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On the numerical simulation of uncertain parameters in a radionuclide transport model

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Abstract

We study a fast algorithm to generate random fields which represent the uncertain parameters in a transport model of radionuclides in the geosphere. This algorithm has been introduced by Mikhailov and is based on a procedure known as Palm process. It can then be applied in a Monte Carlo method in the probabilistic risk assessment of high-level radioactive waste disposal in deep formation. We use this algorithm in order to compute the retardation factor appearing in the radionuclide migration model and we compare the CPU time corresponding to this procedure versus a classical spectral method. **To cite this article:** J.M. Díaz Moreno et al., *C. R. Acad. Sci. Paris, Ser. I* 345 (2007).

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Résumé

Modélisation numérique de paramètres incertains associés à un modèle de transport de radionucléides. On étudie un algorithme rapide pour la génération des champs aléatoires qui représentent les paramètres d'incertitudes d'un modèle de transport de radionucléides dans la géosphère. Cet algorithme peut être appliqué dans une méthode de Monte Carlo lors de l'évaluation du risque de stockage des déchets nucléaires à haute activité dans des couches géologiques en profondeur. À l'aide de cette procédure, on calcule le facteur de retard qui intervient dans les équations du modèle de transport des radionucléides, et on compare le temps de calcul de cet algorithme avec une méthode classique de type spectrale. **Pour citer cet article :** J.M. Díaz Moreno et al., *C. R. Acad. Sci. Paris, Ser. I* 345 (2007).

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Version française abrégée

Les analyses de performance à long terme déterminent si un dépôt et le site d'enfouissement qui le contient sont capables de protéger l'homme et l'environnement des effets des déchets radioactifs, ces analyses sont liées à l'évaluation probabiliste du risque de stockage. Dans ce contexte, nous présentons une étude qui consiste à générer des

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champs aléatoires de paramètres incertains associés à un modèle de type Monte Carlo qui simule le transport des radionucléides dans la géosphère et qui est basé sur un processus d'advection, de diffusion et de dispersion. Les paramètres soumis à des incertitudes sont repérés par des densités de probabilité qui apparaissent dans toutes les activités liées au calcul du risque.

En pratique, les méthodes numériques pour la résolution des équations du modèle du système composé des déchets et des barrières conduisent à un volume important de calculs. Notre étude consiste à générer des champs aléatoires de paramètres à l'aide d'un algorithme probabiliste simple, rapide (voir la Fig. 1) et efficace suggéré par Mikhailov basé sur une procédure appelée ici processus de Palm. Cet algorithme se base essentiellement sur la donnée d'une fonction d'autocorrélation multiéchelles et d'une fonction de distribution décrivant le comportement probabiliste du paramètre incertain.

On considère le système d'équations aux dérivées partielles (1) qui décrit les respectives concentrations d'une chaîne de radionucléides constituée par N_r radioisotopes. Dans ce modèle, les fonctions R_i , connues sous le nom de facteurs de retard, jouent un rôle fondamental dans les processus d'absorption et de désorption des radionucléides dans la roche. En pratique, il est impossible de connaître une expression analytique de R_i avec tous les détails. Cela est dû à la très grande variabilité spatiale de ces fonctions. Les facteurs de retard sont liés au coefficient de distribution, K_d , par les formules (2), ce qui montre que la seule connaissance de K_d donne toutes les fonctions R_i . Or, on sait que K_d est distribué selon une loi lognormale avec moyenne, écart type et fonction d'autocorrélation normalisée (voir Définition 2.3) qu'on sait estimer. Cette information permet de générer des réalisations stochastiques de R_i . Dans ce travail on décrit la procédure de Palm (Section 2) appliquée à la génération des champs aléatoires (dans notre cas, le coefficient de distribution et donc les facteurs de retard) et on compare la rapidité de cette technique par rapport à la méthode de type spectrale (Fig. 1).

La méthode basée sur l'algorithme de Palm exige que la fonction d'autocorrélation vérifie les conditions données par (4). Dans notre cas, on considère souvent des fonctions d'autocorrélation multiéchelles qui s'expriment comme une combinaison de fonctions exponentielles et qui vérifient (4), comme par exemple la fonction donnée par (7). Dans la Fig. 2 on a tracé la fonction d'autocorrélation normalisée avec deux réalisations obtenues par application de la procédure de Palm. Finalement, dans la Fig. 3 on montre une réalisation du facteur de retard obtenue par le processus de Palm en dimension deux ; on peut bien vérifier la grande variabilité spatiale que cette procédure reproduit.

1. Introduction and statement of the problem

Flow and transport models are commonly used to support the decision making process in environmental impact assessment. The modeling process, however, requires knowledge of the fundamental properties of porous media. Field research has shown that these porous media properties change continuously from location to location; this is equivalent to spatial heterogeneity that influences flow and transport processes in the vadose zone. Modeling efforts must inherently cope with uncertain information. Since the model input is uncertain, the model results are uncertain and the validity of the modeling may be questioned. In this study, we focus on the high spatial variability of some uncertain parameters that control radionuclide migration after a release from the repository in the geosphere. The spatial variability of these parameters will be modeled by generating random fields of some parameters as for instance the retardation factor. This work is useful for the study of the propagation of the uncertainty in the radionuclide transport model. In order to solve stochastic problems by a statistical modeling, it is necessary to construct many realizations of the random processes and fields; the problem becomes the computer time. We use a generator of random fields obtained by implementing a simple, fast and efficient numerical algorithm inspired from queuing theory built on a Palm process [6]. Some numerical tests of this algorithm are shown in order to simulate the retardation factor in a contaminant transport model, which can be then solved by finite difference-finite element techniques.

Uncertain parameters that control radionuclide migration are associated to the partial differential equations of the transport process involving several chemical and physical phenomena. As encountered in hydrogeological theory, the processes considered are advection by groundwater, diffusion-dispersion and linear, reversible and instantaneous equilibrium between species in the liquid and the solid phases [1,3], together with radioactive degradation. In this analysis, outputs of the transport process correspond to the concentrations of radionuclides in space and in time.

The transport model relative to a saturated porous medium for a N_r -member radionuclide chain may be written in a parabolic domain $\Omega \times (0, T) \subset \mathbb{R}^N \times (0, +\infty)$ as [7]

$$\frac{\partial(\theta R_i c_i)}{\partial t} + \nabla \cdot (q c_i) - \nabla \cdot [\theta(D_m + D_p) \nabla c_i] + \theta R_i \lambda_i c_i = S_i + \theta \sum_{j=1}^{i-1} \alpha_{ij} R_j \lambda_j c_j, \quad 1 \leq i \leq N_r, \quad (1)$$

where $c_i = c_i(x, t)$ represents the concentration of the i -th radionuclide per unit volume of fluid at location $x \in \Omega$ and time $t \in [0, T]$, R_i its retardation factor, θ the porosity, q the Darcy velocity, D_m the molecular diffusion tensor, D_p the dispersion tensor, λ_i the radioactive decay constant, $T > 0$ the final time of observation, S_i a source term, and α_{ij} are known density values with $0 \leq \alpha_{ij} \leq 1$ for $1 \leq j < i \leq N_r$, and $\alpha_{ii-1} \neq 0$ for $2 \leq i \leq N_r$.

In (1), the retardation factors R_i , $1 \leq i \leq N_r$, are the responsible of the uncertainty due to its highly spatial variability. Geologic statistical measures has shown that it is distributed according to a lognormal law with known mean, standard deviation and normalized autocorrelation function (see Definition 2.3 below). The retardation factors describe the absorption and desorption of radionuclides by the rock of the porous medium. The effect of the retardation factors and Darcy velocity on migration is very important in practical situations [1,3].

We may express R_i in terms of the distribution coefficient, K_d , as follows [1,3,7]

$$R_i = 1 + \gamma_i \frac{\rho_b}{\theta} K_d, \quad \gamma_i = \frac{\langle R_i \rangle - 1}{\langle R_1 \rangle - 1}, \quad 1 \leq i \leq N_r, \quad (2)$$

where ρ_b is the bulk density of the solid phase ($\langle \cdot \rangle$ stands for the average or mean operator). Putting $U = \ln[\rho_b K_d]$, it is straightforward that $\langle U \rangle = \ln[\theta(\langle R_1 \rangle - 1)] - \frac{\sigma_U^2}{2}$, where σ_U is the standard deviation of U . Finally,

$$R_i = 1 + \gamma_i(R_1 - 1), \quad 2 \leq i \leq N_r. \quad (3)$$

Formulae (2), (3) are quite interesting for numerical tests and computation time since every realization of the term $\rho_b K_d$ leads to the respective realizations of all the retardation factors R_i , $1 \leq i \leq N_r$.

In the analysis of the probabilistic risk assessment for the radioactive waste repository, we need to compute the solution of system (1) for every realization of R_i , and this has to be done many times (even tens of millions). It is important to point out that these samples of R_i must fit the given statistical moments (mean, standard deviation and normalized autocorrelation function).

2. Unconditional random field generator

Consider a random function ξ in \mathbb{R}^N (or a subset of \mathbb{R}^N). If $N \geq 2$, the random function is called random field. If $N = 1$, it is called random process. A random function is also called a stochastic process.

Definition 2.1.

- (a) The mean function of a stochastic process is defined as $m(x) = E[\xi(x)]$, $x \in \mathbb{R}^N$, where $E[\cdot]$ is the expectation operator. We also use the notation $m(x) = \langle \xi(x) \rangle$.
- (b) The covariance function is defined as $\text{cov}(x, y) = E[(\xi(x) - m(x))(\xi(y) - m(y))]$, $x, y \in \mathbb{R}^N$. The standard deviation of $\xi(x)$ is given by $\sigma(x) = \text{cov}(x, x)^{1/2}$.

Definition 2.2. A stochastic process ξ is said to be a second stationary process if the following conditions are satisfied:

- (i) The mean is independent of the position: $E[\xi(x)] = m$, for any $x \in \mathbb{R}^N$.
- (ii) The covariance function depends only on the vector difference $d = x - y$, that is

$$\text{cov}(x, y) = \mathbf{C}(x - y) = \mathbf{C}(d), \quad \text{for all } x, y \in \mathbb{R}^N.$$

Definition 2.3. The autocorrelation function of a random process ξ is $\text{acorr}(x, y) = \text{cov}(x + y, y)$. If ξ is second stationary then $\text{acorr}(x, y) = \mathbf{C}(x)$, and the function $C(x) = \mathbf{C}(x)/\mathbf{C}(0)$ is called normalized autocorrelation function of the process ξ .

In order to solve stochastic problems by a statistical modeling, it is necessary to construct many realizations of the random processes and fields. In this kind of analysis, it is important to preserve the normalized autocorrelation function and the probability distribution function (PDF). Many methods are available for simulating one-dimensional realizations of a stationary stochastic process with a given covariance. However, when these procedures are extended to the three-dimensional space, they are often inextricable or prohibitive in terms of computer time. In order to solve this computational challenge, we use a one dimensional simulator of non-Gaussian fields suggested by Mikhailov [5] connected with a stationary fluxes of points that give processes called Palm fluxes [2,6]. Its description now follows.

Let $L > 0$ and suppose that it is required to construct a second stationary random process $\xi : [0, L] \mapsto \mathbb{R}$, with a given PDF, F , and a normalized autocorrelation function, C , satisfying the conditions:

$$C''(x) \geq 0, \quad |C'(0)| < \infty, \quad C(0) = 1, \quad C(\infty) = 0, \quad C'(x) \leq 0. \quad (4)$$

We then consider the following functions

$$f_1(x) = -C'(x), \quad \text{and for } i > 1, \quad f_i(x) = -\frac{C''(x)}{C'(0)}, \quad x \geq 0; \quad f_i(x) = 0, \quad x < 0, \quad i \geq 1. \quad (5)$$

Thanks to (4), every function $f_i(x)$, $i \geq 1$, is a probability density function. Consider now a point flow z_k , $k \geq 0$ of the form

$$z_0 = 0, \quad z_k = \sum_{i=1}^k \eta_i \quad (6)$$

where η_i are independent non-negative random variables which are respectively sampled according to the probability densities $f_i(x)$, $i \geq 1$. The variable η_i is sampled while the condition $z_{i-1} < L$ is verified. If $z_J \geq L$, then we stop the procedure and just put $z_J = L$. In this way, we have built a random partition of the observation interval $[0, L]$.

Finally, we set $\xi(z) = \xi_i$ in each interval $(z_{i-1}, z_i]$, $1 \leq i \leq J$, $\xi(0) = \xi_1$, where ξ_i are independent random variables sampled with the given PDF F . The following result holds [6]:

Theorem 2.4. *The process ξ is a second stationary stochastic process with associated normalized autocorrelation function given by $C(x)$ and distributed according to F .*

Notice that in order to generate the i -th realization of Palm flow (z_k) we may use the inverse distribution method, namely $C(\eta_1) = \alpha_1$, $C'(\eta_i) = \alpha_i C'(0)$, $i \geq 2$, where the α_i , $i \geq 2$, are obtained by a random sampling using the uniform distribution $U(0, 1)$ [4].

One interesting choice of the normalized autocorrelation function C is $C(x) = \sum_{i=1}^M \sigma_i^2 e^{-x/\ell_i}$ where ℓ_i , $1 \leq i \leq M$, represent correlation length scales; heterogeneity of the geological medium can be characterized over the largest scale [3].

This method can be extended to the N -dimensional case. For instance, consider $N = 3$ and let D be the 3-rectangle $[0, L_x] \times [0, L_y] \times [0, L_z]$. Then, a random field ξ using Palm flow can be obtained through the following procedure:

- (i) Sample Palm flow τ_k^i with the normalized autocorrelation $C_i(t)$ on the i -th axis, $1 \leq i \leq 3$.
- (ii) Sample an independent value of ξ according to the distribution function F_ξ for each parallelepiped of the form $[\tau_{k_1-1}^1, \tau_{k_1}^1] \times [\tau_{k_1-1}^2, \tau_{k_1}^2] \times [\tau_{k_1-1}^3, \tau_{k_1}^3]$.

Then, the random field ξ is second stationary and has a normalized autocorrelation function ([6])

$$C(x_1, x_2, x_3) = C_1(|x_1|)C_2(|x_2|)C_3(|x_3|).$$

3. Numerical tests: multiscale model

Numerical results concern the generation of random fields essentially related to the retardation factor. The algorithm associated to Palm process for unconditional generation is built on an exponential autocorrelation function, and values of the generated parameter are sampled according to a lognormal distribution function. Comparison on CPU time with

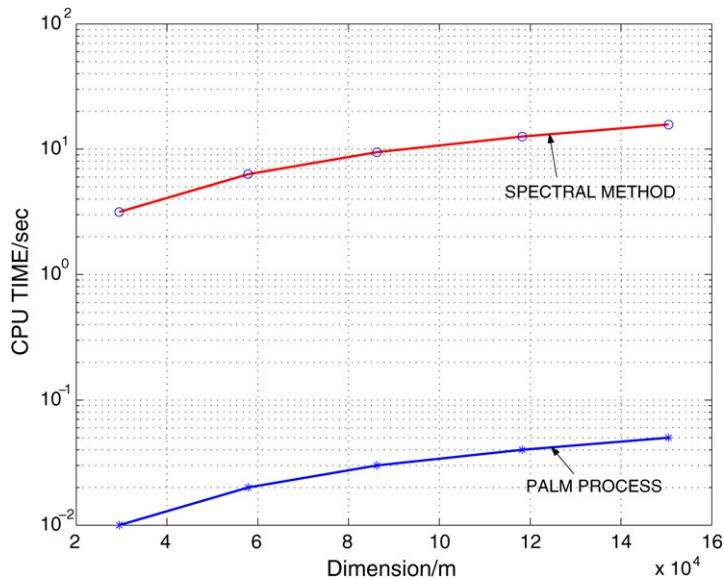


Fig. 1. CPU time comparison between a spectral method and Palm procedure.

Fig. 1. Comparaison entre le temps de calcul d'une méthode spectrale et la procédure de Palm.

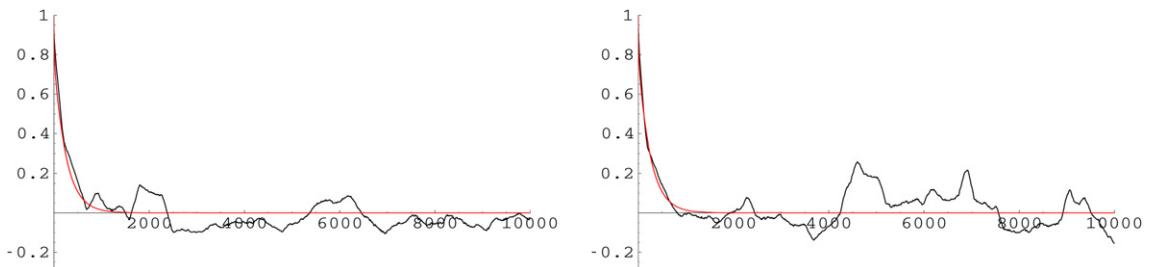


Fig. 2. Normalized autocorrelation functions of two random realizations. The smooth curve represents the exact autocorrelation function.

Fig. 2. Fonctions d'autocorrélation normalisée de deux réalisations aléatoires. La courbe régulière représente la fonction d'autocorrélation exacte.

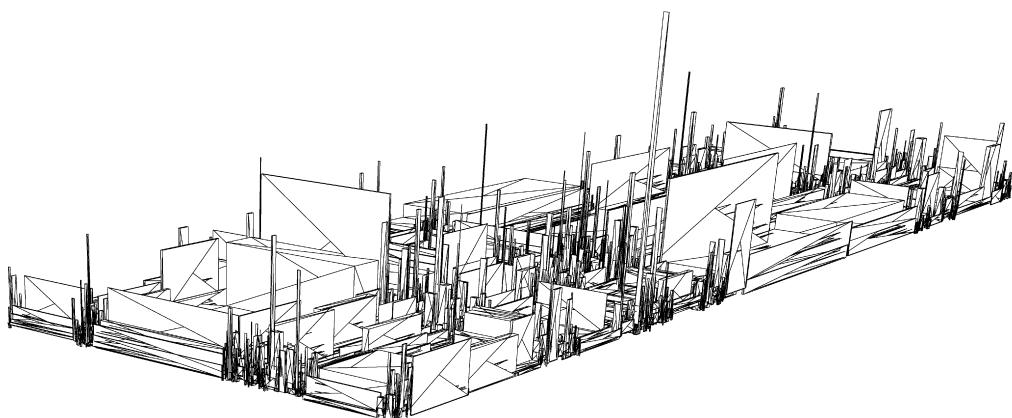


Fig. 3. Sample of a 2D realization of the retardation factor obtained with the Palm process. We can observe the high spatial variability.

Fig. 3. Échantillon d'une réalisation 2D de la fonction de retard obtenu suivant le processus de Palm. On peut observer la grande variabilité spatiale.

a spectral model is shown in Fig. 1. In Fig. 2 we compare the numerical normalized autocorrelation function with the predicted continuous normalized autocorrelation function $C(x)$ defined as

$$C(x) = \sigma_1^2 e^{-x/\ell_1} + \sigma_2^2 e^{-x/\ell_2}, \quad \text{with } \sigma_1^2 = 0.206897, \sigma_2^2 = 0.793103, \ell_1 = 5, \ell_2 = 250. \quad (7)$$

Good agreement of these curves are obtained in both cases. In Fig. 3 we show one sample of a 2D realization of the retardation factor obtained with the Palm process in 2D using a normalized autocorrelation like in (7) and a lognormal distribution to estimate the value on every rectangle. In [2] we may find some numerical simulations of (1) with $N_r = 2$ using two different realizations of the retardation factors obtained with the Palm process.

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