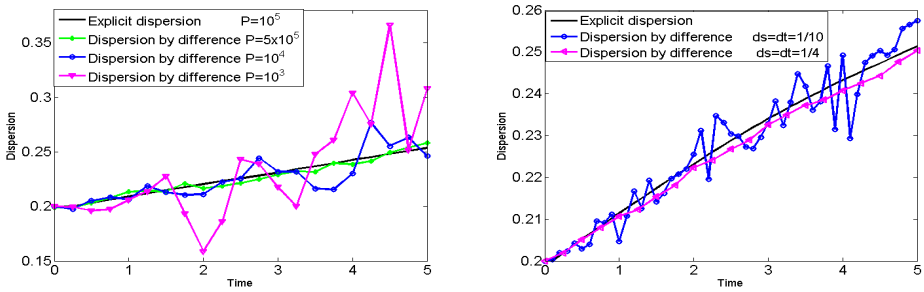

Figure 11: Dispersion computed with finite differences. Left: $dt = ds = \frac{1}{10}$. Right: $ds = \frac{1}{4}$ and $ds = \frac{1}{10}$ with $P = 10^5$ particles. The black curve is the dispersion computed with the explicit formulation, using $dt = \frac{1}{10}$ and $P = 10^5$.

We observe that the approximation (47) is very sensitive to the step ds and to the number of particles P. This sensitivity is explained by the term $\frac{1}{\sqrt{Pds}}$ in the error bound (48). Indeed, it is small for P vary large and ds not too small. Clearly, the explicit dispersion is more accurate and removes oscillations.

5 Conclusion

This paper proposed and analyzed an efficient probabilistic approach to compute quantities of interest quantifying the solute transport in random porous media. The permeability field is modeled by a random log-normal law and characterized by a covariance function having a piecewise regularity. The first step of the numerical approach consists to approximate the permeability through a Karhunen-Loève (K-L) truncation to deal with finite dimensional noise. Monte Carlo simulations are used to estimate mean values of quantities of interest. For each sample, a mixed finite element method is used to solve the flow problem and a probabilistic particle method solves the transport equation. The error estimates derived in this work predict the convergence rate. The behavior is illustrated numerically by a bi-dimensional example, where the permeability field is characterized by an exponential covariance function. We plan to further analyse in future work the truncation error and the effect of ergodicity on the quality of the approximated quantities of interest.

References

[1] I. M. Babuŝka, R. Tempone, and G. E. Zouraris *"Solving elliptic boundary value problems with uncertain coefficients by the finite element method: the stochastic formulation"*, Comput. Methods Appl. Mech. Engrg., 194(12- 16):1251-1294, 2005.

[2] I.M. Babuŝka, F. Nobile, and R. Tempone: *"A stochastic collocation method for elliptic partial differential equations with random input data"*, SIAM J. Numer. Anal, 43(3):1005-1034, 2007.

[3] A. Beaudoin, J.-R. de Dreuzy, J. Erhel and G. Pichot *"Convergence analysis of macro spreading in 3D heterogeneous porous media"*, ESAIM Proceedings. December 2013, Vol. 41, p. 59-76.

[4] A. Beaudoin, J.-R. de Dreuzy, *"Numerical assessment of 3-D macrodispersion in heterogeneous porous media"*, Water Resources Res, Volume 49, Issue 5, pages 2489-2496, May 2013.

[5] Brezzi, F. Fortin, M., *" Mixed and Hybrid Finite Element Methods"*. Springer-Verlag, New York, NY, 1991.

[6] J. Charrier. *"Numerical analysis of the advection-diffusion of a solute in random media"*, INRIA-Report, Num RR-7585 2011.

[7] J. Charrier. *"Numerical analysis of the advection-diffusion of a solute in random media"*, preprint 2013. Marseille University.

[8] J. Charrier and A. Debussche. *"Weak truncation error estimates for elliptic pdes with lognormal coefficients. Stochastic Partial Differential Equations : Analysis and Computations"*, 1:63-93, 2013.

[9] J.-R. de Dreuzy, A. Beaudoin, and J. Erhel. *"Asymptotic dispersion in 2d heterogeneous porous media determined by parallel numerical simulation"*. Water Resourc. Res., 43, 2007.

[10] J. Erhel, J.-R. de Dreuzy, A. Beaudoin, E. Bresciani, and D. Tromeur-Dervout. *"A parallel scientific software for heterogeneous hydrogeology"*. In Ismail H. Tuncer, Ulgen Gulcat, David R. Emerson, and Kenichi Matsuno, editors, Parallel Computational Fluid Dynamics 2007, volume 67 of Lecture Notes in Computational Science and Engineering, pages 39-48. Springer, 2009. invited plenary talk.

[11] J. Erhel, Z. Mghazli, M. Oumouni: *"Calcul de l'espérance de la solution d'une EDP stochastique unidimensionnelle à l'aide d'une base réduite"*, C.R.Acad.Sci.Paris, Ser. I, 349 2011, 861-865.

[12] J. Erhel, Z. Mghazli, M. Oumouni *"An adaptive sparse grid method for elliptic stochastic problem"*. In preparation.

[13] J. Erhel, M. Oumouni, G. Pichot *" About a generation of a stationary Gaussian correlated field"*. INRIA report, In preparation.

[14] Friedman, A. *"Stochastic Differentiel Equations and Applications"*, Academic Press, New-York, 1975

[15] Philipp Frauenfelder, Christoph Schwab, and Radu Alexandru Todor. *"Finite elements for elliptic problems with stochastic coefficients"*. Comput. Methods Appl. Mech. Engrg, 194(2-5):205-228, 2005.

[16] F. Hecht, *" New development in freefem++"*. J. Numer. Math. vol 20, 2012 no. 3-4, 251-265. 65Y15

[17] Ioannis Karatzas and Steven E. Shreve. *"Brownian motion and stochastic calculus"*, volume 113 of Graduate Texts in Mathematics. Springer-Verlag, New York, second edition, 1991.

[18] DENTZ, M. Kinzelbach, H. Attinger, S. and W. Kinzelbach. *"Temporal behavior of a solute cloud in a heterogeneous porous medium"*: 1. Point-like injection, Water Resources Research, 36 (12), pp. 3591-3604, 2000.

[19] Gelhar, L. *"Stochastic Subsurface Hydrology"*, Engelwood Cliffs, New Jersey (1993).

[20] R. G. Ghanem and P. D. Spanos. *"Stochastic finite elements : a spectral approach"*. Springer, 1991.

[21] I. Graham, F. Kuo, D. Nuyens, R. Scheichel, and I. Sloan. *"Quasi-monte carlo methods for elliptic pdes with random coefficients and applications. Journal of Computational Physics"*, 230:3668-3694, 2011.

[22] I. G. Graham, R. Scheichl, and E. Ullmann. *" Mixed Finite Element Analysis of Lognormal Diffusion and Multilevel Monte Carlo Methods"*. arXiv:1312.6047v1 [math.NA].

[23] H. Hoteit, J. Erhel, R. Mosé, B. Philippe, and P. Ackerer. *"Numerical reliability for mixed methods applied to flow problems in porous media"*. Computational Geosciences, 6:161-194, 2002.

[24] Ioannis Karatzas and Steven E. Shreve. *"Brownian motion and stochastic calculus"*, volume 113 of Graduate Texts in Mathematics. Springer-Verlag, New York, second edition, 1991.

[25] Kuo, F.Y., Schwab, C., Sloan, I.H, *"Quasi-monte carlo finite element methods for a class of elliptic partial differential equations with random coefficient"*. SIAM J. Numer. Anal. 50(6), 3351-3374, 2012.

[26] O.P. Le Maître and O.M. Knio. *"Spectral Methods for Uncertainty Quantification With Applications to Computational Fluid Dynamics"*. Scientific Computation. Springer, 2010.

[27] M. Loève: *"Probability Theory I,II"*, fourth edition, in: Graduate Texts in Mathematics, vol. 45,46, Springer-Verlag, New York, 1977-1978.

[28] A. Lunardi. *" Analytic semigroups and optimal regularity in parabolic problems. Progress in Nonlinear Differential Equations and their Applications,"* 16. Birkhäuser Verlag, Basel, 1995.

[29] H. Schwarze, U. Jaekel and H. Vereecken. *"Estimation of Macrodispersion by Different Approximation Methods for Flow and Transport in Randomly Heterogeneous Media"*. Transport in Porous Media 43: 265-287, 2001.

[30] R. Mikulevicius and E. Platen. *" Rate of convergence of the Euler approximation for diffusion processes"*. Math. Nachr., 151:233-239, 1991.

[31] H. Niederreiter, *"Random Number Generation and Quasi-Monte Carlo Methods"*, CBMS-NSF Regional Conf. Ser. in Appl. Math. 63, SIAM, Philadelphia, 1992.

[32] F. Nobile, R. Tempone, and C.Webster: *"An anisotropic sparse grid stochastic collocation method for elliptic partial differential equations with random input data"*, SIAM J. Numer. Anal., 2008, vol. 46/5, pp. 2411-2442.

[33] M. Oumouni, *"Analyse numérique de méthodes performantes pour les EDP stochastiques modélisant l'écoulement et le transport en milieux poreux"*. PhD thesis, Rennes1 University & Ibn Tofaïl University, 2013.

[34] E. Pardo-Iguzquiza and M. Chica-Olmo. *"The Fourier integral method: an efficient spectral method for simulation of random fields"*. Mathematical Geology, 25(2):177-217, 1993.

[35] T. Yao. *"reproduction of the mean, variance, and variogram model in spectral simulation"*. Mathematical Geology, 36:487-506, 2004.

[36] Dongxiao Zhang, Zhiming Lu. *"An efficient, high-order perturbation approach for flow in random porous media via Karhunen-Loève and polynomial expansions"*. Journal of Computational Physics 194 (2004) 773-794.

[37] C. Zheng and G. D. Bennett. *"Applied Contaminant Transport Modeling"*, second edition. John Wiley & Sons, New-York, 2002.