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A new surrogate modeling technique combining Kriging and polynomial chaos expansions – Application to uncertainty analysis in computational dosimetry

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ABSTRACT

In numerical dosimetry, the recent advances in high performance computing led to a strong reduction of the required computational time to assess the *specific absorption rate* (SAR) characterizing the human exposure to electromagnetic waves. However, this procedure remains time-consuming and a single simulation can request several hours. As a consequence, the influence of uncertain input parameters on the SAR cannot be analyzed using crude Monte Carlo simulation. The solution presented here to perform such an analysis is surrogate modeling. This paper proposes a novel approach to build such a surrogate model from a design of experiments. Considering a sparse representation of the *polynomial chaos expansions* using *least-angle regression* as a selection algorithm to retain the most influential polynomials, this paper proposes to use the selected polynomials as regression functions for the *universal Kriging* model. The *leave-one-out* cross validation is used to select the optimal number of polynomials in the deterministic part of the Kriging model. The proposed approach, called LARS-Kriging-PC modeling, is applied to three benchmark examples and then to a full-scale metamodeling problem involving the exposure of a numerical fetus model to a femtocell device. The performances of the LARS-Kriging-PC are compared to an ordinary Kriging model and to a classical sparse polynomial chaos expansion. The LARS-Kriging-PC appears to have better performances than the two other approaches. A significant accuracy improvement is observed compared to the ordinary Kriging or to the sparse polynomial chaos depending on the studied case. This approach seems to be an optimal solution between the two other classical approaches. A global sensitivity analysis is finally performed on the LARS-Kriging-PC model of the fetus exposure problem.

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1. Introduction

The wireless communications are nowadays intensively used, in spite of these heavy usages the risk perception about possible health impacts of the exposure to electromagnetic fields (EMF) is still important. Monitoring the exposure is therefore a key question for local authorities and health protection agencies, as well as manufacturers and network providers. Protection standards have been designed to ensure the compliance of wireless devices to the existing protection limits. To achieve this objective, worst case scenarios are used, but they are not suitable to assess comprehensively the real exposure induced by wireless devices that are nowadays used in versatile ways.

Over the last 20 years, large efforts have been carried out to improve dosimetry and in particular by developing computational methods. As an example, the numerical method known as Finite-Difference Time-Domain approach (FDTD), that does not requires any matrix inversion, [1] has proven efficient to calculate the Specific Absorption Rate (SAR) that characterizes the absorption of waves by a human body or a part of it (e.g. the brain) [2–4]. Despite the large effort carried out for the reduction of the computation time, the numerical SAR analysis remains a computationally expensive procedure. Moreover, the increasingly versatile use of wireless technologies motivates the analysis of the influence of the input parameters variability (e.g. position and type of sources) on the SAR computation. Consequently uncertainty quantification in dosimetry is a true challenge and uncertainty propagation techniques as well as computer experiments have become important topics, as in several other disciplines of engineering and natural sciences. In this paper the exposure induced by a 3G femtocell device is estimated for a numerical model of a pregnant woman developed in two collaborative projects called FEMONUM and FETUS [5,6]. The challenge here is to study the influence of the uncertainty on the position of the femtocell device position in the room space onto the fetus exposure.

Because computer simulation in dosimetry is time consuming, the uncertainty propagation issue cannot be addressed by a classical approach such as crude Monte Carlo simulation. Thus, more advanced statistical methods have to be resorted to. Surrogate models (a.k.a. metamodels) have emerged in the last decade as powerful statistical methods that allow one to emulate the output of a complex computational model. Of great interest here are the so-called polynomial chaos expansion [7–9] and Kriging (a.k.a. Gaussian process modeling) [10–12].

On the one hand, the polynomial chaos (PC) theory has originally been introduced by Wiener in the case of Gaussian random input variables as the finite-dimensional Wiener polynomial chaos [13]. The output in PC theory is explicitly expressed in a suitable space with a basis constituted of multivariate Hermite polynomials that are orthogonal with respect to the joint probability measure of random input variables. This expansion was later extended to other types of random variables with different basis polynomials [14,15] leading to the so-called *generalized polynomial chaos* expansions (gPCE). A major work has been achieved in the direction of the so-called *intrusive* methods and more particularly the *spectral stochastic finite elements* method [7,16] that uses a combination of the Karhunen–Loeve expansion with the finite element method (FEM) for physical systems modeled by elliptic linear boundary-value problems. As an alternative, *non-intrusive* methods appeared in this domain which rely upon solving a number of deterministic problems with different values of the model input vector. In this non-intrusive scope, two approaches are classically distinguished:

- The *projection* method [17,18] that uses the orthogonality of the polynomial basis to compute the coefficients by Monte-Carlo simulation or quadrature.
- The *regression* method [8,19] that is based on the least-square minimization of the error between the model output and its approximation.

In the regression approach, several kind of truncation schemes of the PC expansion have been studied. A classic full truncation has been studied in [20], that has the drawback to require a dramatically increasing number of model evaluations when the dimensionality (i.e. the number of input parameters in the model) increases. To circumvent this issue, some sparse representations of the truncation have been studied in [8,9] in order to reduce the computational cost. Particularly, in [9], the *least-angle regression* (LARS) [21] algorithm is employed to keep in the truncation only the most influential polynomials. Similar sparse representations have been recently obtained using compressive sampling algorithms [22,23].

On the other hand, the universal Kriging theory has been introduced by Matheron [24] in the field of geostatistics as a tool to interpolate discrete data considered as points of a random field trajectory. Later, this approach has been widely used in computer experiment domain [10–12,25], sequential design of experiments [26–28] and global optimization [29]. Because of the lack of a priori knowledge about the output, the Kriging model is often used in its basic configuration known as ordinary Kriging.

It is important to point out that the research communities developing polynomial chaos expansions and Kriging models are essentially different. To our knowledge, no formal link has been established so far between these procedures. In this respect, this paper proposes to combine the *least-angle regression* (LARS) [21] selection algorithm used in a polynomial chaos basis [9] and universal Kriging to obtain a new family of optimized surrogate models. This approach has similarities with the so-called *blind-Kriging* approach developed in [30] but differs by the selection algorithm and the use of a polynomial chaos basis. The paper is organized as follows: in Section 2, the exposure assessment methodology is introduced, and the numerical anatomical model in which the SAR is computed is presented. In Section 3 we summarize both polynomial chaos expansion and universal Kriging approaches. In Section 4, we introduce our hybrid method which is a combination of the