Global sensitivity analysis of computer models with functional inputs

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Abstract

Global sensitivity analysis is used to quantify the influence of uncertain input parameters on the response variability of a numerical model. The common quantitative methods are applicable to computer codes with scalar input variables. This paper aims to illustrate different variance-based sensitivity analysis techniques, based on the so-called Sobol indices, when some input variables are functional, such as stochastic processes or random spatial fields. In this work, we focus on large cpu time computer codes which need a preliminary meta-modeling step before performing the sensitivity analysis. We propose the use of the joint modeling approach, i.e., modeling simultaneously the mean and the dispersion of the code outputs using two interlinked Generalized Linear Models (GLM) or Generalized Additive Models (GAM). The "mean" model allows to estimate the sensitivity indices of each scalar input variables, while the "dispersion" model allows to derive the total sensitivity index of the functional input variables. The proposed approach is compared to some classical SA methodologies on an analytical function. Lastly, the proposed methodology is applied to a concrete industrial computer code that simulates the nuclear fuel irradiation.

Keywords: functional data, Sobol indices, joint modeling, generalized additive model, metamodel

1 INTRODUCTION

Modern computer codes that simulate physical phenomenas often take as inputs a high number of numerical parameters and physical variables, and return several outputs - scalars or functions. For the development and the use of such computer models, Sensitivity Analysis (SA) is an invaluable tool. The original technique, based on the derivative computations of the model outputs with respect to the model inputs, suffers from strong limitations for most of computer models. More recent global SA techniques take into account all the variation ranges of the inputs and aim to apportion the whole output uncertainty to the input factor uncertainties (Saltelli et al. [19]). The global SA methods can also be used for model calibration, model validation, decision making process, i.e., any process where it is useful to know which variables that mostly contribute to the output variability.

The common quantitative methods are applicable to computer codes with scalar input variables. For example, in the nuclear engineering domain, global SA tools have been applied to numerous models where all the uncertain input parameters are modeled by random variables, possibly correlated - such as thermal-hydraulic system codes (Marquès et al. [12]), waste storage safety studies (Helton et al. [6]), environmental model of dose calculations (Iooss et al. [9]), reactor dosimetry processes (Jacques et al [10]). Recent research papers have tried to consider more complex input variables in the global SA process, especially in petroleum and environmental studies:

- Tarantola et al. [23] work on an environmental assessment on soil models which use spatially distributed maps affected by random errors. For the SA, they propose to replace the spatial input by a "trigger" parameter that governs the random field simulation.
- Ruffo et al. [15] evaluate an oil reservoir production using a model that depends on different heterogeneous geological media scenarios. These scenarios, which are of limited number, are then substituted for a discrete factor (a scenario number) before performing the SA.
- Iooss et al. [8] study a groundwater radionuclide migration model which is based on geostatistical simulations of the hydrogeological layer heterogeneity. The authors propose to consider the spatial input parameter as an "uncontrollable" parameter.

In this paper, we tackle the problem of the global SA for numerical models and when

some input parameters ε are functional. $\varepsilon(\boldsymbol{u})$ is a one or multi-dimensional stochastic function where $\boldsymbol{u}$ can be spatial coordinates, time scale or any other physical parameters. Our work focuses with models that depend on scalar parameter vector $\boldsymbol{X}$ and need some stochastic processes simulations or random fields $\varepsilon(\boldsymbol{u})$ as input parameters. The computer code output value Y depends on the realizations of these random functions. These models are typically non linear with strong interactions between input parameters. Therefore, we concentrate our methodology on the variance based sensitivity indices estimation; that is, the so-called Sobol indices (Sobol [22], Saltelli et al. [19]).

To deal with this situation, a first natural approach consists in the discretization of the input functional parameter $\varepsilon(\boldsymbol{u})$ or its decomposition into an appropriate basis of orthogonal functions. Then, for all the new scalar parameters which represent $\varepsilon(\boldsymbol{u})$, sensitivity indices are computed. However, in the case of complex functional parameters, this approach seems to be rapidly intractable as these parameters cannot be represented by a small number of scalar parameters (Tarantola et al. [23]). Moreover, when dealing with non physical parameters (for example coefficients of orthogonal functions used in the decomposition), sensitivity indices interpretation may be labored. Indeed, most often, physicists would prefer to obtain one global sensitivity index related to $\varepsilon(\boldsymbol{u})$.

The following section presents three different strategies to compute the Sobol indices with functional inputs: (a) the macroparameter method, (b) the trigger parameter method and (c) the proposed joint modeling approach. Section 3 compares the relevance of these three strategies an analytical function: the WN-Ishigami function. Then, the proposed approach is illustrated on an industrial computer code simulating fuel irradiation in a nuclear reactor.

2 COMPUTATION METHODS OF SOBOL INDICES

First, let us recall some basic notions about Sobol indices. Let define the model

$$\begin{aligned} f: \quad \mathbb{R}^p \quad &\to \mathbb{R} \\ \boldsymbol{X} \quad &\mapsto Y = f(\boldsymbol{X}) \end{aligned} \tag{1}$$

where Y is the code output, $\boldsymbol{X} = (X_1, \ldots, X_p)$ are p independent inputs, and f is the model function, which is analytically not known. The main idea of the variance-based SA methods is to evaluate how the variance of an input or a group of input parameters

contributes to the output variance. These contributions are described using the following sensitivity indices:

$$S_i = \frac{\mathrm{Var}\left[\mathbb{E}\left(Y|X_i\right)\right]}{\mathrm{Var}(Y)}, \quad S_{ij} = \frac{\mathrm{Var}\left[\mathbb{E}\left(Y|X_iX_j\right)\right]}{\mathrm{Var}(Y)} - S_i - S_j, \quad S_{ijk} = \dots \tag{2}$$

These coefficients, namely the Sobol indices, can be used for any complex model functions f. The second order index S_{ij} expresses the model sensitivity to the interaction between the variables X_i and X_j (without the first order effects of X_i and X_j), and so on for higher orders effects. The interpretation of these indices is natural as all indices lie in $[0, 1]$ and their sums are equal to one. The larger an index value is, the greater is the importance of the variable or the group of variables related to this index.

For a model with p inputs, the number of Sobol indices is $2^p - 1$; leading to an intractable number of indices as p increases. Thus, to express the overall output sensitivity to an input X_i, Homma & Saltelli [7] introduce the total sensitivity index:

$$S_{T_i} = S_i + \sum_{j \neq i} S_{ij} + \sum_{j \neq i, k \neq i, j<k} S_{ijk} + \ldots = \sum_{l \in \#i} S_l \tag{3}$$

where $\#i$ represents all the "non-ordered" subsets of indices containing index i. Thus, $\sum_{l \in \#i} S_l$ is the sum of all the sensitivity indices having i in their index. The estimation of these indices (Eqs. (2) and (3)) can be performed by Monte-Carlo simulations based on independent samples (Sobol [21], Saltelli [17]), or by refined sampling designs introduced to reduce the number of required model evaluations significantly, for instance FAST (Saltelli et al. [20]) and quasi-random designs (Saltelli et al. [18]).

Let us now consider a supplementary input parameter which is a functional input variable $\varepsilon(\boldsymbol{u}) \in \mathbb{R}$ where $\boldsymbol{u} \in \mathbb{R}^d$ is a d-dimensional location vector. $\varepsilon(\boldsymbol{u})$ is defined by all its marginal and joint probability distributions. In this work, it is supposed that random function realizations can be simulated. For example, these realizations can be produced using geostatistical simulations (Lantuéjoul [11]) or stochastic processes simulations (Gentle [4]). Our model writes now

$$Y = f(\boldsymbol{X}, \varepsilon) \tag{4}$$

and in addition to the Sobol indices related to $\boldsymbol{X}$, our goal is to derive methods to compute the sensitivity indices relative to ε, i.e., S_ϵ (first order index), S_{T_ε} (total sensitivity index), $S_{i\varepsilon}$ (second order indices), $S_{ij\varepsilon}$, ...

2.1 The macroparameter method

To resolve the problem of correlated input parameters in the Sobol indices calculations, Jacques et al. [10] propose the use of multi-dimensional sensitivity indices (Sobol [22]): each group of correlated parameters is considered as a multi-dimensional parameter or macroparameter. The different Sobol indices (first order, second order, ..., total) are then computed using independent Monte-Carlo sampling techniques (Sobol [21], Saltelli [17]). These techniques allow correlations between input parameters; while it is prohibited with other methods - for example FAST.

In our context, this approach seems to be relevant as the input functional parameter $\varepsilon(\boldsymbol{u})$ can be considered as an unique input multi-dimensional parameter (i.e. a macroparameter). For instance, the first order Sobol index related to $\varepsilon(\boldsymbol{u})$ is defined as previously by

$$S_\varepsilon = \frac{\mathrm{Var}\left[\mathbb{E}\left(Y|\varepsilon\right)\right]}{\mathrm{Var}(Y)} \tag{5}$$

A simple way to estimate $S_\varepsilon = D_\varepsilon/D$ is based on the Sobol [21] algorithm:

$$\hat{f}_0 = \frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{X}_k^{(1)}, \varepsilon_k) \tag{6a}$$

$$\hat{D} = \frac{1}{N}\sum_{k=1}^{N} f^2(\boldsymbol{X}_k^{(1)}, \varepsilon_k) - \hat{f}_0^2 \tag{6b}$$

$$\hat{D}_\varepsilon = \frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{X}_k^{(1)}, \varepsilon_k) f(\boldsymbol{X}_k^{(2)}, \varepsilon_k) - \hat{f}_0^2 \tag{6c}$$

where $(\boldsymbol{X}_k^{(1)})_{k=1\ldots N}$ and $(\boldsymbol{X}_k^{(2)})_{k=1\ldots N}$ are two independent sets of N simulations of the input vector $\boldsymbol{X}$ and $(\varepsilon_k)_{k=1\ldots N}$ is a sample of N realizations of the random function $\varepsilon(\boldsymbol{u})$. To compute the sensitivity indices S_i, the same algorithm is used with two independent samples of $(\varepsilon_k)_{k=1\ldots N}$. In the same way, the total sensitivity index S_{T_ε} is derived from the algorithm of Saltelli [17].

The major drawback of this method is that it may be cpu time consuming. A precise estimation of Sobol indices by this naive Monte-Carlo method requires more than thousand model evaluations for one input parameter. In complex industrial applications, it is intractable due to the cpu time cost of one model evaluation and the possible large number of input parameters.

2.2 The "trigger" parameter method

Dealing with spatially distributed input variables, Tarantola et al. [23] propose an alternative that uses an additional scalar input parameter ξ - called "trigger" parameter. $\xi \sim U[0,1]$ governs the random function simulation. For each simulation, if $\xi < 0.5$, the functional parameter $\varepsilon(\boldsymbol{u})$ is fixed to a nominal value $\varepsilon_0(\boldsymbol{u})$ (for example the mean $\mathbb{E}[\varepsilon(\boldsymbol{u})]$), while if $\xi > 0.5$, the functional parameter $\varepsilon(\boldsymbol{u})$ is simulated. Using this methodology, it is possible to estimate how sensitive the model output is to the presence of the random function. Tarantola et al. [23] use the Extended FAST method to compute the first order and total sensitivity indices of 6 scalar input factors and 2 additional "trigger" parameters. For their study, the sensitivity indices according to the "trigger" parameters are small and the authors conclude that it is unnecessary to model these spatial errors more accurately.

Contrary to the previous method, there is no restriction about the sensitivity indices estimation procedure - i.e. Monte-Carlo, FAST, quasi Monte-Carlo. However, there are two major drawbacks for this approach:

- As the macroparameter method, it also requires the use of the computer model to perform the SA and it may be problematic for large cpu time computer models. This problem can be compensate by the use of an efficient quasi Monte-Carlo algorithm.
- As underlined by Tarantola et al. [23], ξ reflects only the presence or the absence of the stochastic errors on $\varepsilon_0(\boldsymbol{u})$. Therefore, the term $\mathrm{Var}[\mathbb{E}(Y|\xi)]$ does not quantify the contribution of the random function variability to the output variability $\mathrm{Var}(Y)$. We will discuss about the significance of $\mathrm{Var}[\mathbb{E}(Y|\xi)]$ later, during our analytical function application.

2.3 The joint modeling approach

To perform a variance-based SA for time consuming computer models, some authors propose to approximate the computer code by a mathematical function (Marseguerra et al. [13], Volkova et al. [24]), often called response surface or metamodel (Fang et al. [2]). For metamodels with sufficient prediction capabilities, the bias due to the use of the metamodel instead of the true model is negligible. Several choices of metamodel can be found in the literature: polynomials, splines, Gaussian processes, neural networks, ... Thus, for the functional input problem, one strategy may be to fit a metamodel with

a multi-dimensional scalar parameters representing $\varepsilon(\boldsymbol{u})$ as an input parameter - i.e. its discretization or its decomposition into an appropriate basis. However, this approach seems to be impracticable due to the potential large number of scalar parameters.

A second option is to substitute each random function realization for a discrete number, which can correspond to the scenario parameter of Ruffo et al. [15] (where the number of geostatistical realizations is finite and fixed, and where each different value of the discrete parameter corresponds to a different realization). However, in the general context, this restriction of the possible realizations of the input random function to a few ones is not acceptable.

The last solution considers $\varepsilon(\boldsymbol{u})$ as an uncontrollable parameter and a metamodel is fitted in function of the other scalar parameters $\boldsymbol{X}$:

$$Y_m = \mathbb{E}(Y|\boldsymbol{X}) \tag{7}$$

Therefore, using the relation

$$\mathrm{Var}(Y) = \mathrm{Var}[\mathbb{E}(Y|\boldsymbol{X})] + \mathbb{E}[\mathrm{Var}(Y|\boldsymbol{X})] \tag{8}$$

it can be easily shown that the sensitivity indices of Y according to the scalar parameters $\mathbf{X} = (X_i)_{i=1\ldots p}$ write (Iooss et al. [8])

$$S_i = \frac{\mathrm{Var}[\mathbb{E}(Y_m|X_i)]}{\mathrm{Var}(Y)}, \quad S_{ij} = \frac{\mathrm{Var}[\mathbb{E}(Y_m|X_iX_j)]}{\mathrm{Var}(Y)} - S_i - S_j, \quad \ldots \tag{9}$$

and can be computed by classical Monte-Carlo techniques applied on the metamodel Y_m. Therefore, using equation (8), the total sensitivity index of Y according to $\varepsilon(\boldsymbol{u})$ corresponds to the expectation of the unexplained part of $\mathrm{Var}(Y)$ by the metamodel Y_m:

$$S_{T_\varepsilon} = \frac{\mathbb{E}[\mathrm{Var}(Y|\boldsymbol{X})]}{\mathrm{Var}(Y)} \tag{10}$$

Using this approach, our objective is altered because we cannot decompose the ε effects into elementary effect (S_ε) and interaction effects between ε and the scalar parameters $(X_i)_{i=1\ldots p}$. However, we see below that our technique allows a qualitative appraisal of the interaction indices.

The sensitivity index estimations from equations (9) and (10) raise two difficulties:

1. It is well known that classical parametric metamodels (based on least squares fitting) are not adapted to estimate $\mathbb{E}(Y|\boldsymbol{X})$ accurately due to the presence of heteroscedasticity (induced by the effect of ε). Such cases are analyzed by Iooss et al. [8]. The authors show that heteroscedasticity may lead to sensitivity indices misspecifications.

2. Classical non parametric methods, such as Generalized Additive Model (Hastie and Tibshirani [5]) and Gaussian process (Sacks et al. [16]) which can provide efficient estimation of $\mathbb{E}(Y|\boldsymbol{X})$ (examples are given in Iooss et al. [8]), even in high dimensional input cases ($p > 5$), are based on homoscedasticity hypothesis and do not propose the estimation of $\mathrm{Var}(Y|\boldsymbol{X})$.

To resolve the second problem, Zabalza-Mezghani et al. [26] propose the use of a theory developed for experimental data: the simultaneous fitting of the mean and the dispersion by two interlinked generalized linear models (McCullagh and Nelder [14]), which is called the joint modeling. Besides, to resolve the first problem, this approach has been extended by Iooss et al. [8] to non parametric models. This generalization allows more complexity and flexibility while fitting the data. The authors propose the use of Generalized Additive Models (GAMs) based on penalized smoothing splines (Wood [25]). GAMs allow model and variable selections using quasi-likelihood function, statistical tests on coefficients and graphical display. However, compared to other complex metamodels, GAMs impose an additive effects hypothesis. Therefore, two metamodels are obtained: one for the mean component $Y_m = \mathbb{E}(Y|\boldsymbol{X})$; and the other one for the dispersion component $Y_d = \mathrm{Var}(Y|\boldsymbol{X})$. The sensitivity indices of $\boldsymbol{X}$ are computed using Y_m with the standard procedure (Eq. (9)), while the total sensitivity index of $\varepsilon(\boldsymbol{u})$ is computed from $\mathbb{E}(Y_d)$ (Eq. (10)). Using the explicit formula on Y_d and the associated regression diagnostics, qualitative sensitivity indices for the interactions between $\varepsilon(\boldsymbol{u})$ and the scalar parameters of $\boldsymbol{X}$ can also be deduced.

3 APPLICATION TO AN ANALYTICAL EXAMPLE

The three previously proposed methods are first illustrated on an artificial analytical model with two scalar input variables and one functional input:

$$Y = f(X_1, X_2, \varepsilon(t)) = \sin(X_1) + 7\sin(X_2)^2 + 0.1[\max_t(\varepsilon(t))]^4 \sin(X_1) \qquad (11)$$

where $X_i \sim \mathcal{U}[-\pi;\pi]$ for $i = 1, 2$ and $\varepsilon(t)$ is a white noise, i.e. an i.i.d. stochastic process $\varepsilon(t) \sim \mathcal{N}(0, 1)$. In our model simulations, $\varepsilon(t)$ is discretized in one hundred values: $t = 1 \dots 100$. The function (11) is similar to the well-known Ishigami function (Homma and Saltelli [7]) but substitute the third parameter for the maximum of a stochastic process. Consequently, we call our function the white-noise Ishigami function (WN-Ishigami). Although the WN-Ishigami function is an artificial model, the introduction of the maximum of a stochastic process inside a model is quite realistic. For example, some computer models simulating physical phenomena can use the maximum of time-dependent variable - river height, rainfall quantity, temperature. Such input variable can be modeled by a temporal stochastic process.

As for the Ishigami function, we can immediately deduce from the formula (11) the sensitivity indices which are worse zero:

$$S_\varepsilon = S_{12} = S_{2\varepsilon} = S_{12\varepsilon} = 0 \tag{12}$$

Then, we have

$$S_{T_1} = S_1 + S_{1\varepsilon}, \quad S_{T_2} = S_2, \quad S_{T_\varepsilon} = S_{1\varepsilon} \tag{13}$$

In the following, we focus our attention on the estimation of S_1, S_2 and S_{T_ε}.

Because of a particularly complex probability distribution of the maximum of a white noise, there is no analytical solution for the theoretical Sobol indices S_1, S_2 and $S_{1\varepsilon}$ for the WN-Ishigami function. Even with the asymptotic hypothesis (number of time steps tending to infinity), where the maximum of the white noise follows Generalized Extreme Value distribution, theoretical indices are unreachable. Therefore, our benchmark Sobol indices values are derived from the Monte-Carlo method. However, these benchmark values can be considered as relevant because of the negligible computation time required to evaluate equation (11).

3.1 The macroparameter and "trigger" parameter methods

Table 1 contains the Sobol indices estimates using the macroparameter and "trigger" parameter methods. As explained before, we can only use the two algorithms based on independent Monte-Carlo samples: the algorithm of Sobol [21] which computes S_1, S_2, $S_{1\varepsilon}$, and the algorithm of Saltelli [17] which computes the first order indices S_1, S_2 and

the total sensitivity indices S_{T_1}, S_{T_2}, S_{T_ε}. For the estimation, the size of the Monte-Carlo samples are limited to $N = 10000$ because of memory computer limit. Indeed, the functional input $\varepsilon(\boldsymbol{u})$ contains for each simulation set 100 values. Then, the input sample matrix has the dimension $N \times 102$ which becomes extremely large when N increases. To evaluate the effect of this limited Monte-Carlo sample size N, each Sobol index estimate is associated to a standard-deviation estimated by bootstrap - with 100 replicates of the input-output sample. The obtained standard-deviations are relatively small, of the order of 0.01, which is rather sufficient for our exercise.

[Table 1 about here.]

For the macroparameter method, the theoretical relations between indices given in (13) are verified. We are therefore confident with the estimates obtained with this method (which is in addition theoretically well-founded) and we choose the Sobol indices obtained with Saltelli's algorithm as the indices references:

$$S_1 = 55.1\%, \quad S_2 = 20.7\%, \quad S_{T_\varepsilon} = 24.8\%$$

The S_ε, S_{12}, $S_{\varepsilon 2}$ and $S_{12\varepsilon}$ indices (Eq. (12)) are not reported in table 1 as estimates are negligible.

With the "trigger" parameter method, the obtained values in table 1 are not close to the reference values. The inadequacies are larger than 30% for all the indices, and can be larger than 60% for a few ones. Moreover, the relations given in (13) are not satisfied at all. Actually, replacing the input parameter $\varepsilon(\boldsymbol{u})$ by ξ which governs the presence or absence of the functional input parameter changes the model. When ε is not simulated, it is replaced by its mean (zero) and the WN-Ishigami function becomes $Y = \sin(X_1) + 7\sin(X_2)^2$. Therefore, the mix of the WN-Ishigami model and this new model perturbs the estimation of the sensitivity indices, even those unrelated to ε (like X_2).

This example confirms our intuition: the sensitivity indices derived from the "trigger" parameter method have not the same sense that the classical ones, i.e., the measure of the contribution of the input parameter variability to the output variable variability. The sensitivity indices obtained with these two methods are unconnected because the "trigger" parameter method changes the structure of the model.

3.2 The joint modeling approach

We apply now the joint modeling approach which requires an initial input-output sample to fit the joint metamodel - the mean component Y_m and the dispersion component Y_d. For our application, a learning sample size of $n = 500$ was considered; i.e., n independent random samples of $(X_1, X_2, \varepsilon(\boldsymbol{u}))$ were simulated leading to n observations for Y. Let first remark that this method is extremely less cpu time consuming than the previous ones which needed a 10000-size sample.

Joint GLM and joint GAM fitting procedures are fully described in Iooss et al. [8]. Some graphical residual analyses are particularly well suited to check the relevance of the mean and dispersion components of the joint models. In the following, we give the results of the joint models fitting on a learning sample $(X_1, X_2, \varepsilon(\boldsymbol{u}), Y)$. Let us recall that we fit a model to predict Y in function of (X_1, X_2).

Joint GLM fitting

For the joint GLM, fourth order polynomial for the parametric form of the model is considered. Moreover, only the explanatory terms are retained in our regression model using analysis of deviance and the Fisher statistics. The Student test on the regression coefficients and residuals graphical analysis make it possible to appreciate the model goodness-of-fit. The mean component gives:

```
Deviance Residuals:
     Min        1Q    Median        3Q       Max
-5.79193  -0.59880   0.03988   0.64202   3.51148

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  1.92634    0.22128   8.706   <2e-16 ***
X1           4.74256    0.16198  29.278   <2e-16 ***
I(X2^2)      2.22879    0.14130  15.773   <2e-16 ***
I(X1^3)     -0.51398    0.02453 -20.951   <2e-16 ***
I(X2^4)     -0.28501    0.01588 -17.952   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for quasi family taken to be 1.010101)

    Null deviance: 1901.0  on 499  degrees of freedom
Residual deviance:  500.0  on 495  degrees of freedom
AIC: NA

Number of Fisher Scoring iterations: 2
```

The explained deviance of this model is $D_{expl} = 74\%$. It can be seen that it remains 26% of non explained deviance due to the model inadequacy and/or to the functional input

parameter. The predictivity coefficient, i.e. coefficient of determination R^2 computed on a test sample, is $Q_2 = 71\%$. Q_2 is relatively coherent with the explained deviance.

For the dispersion component, using analysis of deviance techniques, none significant explanatory variable were found: the heteroscedastic character of the data has not been retrieved. Thus, the dispersion component is supposed to be constant; and the joint GLM model is equivalent to a simple GLM - but with a different fitting process.

Joint GAM fitting

At present, we try to model the data by joint GAM. The resulting model is described by the following features ($s(.)$ denotes a penalized spline smoothing term):

```
Mean component:

Family: quasi
Link function: identity
Formula:
y ~ X1 + s(X1) + s(X2)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  4.19914    0.08727   48.12   <2e-16 ***
X1          -5.39131    0.34285  -15.72   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
        edf Est.rank     F p-value
s(X1) 5.503        8 144.1  <2e-16 ***
s(X2) 8.738        9 316.5  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.979   Deviance explained = 90.5%
GCV score = 1.0683   Scale est. = 1.0336    n = 500

Dispersion component:

Family: Gamma
Link function: log
Formula:
d ~ s(X1)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.98812    0.07965   12.41   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
        edf Est.rank     F p-value
s(X1) 8.814        9 28.39  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.0481   Deviance explained = 26.3%
GCV score = 3.2355   Scale est. = 3.172     n = 500
```

The explained deviance of the mean component is $D_{expl} = 90\%$ and the predictivity coefficient is $Q_2 = 77\%$. Therefore, the joint GAM approach outperforms the joint GLM one. Indeed, the proportion of explained deviance is clearly greater for the GAM model. Even if this is obviously related to an increasing number of parameters; this is also explained as GAMs are more adjustable than GLMs. This is confirmed by the increase of the predictivity coefficient - from 71% to 77%. Moreover, due to the GAMs flexibility, the explanatory variable X_1 is identified for the dispersion component. The interaction between X_1 and the functional input parameter $\varepsilon(\boldsymbol{u})$ which governs the heteroscedasticity of this model is therefore retrieved.

Sobol indices

From the joint GLM and the joint GAM, Sobol sensitivity indices can be computed using equations (9) and (10) - see Table 2. The reference values are extracted from the macroparameter method and Saltelli's algorithm in table 1. The standard deviation estimates (sd) are obtained from 100 repetitions of the Monte-Carlo estimation procedure - which uses $N = 10000$ model computations for one index estimation. The joint GLM and joint GAM gives good estimations of S_1 and S_2. Despite the joint GLM leads to an accurate estimation for S_{T_ε}, we will see later that it is a lucky break. A problem occurs with the estimation of S_{T_ε} with joint GAM. In fact, an efficient modeling of $\mathrm{Var}(Y|\boldsymbol{X})$ is difficult, which is a common statistical difficulty in heteroscedastic regression problems (Antoniadis & Lavergne [1]). Another way to estimate the total sensitivity index S_{T_ε} is to compute the unexplained variance of the mean component model given directly by $1 - Q_2$, with Q_2 the predictivity coefficient of the mean component model. In practical applications, Q_2 can be estimated via leave-one-out or cross validation procedures. In our analytical case, the index estimated with this method and the joint GAM gives a correct estimation - 0.23 instead of 0.25.

[Table 2 about here.]

For the other sensitivity indices, the conclusions draw from the GLM formula are completely erroneous: as the dispersion component is constant, the interaction indices are null. Thus, $S_\varepsilon = S_{T_\varepsilon} = 0.25$ while $S_\varepsilon = 0$ in reality. In contrary, the deductions draw from GAM formulas are correct: (X_1, ε) interaction sensitivity is positive, $S_{2\varepsilon} = S_{12\varepsilon} = 0$, $S_{T_2} = S_2$, $S_{12} = S_{23} = S_{123} = 0$. The drawback of this method is that some indices (S_{T_1}

and S_ε) remain unknown due to the non separability of the dispersion component effects.

By estimating Sobol indices with those obtained from other learning samples, we observe that the estimates are rather dispersed: it seems that the estimates are not robust according to different learning samples for the joint models. To examine this effect, we propose to study two different sample sizes: $n = 200$ and $n = 500$. For each sample size, we repeat 25 times, the fitting process on different learning samples, and we compute Sobol indices as previously. In fact, for each sample size, we obtain 25 estimates of each sensitivity index. The variability of the indices is due at present to the learning sample variability. Figures 1 and 2 show the results of this investigation, which are particularly convincing. The boxplots are based on the 25 different estimates. From these figures, several conclusion can be drawn:

- For the joint GAM, the boxplot interquartile interval of each index contains its reference value. In contrary, the joint GLM fails to obtain correct estimates: except for S_1, the sensitivity reference values are outside the interquartile intervals of the obtained boxplots.
- The superiority of the joint GAM with respect to the joint GLM is corroborated, especially for S_2 and S_{T_ε}.
- The increase of the learning sample size has no effect on the joint GLM results (due to the parametric form of this model). However, for the joint GAM, boxplots widths are strongly reduced from $n = 200$ to $n = 500$. In addition, the mean estimates seem to converge to the reference values.
- As explained before, the estimation of S_{T_ε} using the predictivity coefficient Q_2 is markedly better than through the dispersion component model. This is not the case for the joint GLM.

[Figure 1 about here.]

[Figure 2 about here.]

In conclusion, this example shows that the joint models, and specially the joint GAM, can adjust complex heteroscedastic situations. Moreover, the joint models offer a theoretical basis to compute efficiently global sensitivity indices for models with functional input parameter.

4 APPLICATION TO A NUCLEAR FUEL IRRADIATION SIMULATION

The METEOR computer code, developed within the Fuel Studies Department in CEA Cadarache, studies the thermo-mechanical behavior of the fuel rods under irradiation in a nuclear reactor core. In particular, it computes the fission gas swelling and the cladding creep (Garcia et al. [3]). These two output variables are considered in our analysis. These variables are of fundamental importance for the physical comprehension of the fuel behavior and for the monitoring of the nuclear reactor core.

Input parameters of such mechanical models can be evaluated either by database analyses, arguments invoking simplifying hypotheses, expert judgment. All these considerations lead to assign to each input parameter a nominal value associated with an uncertainty. In this study, six uncertain input parameters are considered: the initial internal pressure X_1, the pellet and cladding radius X_2, X_3, the microstructural fuel grain diameter X_4, the fuel porosity X_5 and the time-dependent irradiation power $P(t)$. $X_1, \ldots, X_5$ are all modeled by Gaussian independent random variables with the following coefficient of variations: $\mathrm{cv}(X_1) = 0.019$, $\mathrm{cv}(X_2) = 1.22 \times 10^{-3}$, $\mathrm{cv}(X_3) = 1.05 \times 10^{-3}$, $\mathrm{cv}(X_4) = 0.044$, $\mathrm{cv}(X_5) = 0.25$. The last variable $P(t)$ is a temporal function (discretized in 3558 values) and its uncertainty $\varepsilon(t)$ is modelled like a stochastic process. For simplicity, a temporal white noise (of uniform law ranging between -5% and $+5\%$) was introduced.

As in the previous application, additionally to its scalar random variables, the model includes an input functional variable $P(t)$. To compute Sobol indices of this model, we have first tried to use the macroparameter method. We have succedeed to perform the calculations with $N = 1000$ (for the Monte-Carlo sample sizes of Eqs. (6a), (6b) and (6c)). The sensitivity indices estimates have been obtained after 10 computation days and were extremely imprecise, with strong variations between 0 and 1. Because of the required cpu time, an increase of the sample size N to obtain acceptable sensitivity estimates was unconceivable. Therefore, the goal of this section is to show how the use of the joint modeling approach allows to estimate the sensitivity indices of the METEOR model and, in particular, to quantify the functional input variable influence.

500 METEOR calculations were carried out using 500 Monte-Carlo sampling of the input parameters. As expected, the white noise on $P(t)$ generates an increase in the standard deviation of the output variables (compared to simulations without a white

noise): 6% increase for the variable *fission gas swelling* and 60% for the variable *cladding creep*.

4.1 Gas swelling

We start by studying the gas swelling model output. With a joint GLM, the following result for Y_m and Y_d were obtained:

$$\begin{cases} Y_m & = -76 - 0.4X_1 + 20X_2 + 8X_4 + 134X_5 + 0.02X_4^2 - 2X_2X_4 - 6X_4X_5 \\ \log(Y_d) & = -2.4X_1 \end{cases} \tag{14}$$

The explained deviance of the mean component is $D_{expl} = 86\%$. As the residual analyses of mean and dispersion components do not show any biases, the resulting model seems satisfactory. The joint GAM was also fitted on these data and led to similar results. Thus, it seems that spline terms are useless and that a joint GLM model is suited.

Table 3 shows the results for the Sobol indices estimation using Monte-Carlo methods applied on the metamodel (14). The standard deviation (*sd*) estimates are obtained from 100 repetitions of the Monte-Carlo estimation procedure -which uses 10^5 model computations for one index estimation. It is useless to perform the Monte-Carlo estimation for some indices because they can be deduced from the joint model equations. For example, $S_3 = 0$ (resp. $S_{\varepsilon 2} = 0$) because X_3 (res. X_2) is not involved in the mean (resp. dispersion) component in equation (14). Moreover, we know that $S_{\varepsilon 1} > 0$ because X_1 is an explanatory variable inside the dispersion component Y_d. However, this formulation does not allow to have any idea about S_ϵ which reflects the first order effect of ε. Therefore, some indices are not accessible, such as S_ε and $S_{\varepsilon 1}$ non distinguishable inside the total sensitivity index S_{T_ε}. Finally, we can check that $\sum_{i=1}^{5} S_i + \sum_{i,j=1,i<j}^{5} S_{ij} + S_{T_\varepsilon} = 1$ holds - up to numerical approximations.

It can be seen that X_4 (grain diameter) and X_5 (fuel porosity) are the most influent factors (each one having 40% of influence), and do not interact with the irradiation power $P(t)$ (representing by its uncertainty ε). In addition, the effect of $P(t)$ is not negligible (14%) and parameter X_1 (internal pressure) acts only with its interaction with $P(t)$. A sensitivity analysis by fixing X_1 could allow us to obtain some information about the first order effect of ε in the model.

4.2 Cladding creep

We study now the cladding creep model output. With a joint GLM, the model for Y_m and Y_d is:

$$\begin{cases} Y_m & = -2.75 + 1.05X_2 - 0.15X_3 - 0.58X_5 \\ \log(Y_d) & = 156052 - 76184X_2 + 9298X_2^2 \end{cases} \tag{15}$$

The explained deviance of the mean component is $D_{expl} = 26\%$. As the residual analyses of mean and dispersion components show some biases, the resulting model is not satisfactory.

For the joint GAM, the spline terms $\{s(X_2), s(X_3), s(X_5)\}$ and $s(X_2)$ are added within the mean component and the dispersion component respectively. The explained deviance of the mean component is $D_{expl} = 29\%$ which is not significantly greater than 26%. However, as the mean component residual biases of the joint GAM are smaller than those observed for the joint GLM, the joint GAM seems to be more relevant than the joint GLM.

Table 3 shows the Sobol indices estimates using Monte-Carlo methods and deductions from the joint model equations. For the joint GLM and joint GAM of the cladding creep, $\sum_{i=1}^{5} S_i + \sum_{i,j=1,i<j}^{5} S_{ij} + S_{T_\varepsilon} = 1$ holds – up to numerical imprecisions. Due to the proximity of the two joint models, results are similar. This analysis shows that the parameter X_2 (pellet radius) explains 28% of the uncertainty of the cladding creep phenomenon, while the other scalar parameters have negligible influence. The greater part of the cladding creep variance (70%) is explained by the irradiation power uncertainty. Physicists may be interested in quantifying the interaction influence between the pellet radius and the irradiation power. Unfortunately, this interaction is not available for the moment in our analysis.

[Table 3 about here.]

5 CONCLUSION

This paper has proposed a solution to perform global sensitivity analysis for time consuming computer models which depend on functional input parameters, such as a stochastic process or a random field. Our purpose concerned the computation of variance-based importance measures of the model output according the the uncertain input parameters. We have discussed a first natural solution which consists in integrating the functional input

parameter inside a macroparameter, and using standard Monte-Carlo algorithms to compute sensitivity indices. This solution is not applicable for time consuming computer code. We have discussed another solution, used in previous studies, based on the replacement of the functional input parameter by a "trigger" parameter that governs the integration or not of the functional input uncertainties. However, the estimated sensitivity indices are strongly biased due to changes in the model structure carrying out by the method itself. Finally, we have proposed an innovative solution, the joint modeling method, based on a preliminary step of double (and joint) metamodel fitting, which resolves the large cpu time problem of Monte-Carlo methods. It consists in rejecting the functional input parameters in noisy input variables. Then, two metamodels depending only on the scalar random input variables are simultaneously fitted: one for the mean function and one for the dispersion (variance) function.

Tests on an analytical function have shown the relevance of the joint modeling method, which provides all the sensitivity indices of the scalar input parameters and the total sensitivity index of the functional input parameter. In addition, it reveals in a qualitative way the influential interactions between the functional parameter and the scalar input parameters. A research way for the future would be to distinguish the contributions of several functional input parameters, who are at the moment totally mixed in one sensitivity index. This is the main drawback of the proposed method.

In an industrial application, the feasibility and usefulness of our methodology was established. Indeed, other methods are not applicable in this application because of large cpu time of the computer code. To a better understanding of the model behavior, the information brought by the global sensitivity analysis can be very useful to the physicist or the modeling engineer. The joint model can also serve in propagation uncertainty and reliability studies of complex models, containing input random functions, to obtain some mean predictions with their confidence intervals.

6 ACKNOWLEDGMENTS

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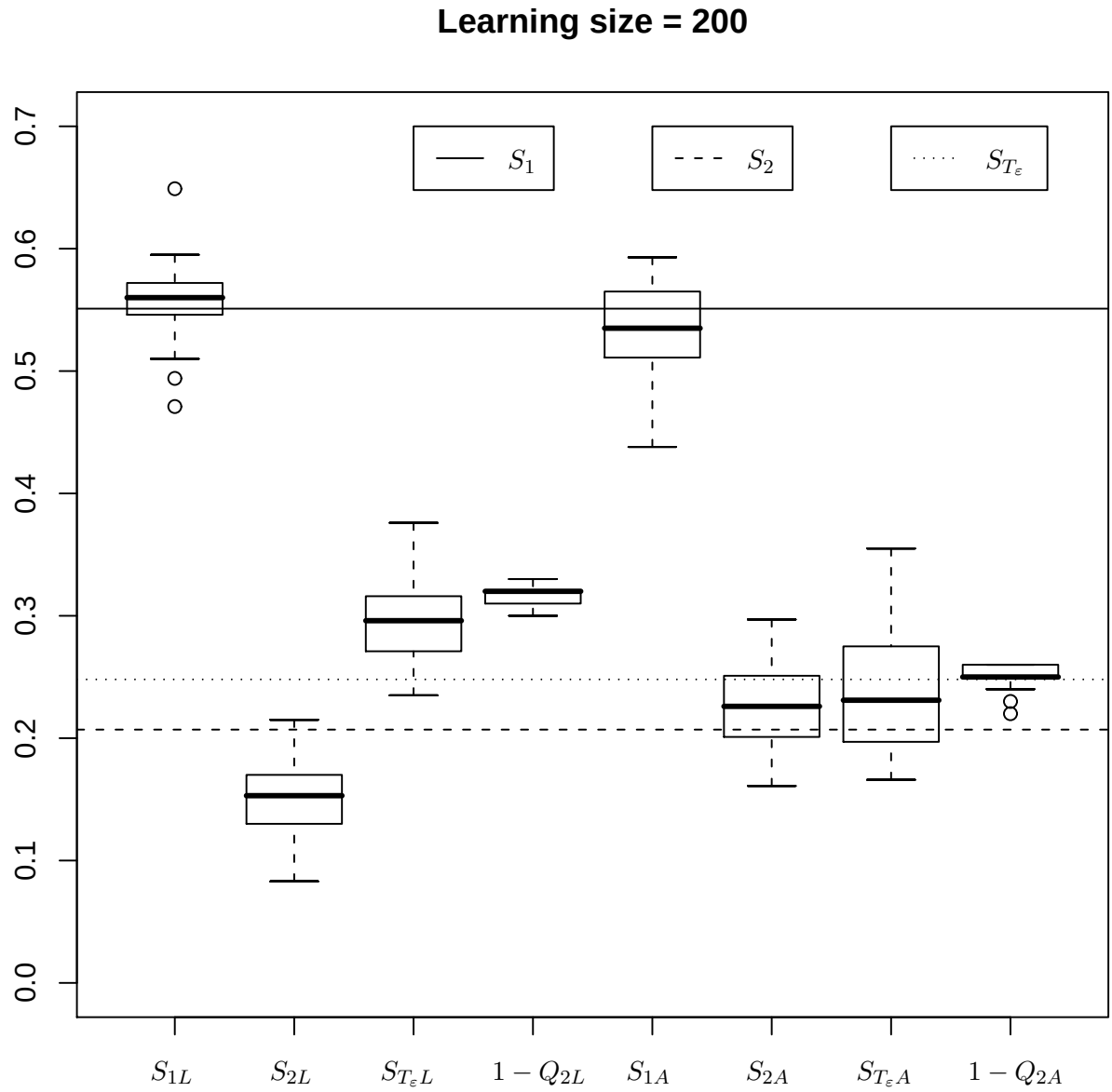

Figure 1: WN-Ishigami application. Comparison of Sobol indices estimates. Reference values: $S_1, S_2, S_{T_\varepsilon}$. Joint GLM: $S_{1L}, S_{2L}, S_{T_\varepsilon L}, 1-Q_{2L}$. Joint GAM: $S_{1A}, S_{2A}, S_{T_\varepsilon A}, 1-Q_{2A}$. $1-Q_{2L}$ (resp. $1-Q_{2A}$) is the estimation of S_{T_ε} via the joint GLM (resp. joint GAM) Q_2 coefficient. Learning sample size: $n = 200$.

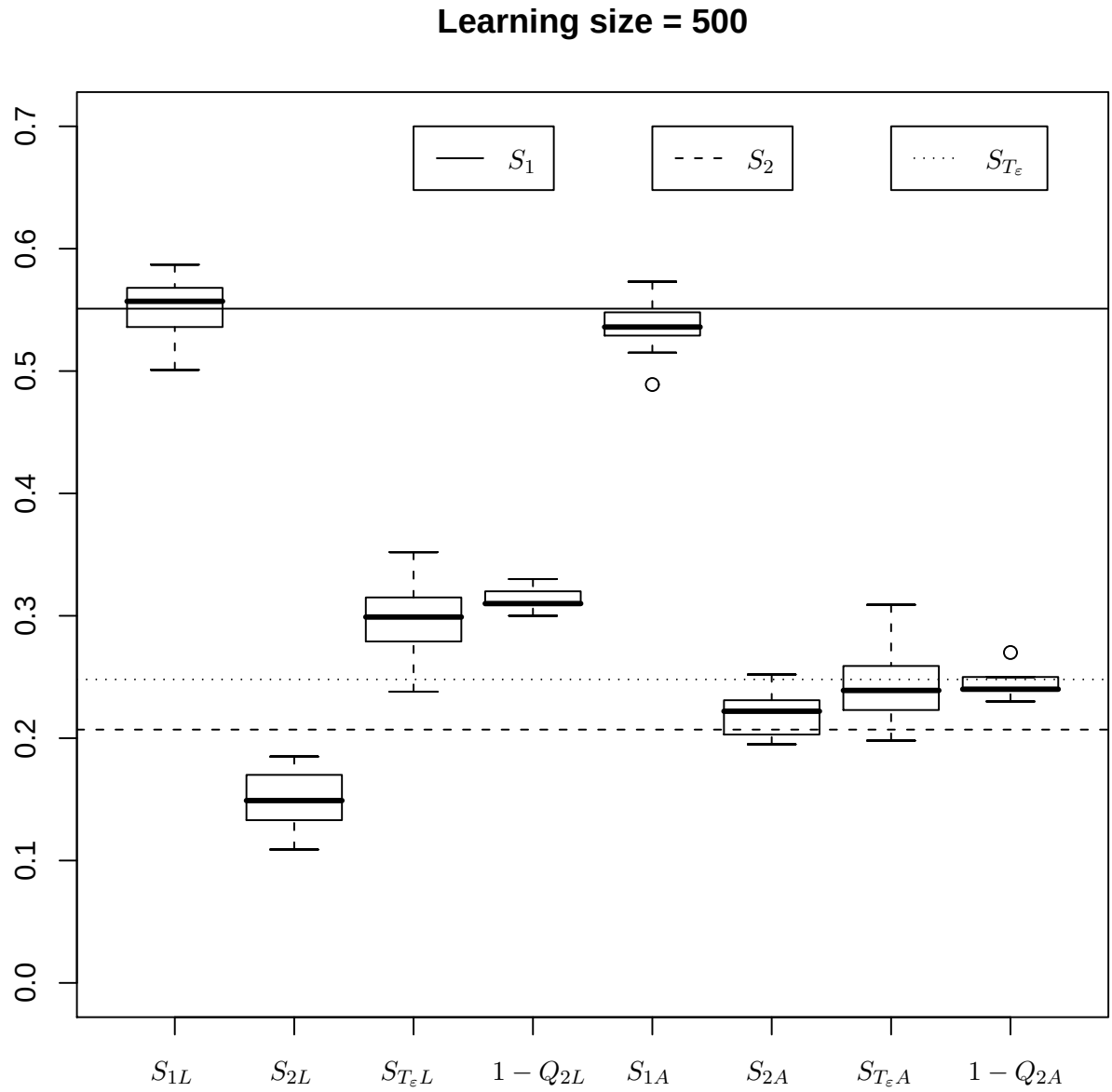

Figure 2: WN-Ishigami application. Comparison of Sobol indices estimates. Reference values: $S_1, S_2, S_{T_\varepsilon}$. Joint GLM: $S_{1L}, S_{2L}, S_{T_\varepsilon L}, 1-Q_{2L}$. Joint GAM: $S_{1A}, S_{2A}, S_{T_\varepsilon A}, 1-Q_{2A}$. $1-Q_{2L}$ (resp. $1-Q_{2A}$) is the estimation of S_{T_ε} via the joint GLM (resp. joint GAM) Q_2 coefficient. Learning sample size: $n = 500$.

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Table 1: Sobol sensitivity indices (with standard deviations *sd*) obtained from two Monte-Carlo algorithms (Sobol [21] and Saltelli [17]) and two integration methods of the functional input ε (macroparameter and "trigger" parameter) on the WN-Ishigami function. "—" indicates that the value is not available.

Indices	Macroparameter				"Trigger" parameter			
	Sobol algo		Saltelli algo		Sobol algo		Saltelli algo	
	Values	*sd*	Values	*sd*	Values	*sd*	Values	*sd*
S_1	0.540	1.3e-2	0.551	1.6e-2	0.304	1.3e-2	0.330	1.8e-2
S_{T_1}	—	—	0.808	2.0e-2	—	—	0.656	1.4e-2
S_2	0.197	1.1e-2	0.207	0.8e-2	0.329	1.4e-2	0.348	1.5e-2
S_{T_2}	—	—	0.212	0.7e-3	—	—	0.532	1.3e-2
$S_{1\varepsilon}$	0.268	2.4e-2	—	—	0.177	2.2e-2	—	—
S_{T_ε}	—	—	0.248	1.3e-2	—	—	0.336	1.4e-2

Table 2: Sobol sensitivity indices (with standard deviations) for the WN-Ishigami function: exact and estimated values from joint GLM and joint GAM (fitted with a 500-size sample). "Method" indicates the estimation method: MC for the Monte-Carlo procedure, Eq for a deduction from the model equations and Q_2 for the deduction of the predictivity coefficient Q_2. "—" indicates that the value is not available.

Indices	Reference Values	Joint GLM			Joint GAM		
		Values	*sd*	Method	Values	*sd*	Method
S_1	0.551	0.572	4e-3	MC	0.569	5e-3	MC
S_2	0.207	0.179	8e-3	MC	0.233	7e-3	MC
S_{T_ε}	0.248	0.250	2e-3	MC	0.197	1e-3	MC
		0.29	—	Q_2	0.23	—	Q_2
S_{12}	0	0	—	Eq	0	—	Eq
$S_{1\varepsilon}$	0.248	0	—	Eq	> 0	—	Eq
$S_{2\varepsilon}$	0	0	—	Eq	0	—	Eq
$S_{12\varepsilon}$	0	0	—	Eq	0	—	Eq
S_{T_1}	0.808	0.832	4e-3	Eq	—	—	—
S_{T_2}	0.212	0.179	8e-3	Eq	0.233	7e-3	Eq
S_ε	0	0.250	2e-3	Eq	—	—	—

Table 3: Sobol sensitivity indices (with standard deviations *sd*) from joint models fitted on the outputs of the METEOR code. "Method" indicates the estimation method: MC for the Monte-Carlo procedure and Eq for a deduction from the joint model equation. "—" indicates that the value is not available.

Indices	Gas swelling			Cladding creep					
	Joint GLM			Joint GLM			Joint GAM		
	Values	*sd*	Method	Values	*sd*	Method	Values	*sd*	Method
S_1	0.029	6e-3	MC	0.000	1e-3	MC	0.000	1e-3	MC
S_2	0.024	5e-3	MC	0.294	1e-4	MC	0.282	2e-4	MC
S_3	0	—	Eq	0.006	1e-3	MC	0.007	1e-3	MC
S_4	0.394	5e-3	MC	0.000	1e-3	MC	0.000	1e-3	MC
S_5	0.409	6e-3	MC	0.006	1e-3	MC	0.006	1e-3	MC
S_{24}	0.002	5e-3	MC	0	—	Eq	0	—	Eq
S_{45}	0.000	9e-3	MC	0	—	Eq	0	—	Eq
other S_{ij}	0	—	Eq	0	—	Eq	0	—	Eq
S_{T_ε}	0.143	1e-4	MC	0.694	1e-4	MC	0.704	3e-4	MC
S_ε	—	—	—	—	—	—	—	—	—
$S_{\varepsilon 1}$	—	—	—	0	—	Eq	0	—	Eq
$S_{\varepsilon 2}$	0	—	Eq	—	—	—	—	—	—
other $S_{\varepsilon i}$	0	—	Eq	0	—	Eq	0	—	Eq
S_{T_1}	—	—	—	0.000	1e-3	Eq	0.000	4e-3	Eq
S_{T_2}	0.026	7e-3	Eq	—	—	—	—	—	—
S_{T_3}	0	—	Eq	0.006	1e-3	Eq	0.007	4e-3	Eq
S_{T_4}	0.396	7e-3	Eq	0.000	1e-3	Eq	0.000	4e-3	Eq
S_{T_5}	0.409	0.011	Eq	0.006	1e-3	Eq	0.006	4e-3	Eq