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Spatial global sensitivity analysis

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Abstract

The global sensitivity analysis of a complex numerical model often requires the estimation of variance-based importance measures, called Sobol indices. Metamodel-based techniques have been developed in order to replace the cpu time expensive computer code with an inexpensive mathematical function, predicting the computer code output. The common metamodel-based sensitivity analysis methods are appropriate with computer codes having scalar model output. However, in the environmental domain, as in many areas of application, numerical models often give as output a spatial map, which is sometimes a spatio-temporal evolution, of some interest variables. In this paper, we introduce a novel way to obtain a spatial map of Sobol indices with a minimal number of numerical model computations. It is based on the functional decomposition of the spatial output onto a wavelet basis and the metamodeling of the wavelet coefficients by Gaussian process. An analytical example allows us to clarify the various steps of our methodology. This technique is then applied to a real case of hydrogeological modeling: for each model input variable, a spatial map of Sobol indices is thus obtained.

Keywords: Computer experiment, Gaussian process, metamodel, functional data, radionuclide migration.

1 INTRODUCTION

Today, in different environments, sites exist with contaminated groundwater formed as a result of the inappropriate handling or disposal of hazardous materials or waste. Such environmental or sanitary problematic needs the development of treatment or remediation strategies and in all cases requires robust long-term behaviour prediction. The

indispensable simulation of global fluxes, as water or pollutants, through the different environmental compartments involves numerous parameters. Numerical modeling of such sites is an efficient tool for an accurate prediction of contamination plume spreading and an assessment of environmental risks associated with the site. However, it has been recognized that in such complex numerical models many input variables are highly uncertain, such as hydrogeological parameters (permeabilities, porosities, etc.) or boundary and initial conditions (contaminant concentrations, aquifer level, etc.). In fact, systematic and exhaustive 3D characterization of sites remains impossible.

To deal with all these uncertainties, computer experiment methodologies based on statistical techniques are useful. For instance, we assume that $Y = f(\mathbf{X})$ is the real-valued output of a computer code f , whose input variables are random and modeled by the random vector $\mathbf{X} = (X_1, \dots, X_d) \in \mathbb{R}^d$ with known distribution. The uncertainty analysis step is used to evaluate statistical parameters, confidence intervals or the density probability distribution of the model response (De Rocquigny et al., 2008), while the global sensitivity analysis step is used to quantify the influence of the uncertainties of the model input variables (in their whole range of variations) on the model response (Saltelli et al., 2000). Recent studies have applied different statistical methods of uncertainty and sensitivity analysis to environmental models (Helton, 1993; Nychka et al., 1998; Fassò et al., 2003; Volkova et al., 2008; Lilburne and Tarantola, 2009). All these methods have shown their efficiency in providing guidance to a better understanding of the modeling act.

However, for the purpose of sensitivity analysis, four main difficulties can arise due to practical problems, especially in the environmental risk domain:

- P1) physical models involve rather complex phenomena (non linear and threshold effects) sometimes with strong interactions between physical variables;
- P2) computer codes are often too cpu time expensive to evaluate a model response, from several minutes to weeks;
- P3) numerical models take as inputs a large number of uncertain variables (typically $d > 10$);
- P4) numerical models give as a result many variables of interest, potentially spatially and temporally dependent.

The first problem P1 is resolved by using variance-based measures, which can deal with non linear and non monotonic relationships between the inputs and the output (Saltelli et al., 2000). These measures are based on the functional ANOVA decomposition of any integrable function f (Efron and Stein, 1981) and determine the weights of the variance of the output resulting from a variable X_i or an interaction between variables (Sobol, 1993):

$$S_i = \frac{\text{Var} [\mathbb{E}(Y|X_i)]}{\text{Var}(Y)}, \quad S_{ij} = \frac{\text{Var} [\mathbb{E}(Y|X_i, X_j)]}{\text{Var}(Y)} - S_i - S_j, \quad S_{ijk} = \dots \quad (1)$$

The interpretation of these coefficients, namely the Sobol indices, is natural as all indices lie in $[0, 1]$ and their sum is equal to one. The larger the index value, the greater the

importance of the variable related to this index. To express the overall output sensitivity to an input X_i , Homma and Saltelli (1996) introduce the total sensitivity index:

$$S_{T_i} = S_i + \sum_{j \neq i} S_{ij} + \sum_{j \neq i, k \neq i, j < k} S_{ijk} + \dots = \sum_{l \in \#i} S_l = 1 - \frac{\text{Var}[\mathbb{E}(Y|X_{\sim i})]}{\text{Var}(Y)} \quad (2)$$

where $\#i$ represents all the “non-ordered” subsets of indices containing index i and $X_{\sim i}$ is the vector of all inputs except X_i . Thus, $\sum_{l \in \#i} S_l$ is the sum of all the sensitivity indices having i in their index.

Unfortunately, the traditional or advanced Monte Carlo methods, used to estimate first order and total Sobol indices, require a large number of model evaluations (Saltelli et al., 1999). To overcome the problem P2 of a too long calculation time in uncertainty and sensitivity analysis, approaches based on metamodeling have recently been developed. This solution consists in replacing the complex computer code by a mathematical approximation, called a metamodel, which is fitted from only a few experiments and simulates the behavior of the computer code in the domain of its influential parameters (Sacks et al., 1989; Fang et al., 2006). Among all the solutions based on metamodels (polynomials, splines, neural networks, etc.), our attention is focused on the Gaussian process (Gp) model, which can be viewed as an extension of the kriging method, a spatial data interpolation method (Chilès and Delfiner, 1999), to computer code data (Sacks et al., 1989). Gp modeling treats the deterministic response $y = f(\mathbf{x})$ (with $y \in \mathbb{R}$, $\mathbf{x} \in \mathbb{R}^d$) of the computer code as a realization of a random function $Y_{\text{Gp}}(\mathbf{x})$:

$$Y_{\text{Gp}}(\mathbf{x}) = f_0(\mathbf{x}) + Z(\mathbf{x}) . \quad (3)$$

$f_0(\mathbf{x})$ is a deterministic function (for example a polynomial) that provides the mean approximation of the computer code, and $Z(\mathbf{x})$ is a Gaussian centered stationary stochastic process fully characterized by its variance σ^2 and correlation function $R(\cdot)$. For a new input vector \mathbf{x}^* , we obtain

$$\mathbb{E}[Y_{\text{Gp}}(\mathbf{x}^*)/X_s, Y_s] = f_0(\mathbf{x}^*) + \mathbf{k}(\mathbf{x}^*)^t \boldsymbol{\Sigma}_s^{-1} (Y_s - f_0(X_s)) , \quad (4)$$

$$\text{Var}[Y_{\text{Gp}}(\mathbf{x}^*)/X_s, Y_s] = \sigma^2 - \mathbf{k}(\mathbf{x}^*)^t \boldsymbol{\Sigma}_s^{-1} \mathbf{k}(\mathbf{x}^*) , \quad (5)$$

where $(X_s, Y_s) = ((\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(n)}, y^{(n)}))$ is the learning sample (n simulation points), $\mathbf{k}(\mathbf{x}^*)$ is the covariance vector between \mathbf{x}^* and the learning sample, and $\boldsymbol{\Sigma}_s$ is the covariance matrix of the learning sample. Numerous authors (for example, Welch et al., 1992; Santner et al., 2003; Marrel et al., 2008) have shown how the Gp model can provide a statistical basis for computing an efficient predictor (given by Eq. (4)) of code response, even in high dimensional cases, when the model contains several tens of random input variables (problem P3).

In this paper, we deal with models affected by the four problems (P1, P2, P3 and P4), which is a common situation in model-based environmental studies. We focus our attention on the problem P4 of high dimensional model output. In fact, in our application case, the costly numerical model computes a spatial concentration map. This spatial output contains several thousands of pixels, each giving a concentration value. This kind of problem cannot be tuned to a vectorial output problem because of its dimensionality: the metamodeling of this vectorial input is intractable via the kriging of each scalar value

or via a cokriging technique (Fang et al., 2006). Therefore, we choose to see the model output as a functional output that we synthesize by its projection on an appropriate basis. This problem of building a metamodel (based on functional decomposition and Gp modeling) for a functional output has recently been addressed for uni-dimensional output by Shi et al. (2007) and Bayarri et al. (2007) and for two-dimensional output by Higdon et al. (2008).

For the sensitivity analysis problem, a functional output is classically treated as a vectorial output and sensitivity indices of each input are computed for each discretized value of the output (De Rocquigny et al., 2008). In order to avoid the large amount of sensitivity index computations by applying such an approach, some authors have applied various basis decompositions, such as the principal component analysis, on the functional output (Campbell et al., 2006; Lamboni et al., 2009). In this approach, sensitivity indices are obtained for the coefficients of the expansion basis.

However, the full functional restitution of Sobol indices remains an unexplored challenge. In this paper, we propose an original complete methodology to compute Sobol indices at each location of the spatial output map. Our approach consists in building a spatial output metamodel based on wavelet decomposition as in Bayarri et al. (2007) (restricted to the case of a temporal output). This metamodel is then used to compute spatial Sobol index maps (one map for each input variable). These visual tools seem to be promising in terms of model understanding, interpretation and prediction.

The next section presents our environmental problem and the associated radionuclide groundwater migration modeling. In the third section, our methodology is fully described step by step. An artificial test function is used to demonstrate the relevance of the choices and the convergence of the algorithms. Section 4 is devoted to the application of this methodology on our real application. Some discussions conclude this paper.

2 THE APPLICATION CASE

In the period between 1943 and 1974 radioactive waste was buried in eleven temporary repositories built on a specially allocated site at the RRC Kurchatov Institute (KI) in the Moscow area (Russia). The site used for radioactive waste interim storage has an area of about 2 hectares and is situated near the KI external perimeter in the immediate vicinity of the city's residential area. A radioactive survey of the site and its adjacent area performed in the late 1980s - early 1990s and in 2002 showed that radioactive contamination is not only present on the surface but has a tendency to spread into groundwater. The porous media of the site is represented principally by sands alternatively with clays that form several horizontal superposed aquifers. To analyze radioactive contamination of groundwater, about a hundred exploration wells were drilled on the site. As a result of the survey, it was discovered that contamination of groundwater is mainly connected to ^{90}Sr . Since the radiation survey results have demonstrated the necessity to clean up the site, rehabilitation activities on radwaste removal and liquidation of old repositories were performed at the site between 2002 and 2006. A network of observation wells is used to control groundwater conditions of the two upper aquifers. This network consists of twenty observation wells for the upper moraine aquifer and nine for the second Jurassic aquifer. It is used for a regular recording of groundwater levels, its chemical and radionuclide

composition (see Velikhov et al., 2007).

A numerical model of ^{90}Sr transport in groundwater was developed for the RRC Kurchatov Institute (KI) radwaste disposal site (Volkova et al., 2008). It aimed to provide a correct prediction of further contamination plume spreading since 2002 (using an interpolated concentration map) and up to the end of the year 2010, to show the risks associated with contamination and to serve as a basis for engineering decision-making. The numerical model has been constructed using the MARTHE hydrogeological program package (developed by BRGM, the French Geological Survey). It is a three-dimensional combined transient flow and transport convection-dispersion model taking into account sorption and radioactive decay. Three layers were singled out; horizontal, vertical and temporal meshes were chosen in accordance with the migration characteristics of the sand. Initial concentration plume in 2002 and spreading prediction made for the year 2010 are shown on Figure 1. As can be seen, contamination plume predicted for the year 2010 is not uniform and is more diffused than the initial one. This is due, above all, to the influence of intensive infiltration assigned to several zones of the model domain that results in local dispersion of contamination plume.

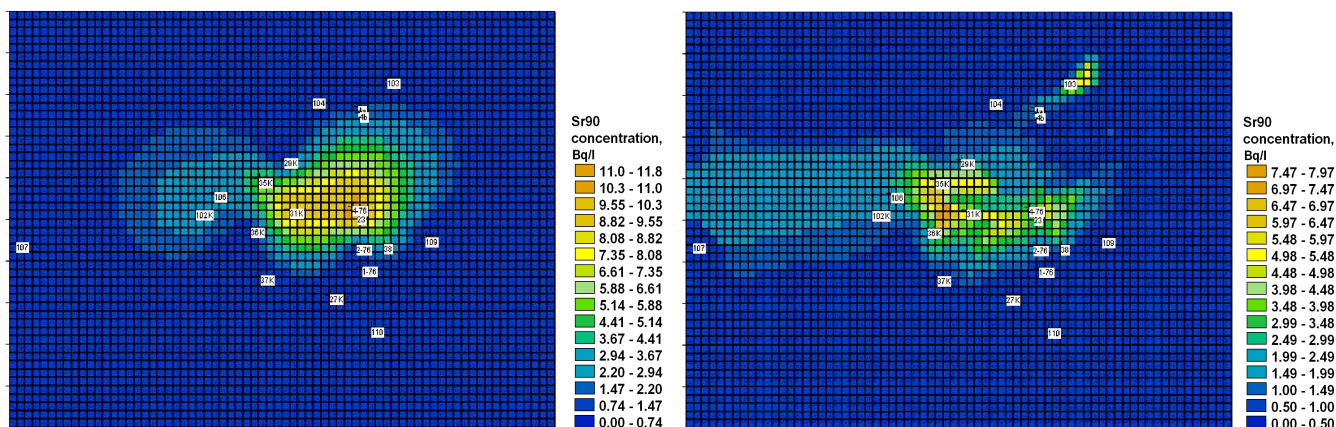


Figure 1: Initial (left, 2002) and predicted (right, 2010) ^{90}Sr concentrations (hot colors represent higher levels of concentration). Initial concentrations range from 0 to 12 Bq/l while final concentrations range from 0 to 8 Bq/l. The small white rectangles represent the location of the observation wells.

It has been shown in Volkova et al. (2008) that the form of predicted contamination plume depends on the model input values (hydraulic conductivity, infiltration parameters, sorption distribution coefficients, etc.). Indeed, a large part of the model input variables are exposed to some uncertainty, since their values have been obtained through expert judgment, model calibration, field experiments and laboratory experiments. These uncertainties lead to uncertainties in model prediction. In order to evaluate the degree of input influence on the resulting contamination plume form and concentration values predicted in observation wells, it has been proposed to perform global sensitivity analysis on this numerical model (called MARTHE in the following sections).

Probability distributions (uniform and Weibull laws) have been assigned to 20 random input variables of MARTHE. 300 Monte Carlo simulations, based on Latin hypercube

sampling of the input variables (McKay et al., 1979), have been performed (requiring four calculation days). For each simulated set of input variables, MARTHE computes transport equations of ^{90}Sr and predicts the evolution of ^{90}Sr concentration. The 20 uncertain model parameters are the permeability of different geological layers composing the simulated field, longitudinal and transverse dispersivity coefficients, and sorption distribution coefficients. To perform global sensitivity analysis and in particular to compute Sobol indices, previous studies have concentrated on 20 scalar outputs of ^{90}Sr concentration values, predicted for the year 2010, in 20 piezometers located on the waste repository site.

Because of the long computing time of MARTHE and of the non linearity of the relationships between inputs and outputs, Volkova et al. (2008) propose to fit a metamodel (based on boosting regression trees) on each output using the learning sample (300 observations). Then Sobol indices are computed by intensive Monte Carlo simulations using this metamodel. In Marrel et al. (2008), each output is modeled by a Gp metamodel: the Gp metamodel outperforms the linear regression and the boosting regression trees metamodel in terms of predictivity of the output values.

As a result of these sensitivity analyses, we note that the calculated concentrations at the piezometer locations are mainly influenced by the distribution coefficient of ^{90}Sr in the first and second layers of the domain and by the intensity infiltration in the pipe leakage zones, and to a lesser extent by the hydrodynamic parameters (dispersivity, porosity, etc.). However, we are aware that spatial information has been lost in these analyses, due to the limited amount of output values that we have considered (concentrations localized at 20 locations). Our goal is now to compute Sobol indices in the whole spatial concentration map, predicted by the model for 2010.

3 METHODOLOGY

In this section, we describe the methodology that we use to perform spatial Sobol index maps (first proposed in Marrel, 2008). We also apply this methodology to an analytical function in order to study the convergence of the algorithms.

3.1 General principles

The computer code that we consider has d input variables denoted by $\mathbf{X} = (X_1, \dots, X_d)$. For a given value \mathbf{x}^* of the vector \mathbf{X} , the code output is a deterministic function $y(\mathbf{x}^*, \mathbf{z})$ where \mathbf{z} denotes a vector of dimension p of spatial coordinates. In this paper, we consider the case $p = 2$, the output of the code is therefore a map corresponding to the values of the function $y(\mathbf{x}^*, \mathbf{z})$, when \mathbf{z} varies in a grid on a compact set D_z of \mathbb{R}^2 . The variables \mathbf{X} and \mathbf{z} are of a completely different nature : the variables X_1, \dots, X_d , corresponding to the inputs of the computer code, are random. They are different for each simulation of the code and we want to perform a sensitivity analysis with respect to these variables. The variables \mathbf{z} are deterministic and vary on a grid of size n_z corresponding to a discretization of D_z . For each simulation of the code, the grid is the same and the output corresponds to the n_z values $y(\mathbf{x}^*, \mathbf{z})$ for \mathbf{z} describing the grid. For example, MARTHE has $d = 20$ input variables and provides at each simulation a map with $n_z = 64 \times 64 = 4096$ points (see Section 4).

Because of the different nature of the variables \mathbf{X} and \mathbf{z} , we model in a different way the dependency of the output with respect to these two kinds of variables. For a fixed value of \mathbf{X} , we will use a projection of the map $\mathbf{z} \mapsto Y(\mathbf{X}, \mathbf{z})$, onto a wavelet orthonormal basis. The coefficients of the projection depend on \mathbf{X} . We select the most important coefficients (to be more precise) and we model the selected coefficients with respect to the d -dimensional input variable \mathbf{X} . In most applications, the dimension of \mathbf{X} is quite large and each simulation of the code is time-expensive. We therefore need a method that is adapted to a situation where we have a limited number of simulations and quite a large dimension of the input vector. It is also expected that the relationship between the input variables and the coefficients is highly non linear. The Gaussian process (Gp) metamodel, described in the introduction (see Eq. (3)), can be efficient to model responses that have a highly non linear behaviour with respect to quite a large number of input variables (Welch et al., 1992; Marrel et al., 2008). We therefore use this methodology to model the dependency of each selected coefficient with respect to \mathbf{X} .

To summarize, given the input design $X_s = (\mathbf{x}^{(i)})_{i=1..n}$, we obtain n simulations of the map $(y(\mathbf{x}^{(i)}, \mathbf{z}_j), j = 1, \dots, n_z), i = 1, \dots, n$. We then have to consider three main steps:

1. Decomposition of the maps $\mathbf{z} \mapsto y(\mathbf{x}^{(i)}, \mathbf{z})$ onto a two-dimensional wavelet basis;
2. Selection of the most important coefficients;
3. Modeling of the coefficients with respect to the input variables using a Gp.

At each step, we will use various criteria to evaluate the performances of our procedures. We are then able to predict a map $(y(\mathbf{x}^*, \mathbf{z}_j), j = 1 \dots, n_z)$ for a new value of the input vector \mathbf{x}^* . Of course, this method of map prediction (which we call a functional metamodel or also, in our case, a spatial metamodel) has the advantage, compared to the simulation of the code, to be much less time-expensive.

Finally, our functional metamodel will allow us to produce maps of sensitivity analysis based on Sobol indices by using Monte Carlo methods (see introduction, Eqs. (1) and (2)). Indeed, as said before, the direct use of the computer code is impossible because of the required number of function evaluations. In this study, we are restricted to the estimation of the first order indices $S_i(\mathbf{z})$ and total Sobol indices $S_{T_i}(\mathbf{z})$ for $\mathbf{z} \in D_z$. For each input, these two indices allow us to quantify respectively its sole influence and its total influence. Then, its degree of interaction with other inputs can be deduced.

3.2 An analytical test case: The Campbell2D function

The analytical function that we will use in this section to perform various tests is inspired from Campbell et al. (2006) who use a function with four inputs and a uni-dimensional output. We have modified it to a function with eight inputs ($d = 8$) and a two-dimensional output ($\mathbf{z} = (\theta, \phi)$):

$$Y = g(\mathbf{X}, \theta, \phi) = X_1 \exp \left[-\frac{(0.8\theta + 0.2\phi - 10X_2)^2}{60X_1^2} \right] + (X_2 + X_4) \exp \left[\frac{(0.5\theta + 0.5\phi)X_1}{500} \right] \\ + X_5(X_3 - 2) \exp \left[-\frac{(0.4\theta + 0.6\phi - 20X_6)^2}{40X_5^2} \right] + (X_6 + X_8) \exp \left[\frac{(0.3\theta + 0.7\phi)X_7}{250} \right], \quad (6)$$

where $(\theta, \phi) \in [-90, 90]^2$ represent azimuthal and polar spatial coordinates and $X_i \sim \mathcal{U}[-1, 5]$ for $i = 1 \dots 8$. This function, called the Campbell2D function, gives as output a spatial map, as shown in Figure 2. The Campbell2D function has been calibrated in order to give strong spatial heterogeneities, sometimes with sharp boundaries, and very different spatial repartitions of the output values in function of the \mathbf{X} values.

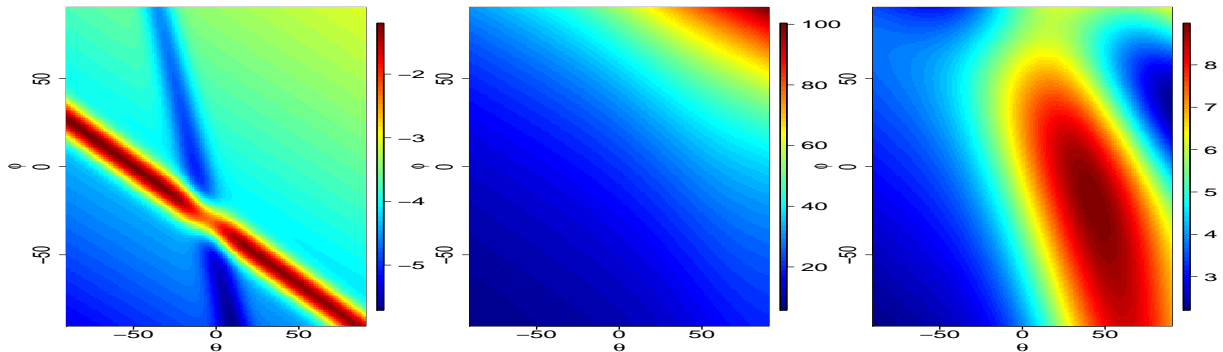


Figure 2: Three different output maps from the Campbell2D function: $\mathbf{x} = (-1, -1, -1, -1, -1, -1, -1, -1)$ (left); $\mathbf{x} = (5, 5, 5, 5, 5, 5, 5, 5)$ (center); $\mathbf{x} = (5, 3, 1, -1, 5, 3, 1, -1)$ (right).

With the Campbell2D function, the analytical calculations of the first order Sobol indices $S_i(\theta, \phi)$ are possible. Appendix A gives the results of these integrations. The obtained analytical expressions (Eqs. (16) to (23)) will serve as the exact solutions of the first order Sobol indices. However, analytical calculations of the total Sobol indices $S_{T_i}(\theta, \phi)$ (Eq. (2)) are not possible. We estimate $S_{T_i}(\theta, \phi)$, $i = 1, \dots, 8$, by using the Saltelli's Monte Carlo algorithm (Saltelli, 2002) using two random samples of $N = 10^5$ computations of the Campbell2D function. The estimated errors with such large sample sizes are of the order of 5×10^{-3} (standard deviation estimated via bootstrap). These estimates $S_{T_i}(\theta, \phi)$ will henceforth be called exact total Sobol indices.

Figure 3 gives the maps of the total Sobol index estimations. Input X_5 has no influence on the output of the Campbell2D function. Input X_1 has a small influence on the output of the Campbell2D function. Input X_3 has a mild influence in a diagonal axis of the spatial domain. Inputs X_4 and X_8 have mild influences in a large part of the spatial domain. Inputs X_2 , X_6 and X_7 have strong influences in different parts of the spatial domain (localized in corners for X_2 and X_7). Moreover, the first order Sobol indices (maps not shown here) for X_3 , X_5 , X_6 and X_7 are far from the total Sobol indices. As shown by the formula (6) of the Campbell2D function, these four variables have some strong interactions (interactions between X_3 , X_5 and X_6 and between X_6 and X_7).

3.3 Spatial metamodeling

The spatial metamodeling process is composed of 5 internal steps.

Step 0 - Preparation of the learning sample

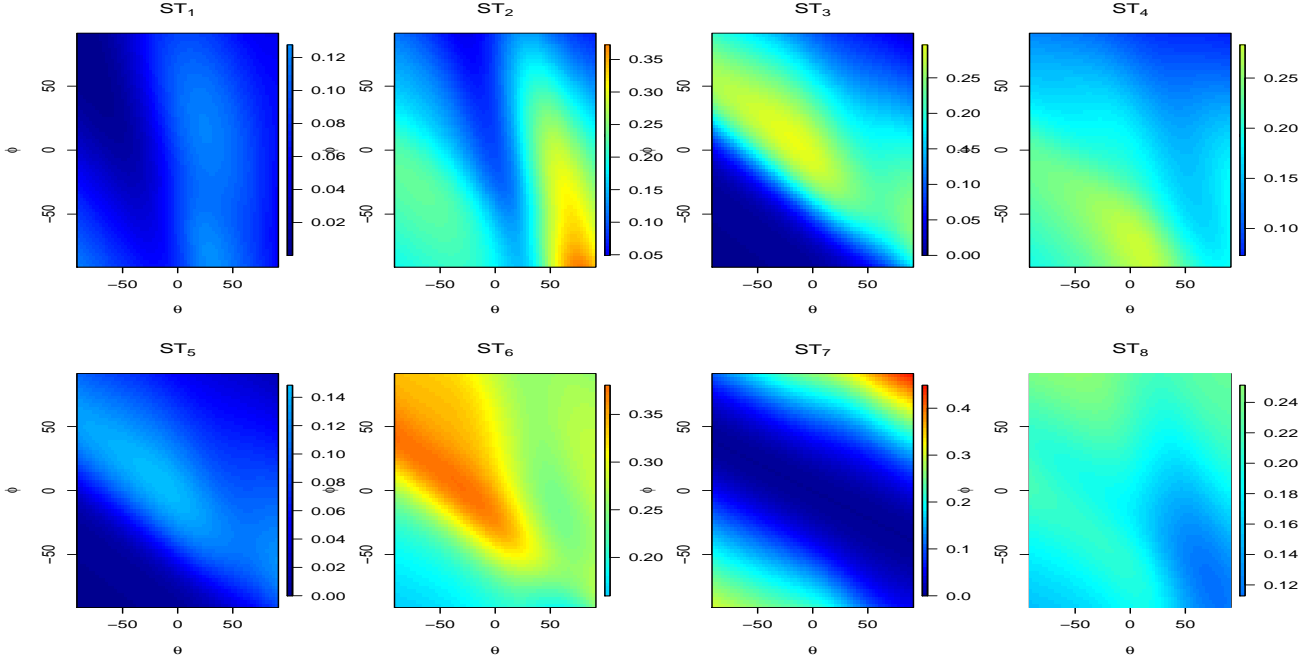


Figure 3: Total Sobol indices of the 8 input variables of the Campbell2D function, estimated by Monte Carlo algorithm.

When dealing with a large input dimension d , the choice of the input design $X_s = (\mathbf{x}^{(i)})_{i=1..n}$ is especially important, and even more so when n is small. For scalar computer model output, numerous authors have shown the strong influence of the input design on the quality of the Gp modeling (Santner et al., 2003; Fang et al., 2006). For instance, maximin Latin hypercube samples and low-discrepancy Latin hypercube samples have shown good results (Marrel, 2008). However, building good input designs for functional output still remains an open question which could be the subject of future work.

For our tests with the Campbell2D function, we use maximin Latin hypercube samples. Once the input design has been defined, we obtain n simulations of the map $(y(\mathbf{x}^{(i)}, \mathbf{z}))_{i=1..n}$ by running the numerical model.

Step 1 - Spatial decomposition and selection of coefficients

The spatial decomposition of the output map is made on a basis of orthogonal functions $\{\phi_j\}_{j \in \mathbb{N}^*}$:

$$Y(\mathbf{X}, \mathbf{z}) = \mu(\mathbf{z}) + \sum_{j=1}^{\infty} \alpha_j(\mathbf{X}) \phi_j(\mathbf{z}) \text{ with } \alpha_j(\mathbf{X}) = \int_{D_z} [Y(\mathbf{X}, \mathbf{z}) - \mu(\mathbf{z})] \phi_j(\mathbf{z}) d\mathbf{z}, \quad (7)$$

where $\mu(\mathbf{z}) = \mathbb{E}_{\mathbf{X}}[Y(\mathbf{X}, \mathbf{z})]$. We define $Y_K(\mathbf{X}, \mathbf{z})$ as the truncated decomposition at the order K :

$$Y_K(\mathbf{X}, \mathbf{z}) = \mu(\mathbf{z}) + \sum_{j=1}^K \alpha_j(\mathbf{X}) \phi_j(\mathbf{z}). \quad (8)$$

For the function basis, we can test various wavelet bases (Haar, Daubechies, Symmlet and Coiflet, see Misiti et al., 2007) in order to optimize the compression of the local and

global information. In our following tests, we use the Daubechies basis which has offered the best results.

The selection of a small number k of coefficients $\alpha_j(\mathbf{X})$ to be modeled with Gp is essential. For instance, MARTHE maps (see Section 4) and Campbell2D maps contain $n_z = 64 \times 64 = 4096$ pixels which lead to $K = 4096$ wavelet coefficients. Modeling such a number of Gp seems intractable because the building process of one Gp is costly (Marrel et al., 2008). It is therefore necessary to model with Gp only the most informative coefficients. The retained criterion for the coefficients' selection process is their variance with respect to \mathbf{X} : priority is given to those coefficients which explain at most the output map variability. Mathematically, the new order of the coefficients $\{\alpha_1, \dots, \alpha_K\}$ is written $\{\alpha_{(1)}, \dots, \alpha_{(K)}\}$ following the inequalities

$$\frac{1}{n} \sum_{i=1}^n (\alpha_{(1)}(\mathbf{x}^{(i)}) - \overline{\alpha_{(1)}})^2 \geq \dots \geq \frac{1}{n} \sum_{i=1}^n (\alpha_{(K)}(\mathbf{x}^{(i)}) - \overline{\alpha_{(K)}})^2 \quad \text{with} \quad \overline{\alpha_j} = \frac{1}{n} \sum_{i=1}^n \alpha_j(\mathbf{x}^{(i)}) . \quad (9)$$

The number k of Gp-modeled coefficients will be discussed in Step 3.

Step 2 - Modeling the coefficients

For $j = 1, \dots, K$, the model $A_j(\mathbf{X})$ used for the coefficient $\alpha_j(\mathbf{X})$ will be one of the following:

- Model 1: the empirical mean: $A_j(\mathbf{X}) = \frac{1}{n} \sum_{i=1}^n \alpha_j(\mathbf{x}^{(i)})$;
- Model 2: the linear regression model:

$$A_j(\mathbf{X}) = \beta_{0,j} + \sum_{l=1}^d \beta_{l,j} X_l \quad (10)$$

fitted on the learning sample $(\mathbf{x}^{(i)}, \alpha_j(\mathbf{x}^{(i)}))_{i=1..n}$. We use an AIC selection process to keep only significant terms in (10);

- Model 3: the Gp model of the form (3) described in Marrel et al. (2008). The deterministic part $f_0(\mathbf{X})$ is a linear regression model as (10) (with an AICC selection process) and the generalized exponential is used for the correlation function $R(\cdot)$ of the stochastic part $Z(\mathbf{X})$. The building of this model is rather costly, especially in a high dimensional context ($d > 10$) because of the specific variable selection process proposed by Marrel et al. (2008).

In the following two steps, we compare three different methodologies in order to prove the benefit of an appropriate metamodel choice:

- Method 1: Model 3 for the k selected coefficients and model 1 for the other coefficients;
- Method 2: Model 2 for the k selected coefficients and model 1 for the other coefficients;

- Method 3: Model 3 for the k selected coefficients, model 2 for k' following coefficients ($k' \gg k$) and model 1 for the $K - k - k'$ other coefficients. For the Campbell2D function, the number $k' = 500$ is a heuristic choice based on the observation that, with 4096 pixels, the information in terms of variability is concentrated into 10% of coefficients. More generally, a convergence study can be made in order to find a convenient value for k' .

We define at present $\widehat{Y}_{K,k}(\mathbf{X}, \mathbf{z})$ the approximation of $Y_K(\mathbf{X}, \mathbf{z})$ (Eq. (8)) using one of the three previous methods.

Several adequacy criteria can be used to measure the discrepancy between the function $Y(\mathbf{X}, \mathbf{z})$ and its approximation $\widehat{Y}_{K,k}(\mathbf{X}, \mathbf{z})$. We use the mean absolute error, the maximal error and the mean squared error but restrict our presentation to mean squared error results for the sake of consistency. The mean squared error $\text{MSE}(\mathbf{X})$ is written

$$\text{MSE}(\mathbf{X}) = \int_{D_z} \left[Y(\mathbf{X}, \mathbf{z}) - \widehat{Y}_{K,k}(\mathbf{X}, \mathbf{z}) \right]^2 d\mathbf{z}. \quad (11)$$

$\text{MSE}(\mathbf{X})$ is estimated by integrating over the n_z grid. For a fixed value of \mathbf{X} , this criterion measures the restitution quality in the mean of the overall map. We denote by MSE the expectation (with respect to the variable \mathbf{X}) of $\text{MSE}(\mathbf{X})$. When it is possible, we provide new simulations of the map $Y(\mathbf{X}, \mathbf{z})$ for randomized values of \mathbf{X} , and we use this test sample to estimate the MSE. For some applications, this is not possible and cross-validation methods can be used to estimate the MSE (see Section 4).

The MSE can also be obtained by first integrating $\left[Y(\mathbf{X}, \mathbf{z}) - \widehat{Y}_{K,k}(\mathbf{X}, \mathbf{z}) \right]^2$ over \mathbf{X} and then by taking the expectation with respect to \mathbf{z} . From the MSE, we also define the predictivity coefficient Q_2 which gives us the percentage of the mean explained variance of the output map:

$$Q_2 = 1 - \frac{\text{MSE}}{\mathbb{E}_{\mathbf{z}} \{ \text{Var}_{\mathbf{X}} [Y(\mathbf{X}, \mathbf{z})] \}}. \quad (12)$$

The variance is taken with respect to \mathbf{X} because we are interested in the variability induced by the model input vector \mathbf{X} . Q_2 corresponds to the coefficient of determination R^2 computed in prediction (on a test sample or by cross-validation).

Step 3 - Choosing k^* , an optimal value for k

We perform simulations using the Campbell2D function and study convergence of MSE (Eq. (11)) in function of k . Our goal is to compare the three methods proposed in step 2, then to heuristically find an optimal value k^* for k . Indeed, there is a trade-off between keeping k small and minimizing the MSE. The MSE is computed using a test sample of 1000 independent Monte Carlo simulations, giving 1000 output maps.

Figure 4 gives the MSE results in function of k for different values of the learning sample size n . For each method, the MSE curves regularly turn downward as n increases. As expected, method 3, which is the richest in terms of model complexity, gives the best results, especially for small values of k . The usefulness of Gp is proved as we see that method 2 performs badly. It is certainly caused by the behaviour of the first selected coefficients, which offer strong and non linear variations: linear models are irrelevant for modeling these coefficients. For each method, the convergence is reached for k around 20

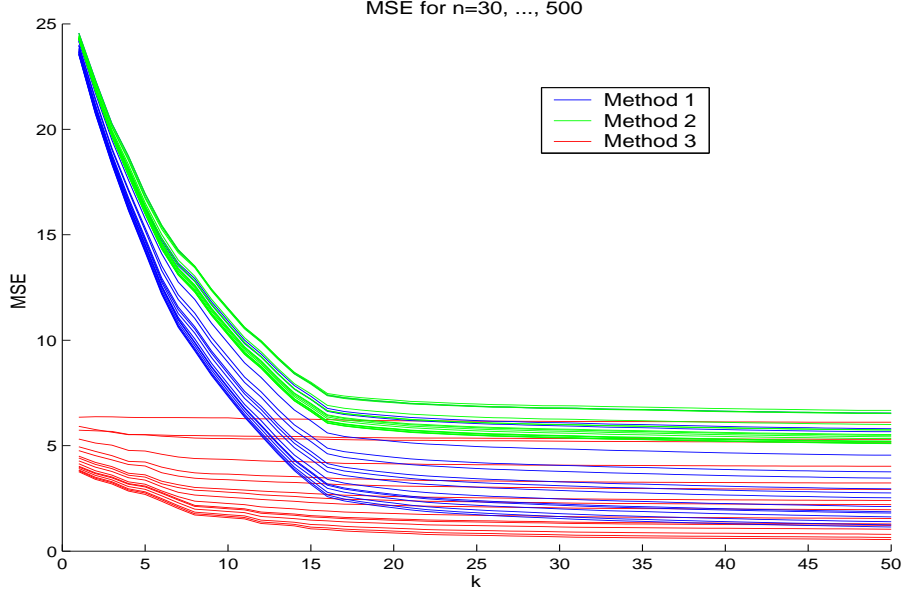


Figure 4: For the Campbell2D function, MSE convergence (in function of k) for the three methods and for various learning sample sizes ($n = 30, 40, 50, 60, 70, 80, 90, 100, 120, 140, 160, 180, 200, 300, 400, 500$).

- 25. We decide to fix the optimal value at $k^* = 30$, which is a reasonable number of Gp models to be built.

In real applications, this methodology for choosing k^* can be applied even if the learning sample size n is limited. For a fixed n , we look for a stabilization of the MSE. If this convergence is not reached, we use a predefined maximal value for k .

Step 4 - Convergence in function of the learning sample size n

Finally, it is important to study the convergence of the adequacy criteria in function of the learning sample size n . It would allow us to eventually prescribe the need to make new simulations with the code. For the Campbell2D function, Figure 5 gives the MSE results in function of n for different values of k . For each method, the MSE curves regularly turn downward as k increases. In real applications, one can restrict this to the visualization of the k^* curves.

Method 2 performs badly and the stabilization of its curves is obtained earlier. Indeed, adding simulations does not improve the linear models fitted on the k coefficients. For methods 1 and 3, the curve stabilization is not reached at $n = 500$. MSE would decrease for larger values of n , but this decrease becomes slower from $n = 200$ and MSE results are rather satisfactory for this value $n = 200$. In terms of predictivity coefficient (Eq. (12)), we obtain $Q_2 = 96.6\%$ for $n = 500$ and $Q_2 = 92.9\%$ for $n = 200$. For methods 1 and 3, increasing k and n leads to a systematic decrease of the MSE. Therefore, one can argue that MSE tends to zero and that our methodology converges.

In real applications, if no additional simulation can be made, this step can be optional. However, in the opposite case, these curves would help us to decide if our simulation number is sufficient and which method we have to choose. Moreover, knowing that method 3 can be costly, we can decide to choose method 1 if their MSEs are similar. In

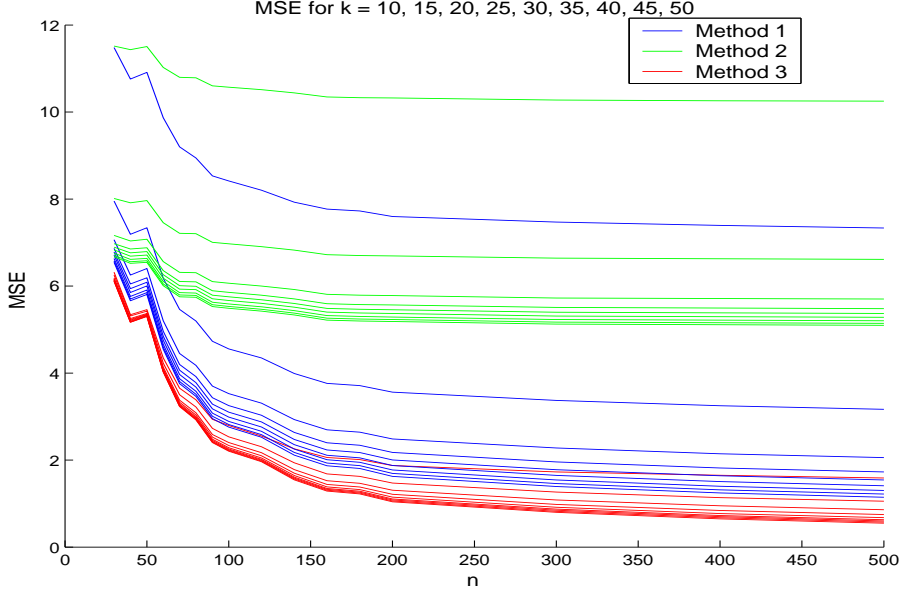


Figure 5: For the Campbell2D function, MSE convergence (in function of n) for the three methods and for various numbers k of Gp-modeled coefficients.

practical terms, we start from an initial n_0 (random selection of n_0 simulations among the n simulations) and randomly add simulations until n .

In conclusion, by analyzing all these convergence plots, we choose in the next section to use a learning sample size $n = 200$ and to model $k^* = 30$ Gps using method 3 in order to compute Sobol indices.

3.4 Global sensitivity analysis

At this stage, we have a functional metamodel allowing us to predict new output concentration maps for any new set of input variables. This metamodel has been obtained with only $n = 200$ computations with the Campbell2D function. To estimate Sobol indices of the overall output map of the Campbell2D function, we will then perform thousands of simulations on our functional metamodel. This method is called in the following the functional metamodel-based approach.

However, problems of memory allocation (due to the size of the output map and our vectorial programming constraints) do not make it possible to use Saltelli's Monte Carlo algorithm (Saltelli, 2002). Therefore, we use the following procedure for each node of the n_z grid:

- For the variance of the conditional expectation of each input variable X_i ($i = 1, \dots, 8$), we perform 1000 Monte Carlo computations to estimate $\mathbb{E}(Y|X_i)$ (integration over 7 dimensions) and 200 Monte Carlo computations to estimate $\text{Var}[\mathbb{E}(Y|X_i)]$ (integration over one dimension).
- For the variance of the conditional expectation of each $X_{\sim i}$ ($i = 1, \dots, 8$), we perform 100 Monte Carlo computations to estimate $\mathbb{E}(Y|X_{\sim i})$ (integration over

Table 1: For the Campbell2D function, relative mean absolute errors (in percent) of the first order sensitivity indices estimated via the functional metamodel-based approach.

X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8
8.75	16.25	16.35	12.8	—	13.17	11.80	9.96

one dimension) and 1000 Monte Carlo computations to estimate $\text{Var}[\mathbb{E}(Y|X_{\sim i})]$ (integration over 7 dimensions).

- The variance of the output $\text{Var}(Y)$ is obtained using 2×10^4 simulations (integration over 8 dimensions).
- Thus, the first order Sobol index estimates (noticed S_i^{Gp}) are obtained from Eq. (1) and the total Sobol index estimates (noticed $S_{T_i}^{\text{Gp}}$) are obtained from Eq. (2).

Finally, we obtain the Sobol indices $S_i^{\text{Gp}}(\mathbf{z})$ and $S_{T_i}^{\text{Gp}}(\mathbf{z})$ for all the n_z grid points.

Figure 6 shows the Sobol index maps for X_2 and X_6 , which are the most influential input variables in the Campbell2D function (see Fig. 3). Results for X_2 are particularly convincing: first order and total sensitivity values obtained with the functional metamodel-based approach are accurate everywhere in the spatial domain D_z . Results for X_6 are rather good for the first order Sobol index and less precise for the total Sobol index. However, the spatial influence zone of X_6 in the upper left corner is well retrieved by the functional metamodel-based approach. In fact, X_2 corresponds to a solely influential input variable while X_6 has important interactions with other input variables (mainly with X_3). Therefore, because of a more difficult Gp fitting process, the Gp models of the wavelet coefficients of X_6 are less precise than the Gp models of the wavelet coefficients of X_2 . However, we argue that the important information is present in the spatial Sobol map of $S_{T_6}^{\text{Gp}}(\mathbf{z})$.

For all the input variables, the relative mean absolute errors of the first order Sobol indices,

$$\text{rMAE}(S_i) = \frac{\mathbb{E}_{\mathbf{z}} |S_i^{\text{Gp}}(\mathbf{z}) - S_i(\mathbf{z})|}{\mathbb{E}_{\mathbf{z}} [S_i(\mathbf{z})]}, \quad (13)$$

have been estimated for $i = 1, \dots, 8$ (see Table 1). The results of Table 1 show that the estimations of the sensitivity maps for X_2 and X_6 correspond to one of the most difficult cases. Figure 6 shows that a mean absolute error of a 15%-order is rather satisfactory in terms of sensitivity maps. Therefore, all the results for the other input variables show that our functional metamodel-based approach gives precise results. Note that the rMAE value for X_5 is not given because $S_5(\theta, \phi) = 0 \quad \forall(\theta, \phi) \in [-90, 90]^2$, so Eq (13) tends to infinity.

In conclusion, we have shown the efficiency of this new spatial global sensitivity analysis method for this analytical and relatively complex test function: all sensitivity index spatial maps have been obtained using only $n = 200$ computations of the Campbell2D function.

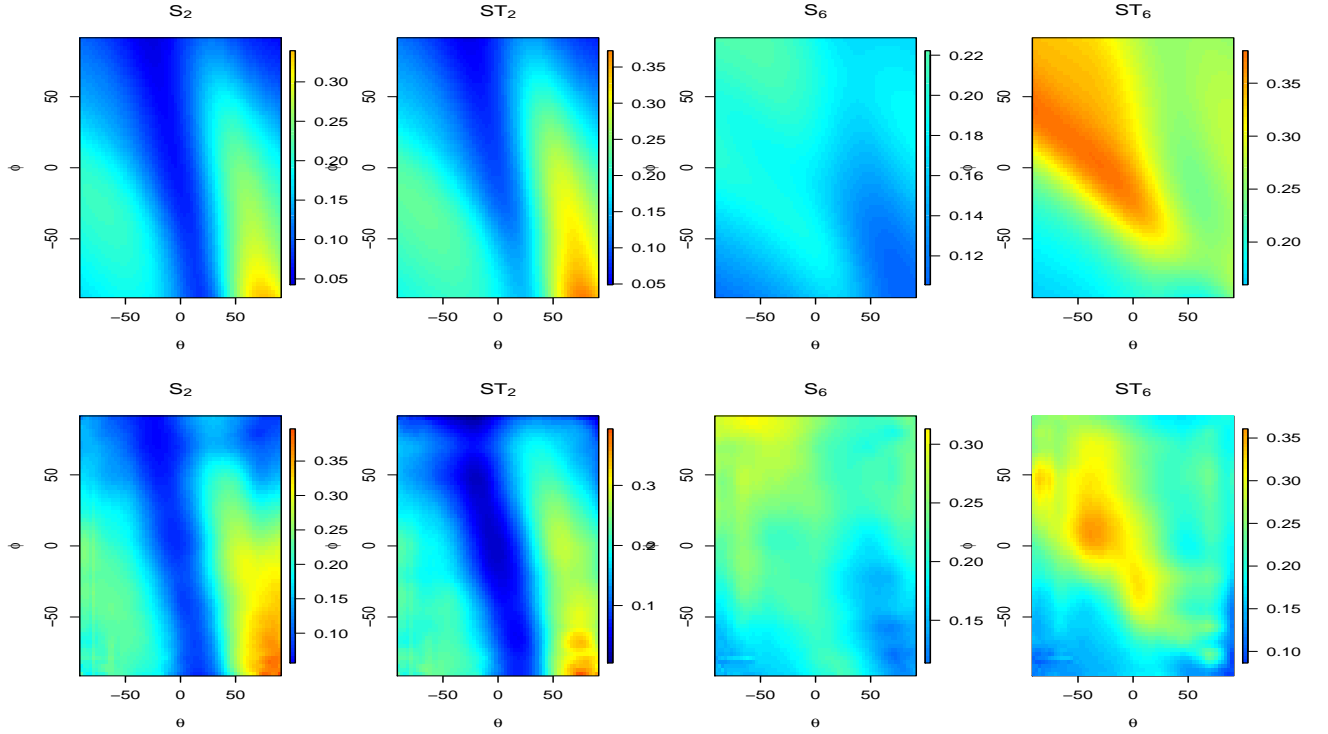


Figure 6: For the Campbell2D function and variables X_2 and X_6 , comparison between exact first order and total Sobol indices (top) and functional metamodel-based Sobol indices (bottom).

4 APPLICATION

The spatial global sensitivity analysis methodology is now applied to the application case MARTHE presented in Section 2. We recall that MARTHE contains $d = 20$ input random variables and that the $n = 300$ simulations have been performed following a Latin hypercube sample in a previous work. In previous studies (Volkova et al., 2008; Marrel et al., 2008), 20 scalar output variables have been considered and we hope to obtain more information by using all the spatial information contained in the maps. We will then use the 300 spatial output maps, discretized in $n_z = 4096$ pixels and predicting the ^{90}Sr concentration values in 2010.

Figure 7 (a) and (b) shows two output maps and exemplifies the potential variability between the maps and their contour irregularity. Another output map (Figure 1, right) confirms this observation. The variance of the 300 maps (Figure 7 (c)) allows us to illuminate the strong-variability zones (central spot), the mild-variability zones (on the left and at the top of the central spot) and the zones with no variability where the concentration values are equal to zero (the major part of the maps). All this corroborates the need for a non-trivial functional metamodel, such as our wavelet-Gp based metamodel described in Section 3.3.

As step 0 is already done, we apply the remaining steps of the spatial global sensitivity

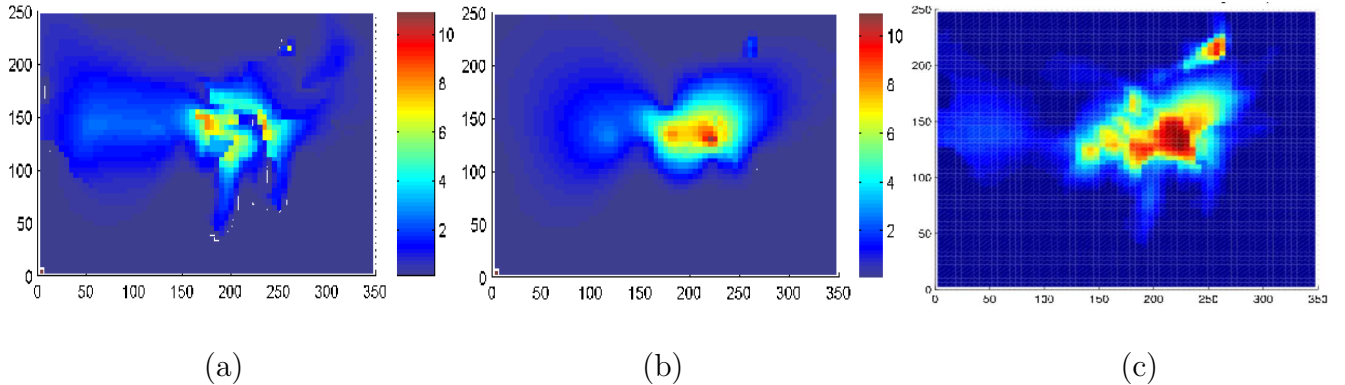


Figure 7: (a) and (b): Two final concentration maps of MARTHE (units in Bq/l). (c): Variance of the 300 concentration maps (colors are in logarithmic scales, ranging from 0 to 10).

analysis methodology (see Section 3) using our learning sample of size $n = 300$. From steps 2 and 3, we retain method 3 with the choice of $k^* = 100$ modeled coefficients with Gp: the stabilization of MSE has been observed for this value of k^* . The number of coefficients modeled with linear models is $k' = 900$. Step 4 is not applied to this application case. Indeed, MARTHE simulations have been performed in a previous study (Volkova et al., 2008) and the computer code is no longer available. Therefore, no additional point could be added and step 4 would be useless.

In the MARTHE application, no test basis is available to compute the MSE in prediction. The MSE estimate is obtained via a 10-fold cross-validation technique. The learning sample is randomly divided into 10 sub-samples. Then, we iterate 10 times the following process: learning the functional metamodel on 9 sub-samples and estimating the MSE on the remaining sub-sample. Our final MSE estimate is the mean of the 10 obtained MSE values: $\text{MSE} = 0.039$. In terms of predictivity coefficient (Eq. (12)), we obtain $Q_2 = 72.1\%$. All the details of this study are given in Marrel (2008).

At present, the functional metamodel can be used to estimate first order and total Sobol indices. We use Saltelli's Monte Carlo algorithm (as for the total Sobol indices in Section 3.2) with two random samples of $N = 10^3$ computations. Indeed, the low computational cost of our metamodel makes possible the realization of thousands of simulations, but not billions because of memory allocation problems (see Section 3.4). The final computation cost of Saltelli's algorithm is $N(d + 2)$, which leads to a number of 22000 metamodel-based simulations in our case. As a final result, we obtain 20 maps of first order Sobol indices and 20 maps of total Sobol indices (two maps for each input).

Figure 8 (a), (b) and (c) shows three maps of total Sobol indices S_{T_i} corresponding to the three main influent variables. The 17 remaining input variables have no influence in any zone of the spatial output domain. These results are completely coherent with previous studies which have detected the predominant influence of these three variables. Some spatial additional information is now brought by our new results. For example, we precisely localize the influence zones of the distribution coefficient of the first hydrogeological layer. Such information is precious for the model engineers. It could help them to determine in function of the spatial localization of large variability zones the kind

of additional information which is needed. Subsequent decisions could be to place new piezometers in specific geographical zones. The methodological developments highlight not only the direct involving in post-treatment processes but also allow purposing an a priori measurement or characterization strategy.

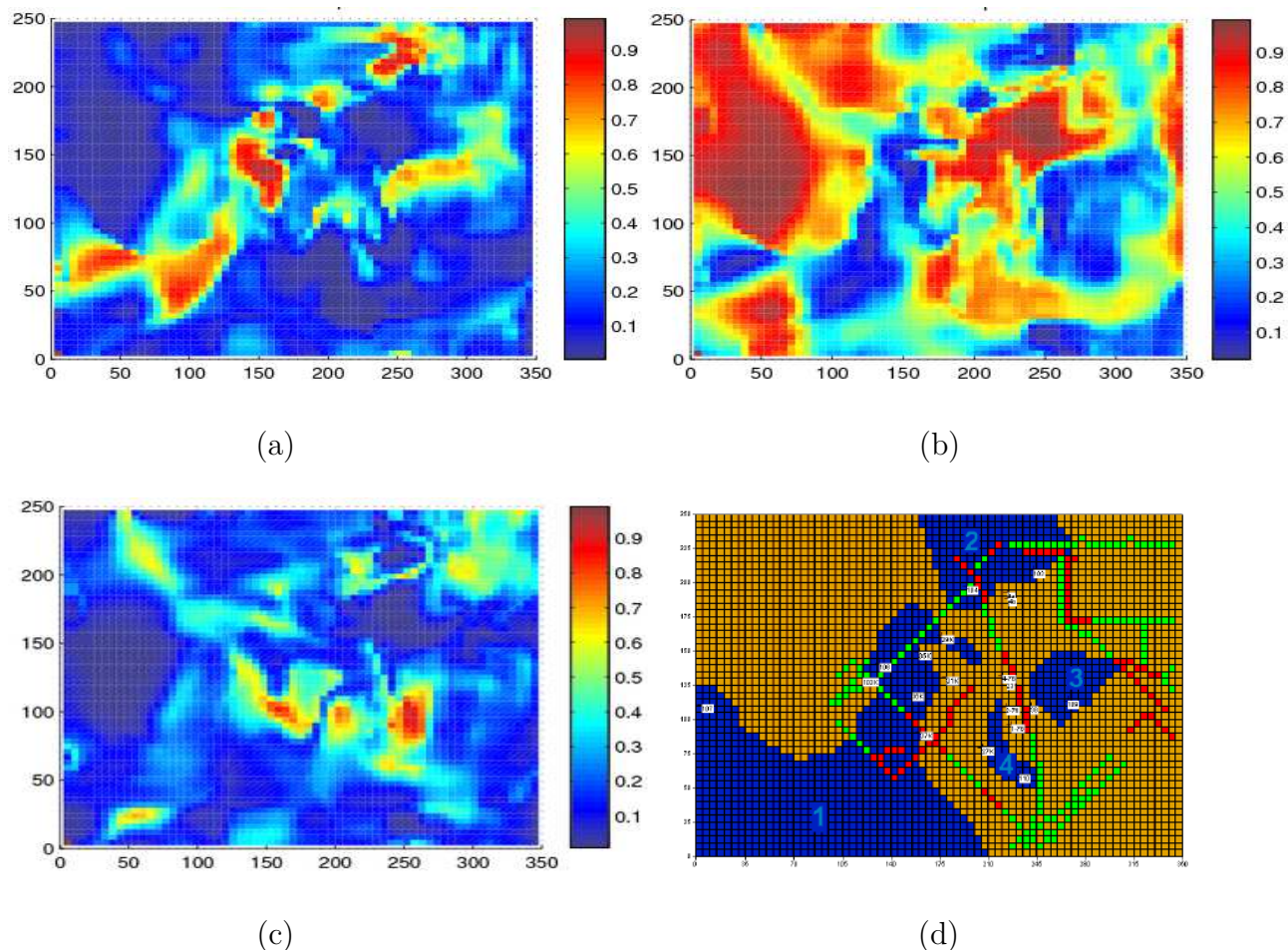


Figure 8: Total Sobol indices of three input variables of MARTHE: (a) $kd1$ (distribution coefficient of the first layer), (b) $kd2$ (distribution coefficient of the second layer) and (c) $i3$ (high infiltration rate). (d): MARTHE hydrogeological model: blue zones (numbered from 1 to 4) correspond to low conductivity zones (absence of coarse sand in the second layer); lines present zones of high infiltration rates.

Figure 8 (d) gives spatial information about the MARTHE model. It clarifies the obvious correlation between the MARTHE hydrogeological scenario and our obtained spatial maps of sensitivity indices: influent $kd1$ zones correspond to the absence of the second hydrogeological layer while influent $kd2$ zones correspond to its presence. In Figure 8 (c), we also retrieve the high infiltration lines of Figure 8 (d) and see their spatial area of influence.

5 CONCLUSION

In this paper, a new methodology has been introduced in order to compute spatial maps of variance-based sensitivity indices (such as the Sobol indices) for numerical models giving a spatial map as output. Such situations are often encountered in environmental modeling problems. The critical issue of our method is due to the small number of available model output maps because of the large cpu time cost of the numerical model. A functional basis decomposition (wavelet basis) linked to a metamodel technique (based on the Gp model) is proposed and used to solve this problem. The wavelet basis choice is well adapted in our application cases (analytical and real models) because of strong spatial heterogeneities and sharp boundaries present in the model output maps. The Gp model choice is adequate because of strong variations between the output maps for different inputs, leading to strong and non linear variations of the Gp-modeled wavelet coefficients. The obtained functional metamodel can serve as a rapid emulator (i.e. with negligible cpu time) of the computer code. It could be used for uncertainty propagation issues, optimization problems and, as advocated in this paper, for sensitivity index estimation.

An analytical test function serves to define the different steps, criteria and modeling choices involved in our methodology. The convergence of our Gp-based functional metamodel is also shown. Then, a real application illustrates the concrete applicability of the methodology. We particularly emphasize the relevance of the additional information (in addition to the expert and model knowledge) brought by the spatial maps of first order and total sensitivity indices. These kinds of sensitivity maps allow us to spatially detect the inputs which have the main influence, to find the geographical zones where some inputs interact with each other and to analyze the spatial zone of influence of each input. The ranking of input variables as function of their direct influence in mapping model allows an expected robust expert opinion. In fine, such efficient methodology supports global decision process, from interpretation and prediction modelling to the deployment of measurement and characterization targeted and pragmatic strategies. The economic and time gains are evident.

Our methodology can be extended to any computer codes with functional output: temporal output, other physical dependencies (such as a function of temperature) and spatio-temporal evolution. In the third case, special attention would be paid to the distinction between the temporal scale and the spatial scales. It would be interesting in a future work to apply our method to the MARTHE spatio-temporal evolutions (between 2002 and 2010) of the concentration values. Moreover, improvements of our model are possible. For example, the vaguelette-wavelet decomposition (Abramovich and Silverman, 1997; Ruiz-Medina et al., 2007) would be an interesting substitute for the wavelet decomposition. It would allow a simultaneous treatment of all the spatial output maps and a direct standardization of all the decomposition coefficients. Finally, in order to disseminate the global sensitivity analysis in environmental modeling communities, dealing with the functional input case remains an important and challenging issue. Iooss and Ribatet (2009) and Lilburne and Tarantola (2009) have proposed some preliminary methodologies to take into account the spatially distributed inputs in the computation of Sobol indices.

6 ACKNOWLEDGMENTS

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APPENDIX A: SOBOL INDICES FOR THE CAMPBELL2D FUNCTION

The analytical derivations of the first order Sobol indices S_i (Eq. (1)) of the Campbell2D function (6) consists, at first, in obtaining analytical expressions of the conditional expectations $\mathbb{E}(Y|X_i)$ (for $i = 1, \dots, 8$). The multiple integrations are made following the uniform distribution on $[-1, 5]$ (we have $\mathbb{E}(X_i) = 2$ and $\text{Var}(X_i) = 3 \forall i = 1, \dots, 8$). The terms of these integrals which do not depend on X_i can be directly put to zero (because these terms will next disappear when the variance over X_i is taken). In the next step, we take the variance over X_i of the expressions of the conditional expectations (which leads to simple integrals). In some cases, analytical simplifications can be done but in other cases, these variances cannot be simplified and the integrals will be evaluated by Monte Carlo.

We recall that $(\theta, \phi) \in [-90, 90]^2$ and we define the following variable changes:

$$\theta_1 = 0.8\theta + 0.2\phi, \theta_2 = 0.5\theta + 0.5\phi, \phi_1 = 0.4\theta + 0.6\phi, \phi_2 = 0.3\theta + 0.7\phi. \quad (14)$$

The Campbell2D function is now written

$$g(\mathbf{X}, \theta, \phi) = X_1 \exp \left[-\frac{(\theta_1 - 10X_2)^2}{60X_1^2} \right] + (X_2 + X_4) \exp \left[\frac{\theta_2 X_1}{500} \right] + X_5(X_3 - 2) \exp \left[-\frac{(\phi_1 - 20X_6)^2}{40X_5^2} \right] + (X_6 + X_8) \exp \left[\frac{\phi_2 X_7}{250} \right], \quad (15)$$

We also define $\Phi(x)$ as the cumulative distribution function of a standardized Gaussian variable. The first order Sobol indices for the 8 input variables is written:

$$S_1(\theta, \phi) = \text{Var} \left\{ \sqrt{\frac{\pi}{60}} X_1^2 \left[\Phi \left(\frac{50 - \theta_1}{\sqrt{30}X_1} \right) - \Phi \left(-\frac{10 + \theta_1}{\sqrt{30}X_1} \right) \right] + 4 \exp \left(\frac{\theta_2 X_1}{500} \right) \right\}, \quad (16)$$

$$S_2(\theta, \phi) = \begin{cases} \text{Var} \left\{ \frac{250X_2}{3\theta_2} \left[\exp \left(\frac{\theta_2}{100} \right) - \exp \left(-\frac{\theta_2}{500} \right) \right] + \int_{-1}^5 \frac{x}{6} \exp \left[-\frac{1}{2} \left(\frac{\theta_1 - 10X_2}{\sqrt{30}x} \right)^2 \right] dx \right\} & \text{if } \theta_2 \neq 0 \\ \text{Var} \left\{ X_2 + \int_{-1}^5 \frac{x}{6} \exp \left[-\frac{1}{2} \left(\frac{\theta_1 - 10X_2}{\sqrt{30}x} \right)^2 \right] dx \right\} & \text{if } \theta_2 = 0, \end{cases} \quad (17)$$

$$S_3(\theta, \phi) = \frac{\pi}{120} \left\{ \int_{-1}^5 \frac{x^2}{6} \left[\Phi \left(\frac{100 - \phi_1}{\sqrt{20}x} \right) - \Phi \left(\frac{-20 - \phi_1}{\sqrt{20}x} \right) \right] dx \right\}^2, \quad (18)$$

$$S_4(\theta, \phi) = \begin{cases} \frac{1}{3} \left\{ \frac{250}{\theta_2} \left[\exp\left(\frac{\theta_2}{100}\right) - \exp\left(-\frac{\theta_2}{500}\right) \right] \right\}^2 & \text{if } \theta_2 \neq 0, \\ 3 & \text{if } \theta_2 = 0, \end{cases} \quad (19)$$

$$S_5(\theta, \phi) = 0, \quad (20)$$

$$S_6(\theta, \phi) = \begin{cases} \frac{1}{3} \left\{ \frac{125}{\phi_2} \left[\exp\left(\frac{\phi_2}{50}\right) - \exp\left(-\frac{\phi_2}{250}\right) \right] \right\}^2 & \text{if } \phi_2 \neq 0, \\ 3 & \text{if } \phi_2 = 0, \end{cases} \quad (21)$$

$$S_7(\theta, \phi) = \begin{cases} \frac{8}{3} \frac{125}{\phi_2} \left[\exp\left(\frac{\phi_2}{25}\right) - \exp\left(-\frac{\phi_2}{125}\right) \right] - \frac{4}{9} \left\{ \frac{250}{\phi_2} \left[\exp\left(\frac{\phi_2}{50}\right) - \exp\left(-\frac{\phi_2}{250}\right) \right] \right\}^2 & \text{if } \phi_2 \neq 0, \\ 0 & \text{if } \phi_2 = 0, \end{cases} \quad (22)$$

$$S_8(\theta, \phi) = S_6(\theta, \phi). \quad (23)$$

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