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Résumé — **Méthode de criblage basée sur les indices de sensibilité DGSM : application au simulateur de réservoir** — Les simulateurs d'écoulements en milieux poreux sont utilisés pour effectuer des prévisions de la production de gisements pétroliers. Les modèles de réservoir étudiés sont caractérisés par un grand nombre de propriétés qui sont souvent très incertaines. Afin de construire des modèles prédictifs il est donc nécessaire de réduire cette incertitude en se focalisant sur les variables les plus influentes. Les méthodes d'analyse de sensibilité permettent de résoudre ce problème, mais sont souvent très coûteuses en nombre de simulations. Afin de réduire le nombre d'appels au simulateur des nouveaux indices, nommés DGSM (*Derivative-based Global Sensitivity Measures*) basés sur la moyenne des dérivés partielles, ont été introduits. Dans cet article, une version révisée des indices DGSM est proposée afin d'améliorer leur efficacité et leur convergence dans le cas où très peu de simulations peuvent être effectuées. L'efficacité de ces indices est montrée sur des cas test analytiques ainsi que sur un modèle synthétique de réservoir.

Abstract — ***Screening Method Using the Derivative-based Global Sensitivity Indices with Application to Reservoir Simulator*** — *Reservoir simulator can involve a large number of uncertain input parameters. Sensitivity analysis can help reservoir engineers focusing on the inputs whose uncertainties have an impact on the model output, which allows reducing the complexity of the model. There are several ways to define the sensitivity indices. A possible quantitative definition is the variance-based sensitivity indices which can quantify the amount of output uncertainty due to the uncertainty of inputs. However, the classical methods to estimate such sensitivity indices in a high-dimensional problem can require a huge number of reservoir model evaluations. Recently, new sensitivity indices based on averaging local derivatives of the model output over the input domain have been introduced. These so-called Derivative-based Global Sensitivity Measures (DGSM) have been proposed to overcome the problem of dimensionality and are linked to total effect indices, which are variance-based sensitivity indices. In this work, we propose a screening method based on revised DGSM indices, which increases the interpretability in some complex cases and has a lower computational cost, as demonstrated by numerical test cases and by an application to a synthetic reservoir test model.*

INTRODUCTION

Reservoir simulators are complex computer codes that model the physical laws governing the recovery process, and which are mainly modeled by mathematical equations for the three-phases flow (oil, gas and water) through porous media. These simulators involve a large number of input parameters. The information gathered on such inputs comes from direct measurements, which are clearly very limited and are marred by considerable uncertainty. Thus, it is important to detect influential inputs, whose uncertainties have an impact on the model output. Once identified, one can reduce the complexity of the model by fixing the non-influential inputs at default values (defined by experts) and focus the attention on the influential inputs.

Sensitivity Analysis (SA) is the study of how the variation (uncertainty) in the output of the computer model can be apportioned, qualitatively or quantitatively, to different sources of variation in the input of the model. Put in another way, it is a technique for systematically changing parameters in a model to determine the effects of such changes on the output. The local SA methods refer to the study of the sensitivity at a fixed point in the input domain, typically the simple derivative $\partial Y / \partial x^{(i)}$ of the output Y with respect to a given input $X^{(i)}$ taken at some fixed point $\mathbf{x}_0$ in the input domain. The Global Sensitivity Analysis (GSA) methods [1-4] refer to the sampling-based methods in which the model is evaluated for combinations of values sampled from the distribution (assumed known) of the inputs. Once the sample is generated, several strategies (including simple input-output scatterplots) can be used to derive global sensitivity measures for the factors.

The variance-based methods are non-linear with respect to the input parameters, and are based on analysis of variance (ANOVA) decomposition, which is the decomposition of the total variance V of output into terms due to individual factors plus terms due to interaction among inputs. Most variance-based methods are quantitative, and in this work, we will focus on this class of methods, and more specifically on Sobol's indices.

One of the main issues with variance-based methods is computational time. Indeed, a reservoir simulator is often very costly in terms of computational time. Furthermore, such variance-based methods generally require several thousands simulations that are usually not affordable in common applications. In order to perform SA with a limited number of runs, metamodel methods can therefore be used. In the latter, the simulator input/output relation is approximated using different statistical regression techniques starting from an initial set of carefully chosen training runs. Then, if a reasonably good approximation is obtained, the estimated metamodel is used instead of the complex simulator to compute the sensitivity indices. Metamodel methods have known a quick development in the last decade and different approaches have been suggested in many different scientific disciplines [5-13]. However, despite significant advances in the area, construction of a sufficiently accurate approximation for high-dimensional computer code using a relatively low number of model evaluations is problematic.

Screening methods aim at reducing the input dimensionality by identifying the non-influential inputs with a low computational cost in terms of model evaluation. The screening design proposed by Morris [14] is adapted for high-dimensional expensive computer models. This method is a One-factor-At-a-Time (OAT) technique that varies one input parameter at a time and measures the impact on the output. Indeed, the method is based on calculating a sensitivity index called an elementary effect, which provides a good compromise between accuracy and efficiency. However, although this method is computationally cheaper than other SA methods, it involves hundreds or thousands (depending on the number of inputs and the complexity of the model) of model evaluations, which is still computationally intensive with realistic reservoir simulators, for which each simulation requires several hours or days.

Recently, Sobol and Kucherenko [15, 16] have proposed new sensitivity indices based on averaging local derivatives of the model output over the input domain. It was shown that the so-called Derivative-based Global Sensitivity Measures (DGSM) can be easily estimated and much faster than the global sensitivity indices. In addition, different methods exist to efficiently compute the derivatives of reservoir simulators; in this case, DGSM represent a valid alternative to the Morris method for screening the input parameters.

In this work, we propose a revised derivative-based sensitivity index that allows a better convergence of the estimation and increases the interpretability in some complex cases. We propose a screening method based on the defined indices. We then employ the method to perform a screening of a high-dimensional analytical test case and of a synthetic reservoir model application.

1 GLOBAL SENSITIVITY ANALYSIS AND MORRIS DESIGN

First, let us consider a mathematical model for a reservoir simulator:

$$Y = f(\mathbf{X}) \tag{1}$$

where Y is a scalar output of the computer code, $\mathbf{X} = (X^{(1)}, \ldots, X^{(d)})$ a unit d-dimensional input vector ($\mathbf{X} \in [0,1]^d$) which represents the uncertain parameters/factors of the simulator and $f: [0,1]^d \to \mathbb{R}$ is a function that models the relationship between the input factors and the output of the computer code.

1.1 Global Sensitivity Analysis

The main idea of Sobol's approach [4] is to decompose the response $Y = f(\mathbf{X})$ into summands of different dimensions *via* analysis of variance decomposition (ANOVA) defined as:

$$f(\mathbf{X}) = f_0 + \sum_{j=1}^{d} f_j\left(X^{(j)}\right) + \sum_{j<l} f_{jk}\left(X^{(j)}, X^{(l)}\right) + \ldots \\ + f_{1,\ldots,d}\left(X^{(1)}, \ldots, X^{(d)}\right) \quad (2)$$

where f_0 is a constant, f_j's are univariate functions representing the main effects, f_{jl}'s are bivariate functions representing the two-way interactions, and so on.

The integrals of every summand of this decomposition over any of its own variables is assumed to be equal to zero, *i.e*:

$$\int_0^1 f_{j_1,\ldots,j_s}(X^{(j_1)}, \ldots, X^{(j_s)})dX^{(j_k)} = 0 \quad (3)$$

where $1 \leq j_1 < \ldots < j_s \leq d$, $s = 1, \ldots, d$ and $1 \leq k \leq s$. It follows from this property that all the summands in Equation (2) are orthogonal, *i.e.*, if $(i_1, \ldots, i_s) \neq (j_1, \ldots, j_l)$, then:

$$\int_{\Omega^d} f_{i_1,\ldots,i_s} f_{j_1,\ldots,j_l} d\mathbf{X} = 0 \quad (4)$$

Using the orthogonality, Sobol [4] showed that such decomposition of $f(\mathbf{X})$ is unique and that all the terms in Equation (2) can be evaluated *via* multidimensional integrals:

$$f_0 = E(Y) \quad (5)$$

$$f_j(X^{(j)}) = E(Y|X^{(j)}) - E(Y) \quad (6)$$

$$f_{j,l}(X^{(j)}, X^{(l)}) = E(Y|X^{(j)}, X^{(l)}) - f_j - f_l - E(Y) \quad (7)$$

where $E(Y)$ and $E(Y|X^{(j)})$ are, respectively, the expectation and the conditional expectation of the output Y. Analogous formulae can be obtained for the higher-order terms. If all the input factors are mutually independent, the ANOVA decomposition is valid for any

distribution function of the $X^{(i)}$s and using this fact, squaring and integrating (2) over $[0,1]^d$, and by Equation (4), we obtain:

$$V = \sum_{j=1}^{d} V_j + \sum_{1 \leq j < l \leq d} V_{jl} + \ldots + V_{1,2,\ldots,d} \quad (8)$$

where $V_j = V[E(Y|X^{(j)})]$ is the variance of the conditional expectation that measures the main effect of X_j on Y and $V_{jl} = V[E(Y|X^{(j)}, X^{(l)})] - V_j - V_l$ measures the joint effect of the pair $(X^{(j)}, X^{(l)})$ on Y. The total variance V of Y is defined to be:

$$V = E(Y^2) - f_0^2 \quad (9)$$

Variance-based sensitivity indices, also called Sobol indices, are therefore defined by:

$$S_{j_1,\ldots,j_s} = \frac{V_{j_1,\ldots,j_s}}{V} \quad (10)$$

where $1 \leq j_1 < \ldots < j_s \leq d$ and $s = 1, \ldots, d$. Thus, $S_j = V_j/V$ is called the first-order sensitivity index (or the main effect) for factor $X^{(j)}$, which measures the main effect of $X^{(j)}$ on the output Y, the second-order index $S_{jl} = V_{jl}/V$, for $j \neq l$, is called the second-order sensitivity index and expresses the sensitivity of the model to the interaction between the variables $X^{(i)}$ and $X^{(j)}$ on Y, and so on for higher-orders effects. The decomposition in (8) has the useful property that all sensitivity indices sum up to one:

$$\sum_{j=1}^{p} S_j + \sum_{1 \leq j < l \leq p} S_{jl} + \ldots + S_{1,2,\ldots,p} = 1 \quad (11)$$

The total sensitivity index (or total effect) of a given factor is defined as the sum of all the sensitivity indices involving the factor in question:

$$S_{T_i} = \sum_{l \# i} \frac{V_l}{V} = \frac{V_{T_i}}{V} \quad (12)$$

where #i represents all the $S_{j_1,\ldots,j_s}$ terms that include the index i. The total effect index of an input $X^{(i)}$ measures the part of output variance explained by all the effects in which it plays a role. Note, however, that the sum of all S_{T_i} is higher than one because interaction terms are counted several times. It is also important to note that total effect indices can be computed by a single multidimensional integration and do not require computing all high-order indices (Sobol [4]). Therefore, comparing the total effect indices provides information about influential parameters. Indeed, one can suppose that the input is non-influential if its total effect S_{T_i} is less than 0.01.

GSA enables the explanation of the variability of the output response as a function of the input parameters through the definition of total and partial sensitivity indices. The computation of these indices involves the computation of several multidimensional integrals that are estimated by the Monte-Carlo method and thus requires huge random samples. For this reason, GSA techniques are prohibitive if used directly using the computer code (fluid flow simulator, for example).

1.2 Morris's Screening Method

The screening method introduced by Morris [14] is based on a OAT experimental design. The points of the Morris design are sampled from a d-dimensional p-level grid, as the range of each input $X^{(i)}$ is divided into p equal levels. The impact of varying one input at a time is evaluated by the so-called elementary effect that, for $i = 1, \ldots, d$, is defined as:

$$d_i^r(\mathbf{X}^r) = \frac{f(\mathbf{X}_i^r) - f(\mathbf{X}^r)}{\Delta} \tag{13}$$

where Δ is a multiple of $1/(p-1)$ with p the number of levels, $\mathbf{X}^r$ is a randomly chosen point in $[0,1]^d$ such that $X^{(i)} + \Delta$ is still in $[0,1]$ and:

$$\mathbf{X}_i^r = X^{(1)}, \ldots, X^{(i-1)}, X^{(i)} + \Delta, X^{(i+1)}, \ldots, X^{(d)}$$

The group of points composed of $\mathbf{X}^r$ and $\mathbf{X}_i^r$s are called trajectories. Thus, the Morris design is structured in R random trajectories composed of $R(d+1)$ points.

The sensitivity measures proposed by Morris [14] are defined as a statistics of the elementary effect. The first one is the mean $\hat{\mu}_i$:

$$\hat{\mu}_i = \frac{1}{R} \sum_{r=1}^{R} d_i^r \tag{14}$$

which is a measure of the ith input importance. The second statistic is the standard deviation of the elementary effect $\hat{\sigma}_i$:

$$\hat{\sigma}_i = \sqrt{\frac{1}{R-1} \sum_{r=1}^{R} (d_i^r - \hat{\mu}_i)^2} \tag{15}$$

which is a measure of the non-linearity and the interactions involved in the ith input. However, $\hat{\sigma}_i$ does not allow one to distinguish between non-linearities and interactions.

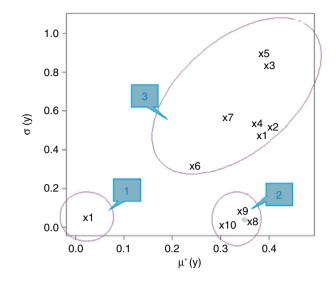Noting that when the model is non-monotonic the elementary effects of opposite signs cancel each other,

Figure 1

An example of a graph displaying the Morris sensitivity measures $\hat{\mu}_i^*$ and $\hat{\sigma}_i$.

Campolongo *et al.* [17] proposed the sensitivity measure $\hat{\mu}_i^*$, which is a revised version of $\hat{\mu}_i$:

$$\hat{\mu}_i^* = \frac{1}{R} \sum_{r=1}^{R} |d_i^r| \tag{16}$$

To identify the non-influential inputs, the sensitivity measures $\hat{\mu}_i^*$ and $\hat{\sigma}_i$ are simultaneously considered. Typically, for more interpretability, $\hat{\mu}_i^*$ and $\hat{\sigma}_i$ are displayed on a 2D graph. An example is shown in Figure 1; we can distinguish three groups of inputs. The inputs of group 1, group 2 and group 3 will be respectively classified as non-influential, having linear effects, and having non-linear and/or interaction effects.

2 DERIVATIVE-BASED SENSITIVITY ANALYSIS

2.1 Derivative-based Global Sensitivity Measures

First introduced by Sobol and Gresham [18] and then studied in Kucherenko *et al.* [19], Sobol and Kucherenko [15, 16] and Lamboni *et al.* [20], DGSM are a new sensitivity indices based on averaging local derivatives of the model output over the input domain.

Assume that $\partial f(\mathbf{X})/\partial x^{(i)}$, for $i = 1, \cdots, d$, are square-differentiable. The DGSM indices are defined as:

$$v_i = \mathbb{E}\left[\left(\frac{\partial f(\mathbf{X})}{\partial x^{(i)}}\right)^2\right] = \int \left(\frac{\partial f(\mathbf{X})}{\partial x^{(i)}}\right)^2 d\mathbf{x} \tag{17}$$

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Thus, calculation of DGSM indices is based on the evaluation of integrals, which is easily performed using classical Monte-Carlo (MC), Quasi-Monte-Carlo (QMC) or Latin Hypercube Sampling (LHS). The empirical estimator of v_i is given by:

$$\hat{v}_i = \frac{1}{n} \sum_{j=1}^{n} \left(\frac{\partial f(\mathbf{X}_j)}{\partial x^{(i)}} \right)^2 \qquad (18)$$

It is important to note that the ability to calculate derivatives efficiently is important for estimating DGSM indices within an acceptable computational cost.

2.1.1 Link between DGSM and GSA

Recently, Sobol and Kucherenko [15] have established the link between the DGSM index v_i and the total effect index S_{T_i} for input variables following uniform and normal distributions. These results have been extended to the standard log-concave distributions by Lamboni et al. [20]. Here, we assume that $X^{(i)} \sim \mathbb{U}[a_i, b_i]$, for $i = 1, \ldots, d$, the link between V_{T_i} and v_i is defined by the following inequality:

$$V_{T_i} \leq \frac{(b_i - a_i)^2}{\pi^2} v_i = v_i^* \qquad (19)$$

Thereby, the total effect indices have the following upper bound:

$$S_{T_i} \leq \frac{v_i^*}{V} = \Upsilon_i \qquad (20)$$

where V is the total variance of the model. If $\Upsilon_i \simeq 0$, then $X^{(i)}$ can be considered as non-influential input, which makes Υ_i a good candidate for a screening procedure. However, as has been shown in Sobol and Kucherenko [15], for highly non-linear functions the ranking of important inputs obtained with Υ and total effect indices may not be the same.

2.1.2 Link between DGSM and the Morris Method

Kucherenko et al. [19] have introduced two derivative-based sensitivity indices that are very similar to the Morris indices μ_i and σ_i. These indices are defined, for $i = 1, \ldots, d$, as:

$$\bar{M}_i = \int \frac{\partial f(\mathbf{X})}{\partial x^{(i)}} d\mathbf{x} \qquad (21)$$

and

$$\bar{\Sigma}_i^2 = \int \left(\frac{\partial f(\mathbf{X})}{\partial x^{(i)}} \right)^2 d\mathbf{x} - \bar{M}_i^2 \qquad (22)$$

where $\bar{M}_i$ is equivalent to μ_i and $\bar{\Sigma}_i^2$ equivalent to σ_i^2. In addition, these indices are more accurate than Morris's indices, which cannot correctly consider effects with characteristic dimensions less than Δ. Indeed, in (13) the elementary effects d_i^r are calculated as finite differences with the increment Δ, which has the same order of magnitude as the uncertainty range of inputs, in contrast with the derivative-based indices $\bar{M}_i$ and $\bar{\Sigma}_i^2$, where the elementary effects are substituted by the local derivatives.

We can also note that the DGSM indices v_i can be defined as:

$$v_i = \int \left(\frac{\partial f(\mathbf{X})}{\partial x^{(i)}} \right)^2 d\mathbf{x} = \bar{M}_i^2 + \bar{\Sigma}_i^2 \qquad (23)$$

2.2 Refining the DGSM Index Υ

In the previous section, we have shown that the sensitivity index Υ is an upper bound of the total effect index. However, for some complex models, Υ can be much larger than the corresponding total effect index (Lamboni et al. [20]). In this case, it is difficult to decide which inputs are influential and which are not. In addition, Υ estimation involves the variance of the model output V. Empirical results (see next section) show that estimation of V requires more model evaluation than estimation of v.

We propose here a normalized version of Υ that we call Υ^*, which is defined, for $i = 1, \ldots, d$, as:

$$\Upsilon_i^* = \frac{v_i^*}{\sum\limits_{j=1}^{d} v_j^*} \qquad (24)$$

This index is a normalized upper bound of V_{T_i}. Indeed, the link between Υ_i^* and V_{T_i} is defined as:

$$\frac{V_{T_i}}{\sum\limits_{j=1}^{d} v_j^*} \leq \Upsilon_i^* \qquad (25)$$

In addition, Υ^* has the following useful properties:

$$0 \leq \Upsilon_i^* \leq 1 \qquad (26)$$

and

$$\sum_{i=1}^{d} \Upsilon_i^* = 1 \qquad (27)$$

The drawback of Υ^* is the loss of the link with the total effect indices. Nevertheless, the use of Υ^* offers a
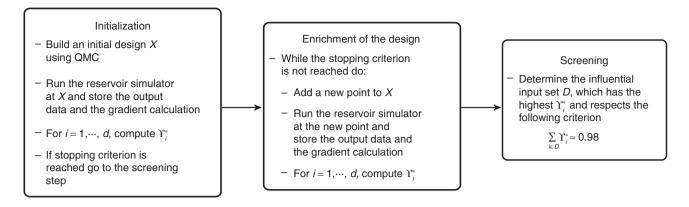
Figure 2

Schematic representation of the screening method.

stronger measure to define the non-influential inputs, as we will see in the next sections.

3 DGSM-BASED SCREENING METHOD

As shown in Section 2, estimating Υ^* for each input allows one to detect the influential inputs in the model. Indeed, one can state that if $\hat{\Upsilon}_i^* \leq 0.01$, the corresponding input $X^{(i)}$ can be defined as non-influential. However, such a criterion may be too strong in the case of very high-dimensional models (typically more than 100 input parameters); the fact is that the sum of effects due to inputs with small sensitivity indices may be significant on the output model variance. Because of this, and by using the property (27) of the Υ^* measures, it is more robust to state that the influential inputs are the set D of d^* inputs whose Υ_i^* are the highest, and which respect the following criterion:

$$\sum_{i \in D} \Upsilon_i^* \approx 0.98 \tag{28}$$

Given that the reservoir simulator evaluation may be computationally demanding, it is important to use a sequential strategy to build the design of points by reusing at each step the already evaluated points. The use of the so-called QMC Sobol sequence [21, 22] is an efficient way to build a sequential design. Our choice is motivated by two main properties of the QMC Sobol sequences. First, this technique is based on the generation of deterministic quasi-random sequences with a good space-filling property of the unit hypercube; in other words, the input domains are well covered for fairly small sets.

Second, the points of the Sobol sequence are independent. That is, by enriching the design sequentially, one keeps the space-filling properties of the Sobol sequence.

Since a sequential method computes successive estimation of the Υ_i^* indices, a practical test is needed to determine when to stop the iteration. In this work, we propose to use the following error criterion:

$$err_l = \frac{1/10 \sum_{k=1}^{10} ||\boldsymbol{\Upsilon}_{(l)}^* - \boldsymbol{\Upsilon}_{(l-k)}^*||}{||\boldsymbol{\Upsilon}_{(l)}^*||} \tag{29}$$

where vectors $\boldsymbol{\Upsilon}_{(l)}^* = (\Upsilon_1^*, \ldots, \Upsilon_d^*)$ are the lth estimation of Υ_i^* indices and $||\cdot||$ is the Euclidean norm. Thus, we define the stopping criterion as $err \leq 0.05$. Note that the proposed stopping criterion was not chosen as a convergence criterion for each of the indices, because this might be very long. The criterion chosen is more global and it is intended to detect as soon as possible influential or not-influential parameters in order to perform the screening. A schematic representation of the entire screening method is shown in Figure 2. Note that one can use the same stopping criterion (29) to estimate Υ_i indices.

4 NUMERICAL TESTS

In this section, two numerical test cases are used to demonstrate the estimation performance of the DGSM index Υ^* and the accuracy of the proposed screening method to detect the influential inputs. Adopting the QMC sampling method, each input parameter $X^{(i)}$ is uniformly distributed in $[0, 1]$.

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TABLE 1

Results of averaging, over 100 realizations, the estimated Υ_i and Υ_i^* sensitivity indices *versus* the sample size for the Morris function. The estimated standard deviation is given in parentheses

	Υ_i^* ($n = 50$)	Υ_i ($n = 50$)	Υ_i^* ($n = 500$)	Υ_i ($n = 500$)
$X^{(1)}$	0.158 (0.020)	0.322 (0.079)	0.158 (0.007)	0.310 (0.026)
$X^{(2)}$	0.158 (0.019)	0.322 (0.073)	0.157 (0.007)	0.307 (0.021)
$X^{(3)}$	0.084 (0.010)	0.169 (0.036)	0.085 (0.004)	0.167 (0.012)
$X^{(4)}$	0.157 (0.019)	0.319 (0.077)	0.159 (0.006)	0.311 (0.025)
$X^{(5)}$	0.086 (0.011)	0.174 (0.037)	0.085 (0.004)	0.166 (0.013)
$X^{(6)}$	0.058 (0.008)	0.117 (0.024)	0.058 (0.003)	0.114 (0.009)
$X^{(7)}$	0.047 (0.005)	0.095 (0.023)	0.046 (0.004)	0.091 (0.011)
$X^{(8)}$	0.077 (0.012)	0.158 (0.043)	0.079 (0.010)	0.156 (0.024)
$X^{(9)}$	0.081 (0.010)	0.166 (0.046)	0.079 (0.009)	0.154 (0.021)
$X^{(10)}$	0.079 (0.011)	0.161 (0.041)	0.077 (0.007)	0.152 (0.020)
$X^{(11)}$	0.002 (0.001)	0.003 (0.002)	0.002 (0.001)	0.003 (0.002)
$X^{(12)}$	0.002 (0.001)	0.003 (0.002)	0.001 (0.001)	0.003 (0.001)
$X^{(13)}$	0.002 (0.001)	0.003 (0.002)	0.002 (0.001)	0.003 (0.002)
$X^{(14)}$	0.002 (0.001)	0.003 (0.002)	0.002 (0.001)	0.003 (0.001)
$X^{(15)}$	0.002 (0.001)	0.003 (0.002)	0.002 (0.001)	0.003 (0.002)
$X^{(16)}$	0.002 (0.001)	0.003 (0.002)	0.002 (0.001)	0.003 (0.001)
$X^{(17)}$	0.002 (0.001)	0.003 (0.002)	0.002 (0.001)	0.003 (0.002)
$X^{(18)}$	0.001 (0.001)	0.003 (0.002)	0.002 (0.001)	0.003 (0.001)
$X^{(19)}$	0.002 (0.001)	0.003 (0.002)	0.002 (0.001)	0.003 (0.002)
$X^{(20)}$	0.002 (0.001)	0.003 (0.002)	0.002 (0.001)	0.003 (0.002)

4.1 The Test Case of Morris

The test function proposed by Morris [14] contains 20 input parameters and is defined as follows:

$$y = \beta_0 + \sum_{i=1}^{20} \beta_i w_i + \sum_{i<j}^{20} \beta_{i,j} w_i w_j + \sum_{i<j<l}^{20} \beta_{i,j,l} w_i w_j w_l + \sum_{i<j<l<s}^{20} \beta_{i,j,l,s} w_i w_j w_l w_s$$

where $w_i = 2 \times (X^{(i)} - 1/2)$ except for i = 3, 5, and 7, where $w_i = 2 \times (1.1 X^{(i)}/(X^{(i)} + 1) - 1/2)$. Coefficients with relatively large values are:

$$\begin{cases} \beta_i = 20 \text{ for } i = 1, \cdots, 10 \\ \beta_{i,j} = -15 \text{ for } i,j = 1, \cdots, 6 \\ \beta_{i,j,l} = -10 \text{ for } i,j,l = 1, \cdots, 5 \\ \beta_{i,j,l,s} = 5 \text{ for } i,j,l,s = 1, \cdots, 4 \end{cases}$$

the remaining β_i and $\beta_{i,j}$ are independently generated from a standard normal distribution. The remaining $\beta_{i,j,l}$ and $\beta_{i,j,l,s}$ are set to zero.

Table 1 summarizes the results of Υ_i and Υ_i^* estimation using 100 realizations of two sizes ($n = 50$ and $n = 500$) built by the Latin hypercube design procedure [23]. The goal here is to compare the robustness of the estimators. It is clear that the Υ_i^* estimators are more robust than the Υ_i estimator, which can be explained by the fact that the estimation of the model variance requires more model evaluations than estimation of DGSM v_i.

In Figure 3, one can see the results of computing Υ_i and Υ_i^* sequentially with a QMC design ranging from $n = 5$ to $n = 256$. In addition, the sample size when the stopping criterion of the proposed screening method is reached is represented by the red vertical line. Thereby, we can notice that Υ_i^* converge faster than Υ_i. Indeed,
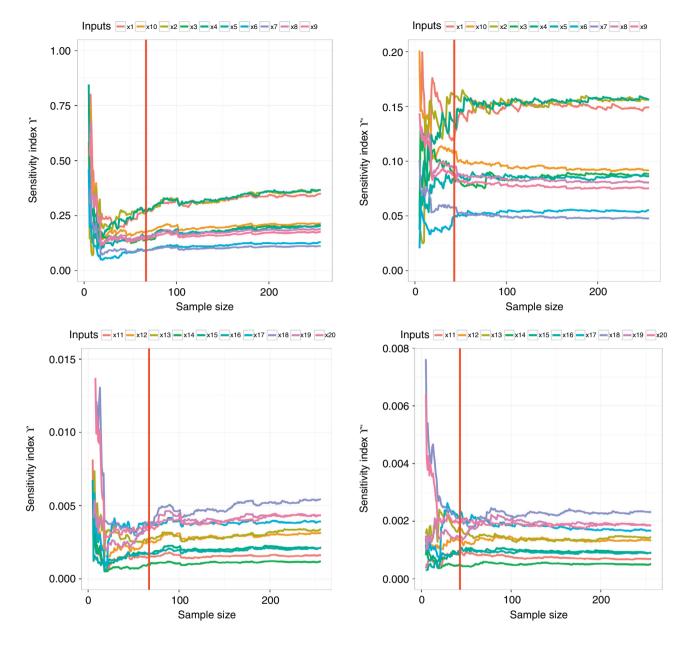
Figure 3

Convergence of the Υ_i and Υ_i^* indices estimates *versus* the sample size for the Morris function. The red vertical line corresponds to the sample size when the stopping criterion (29) is reached.

the stopping criterion is reached at $n = 43$ for Υ_i^* and at $n = 67$ for Υ_i estimations. In Table 2, for the inputs selected by the proposed screening method, the values of the total effect indices (obtained by the so-called extended FAST method [2] using a sample of size $N = 3.5 \times 10^4$) as well as the values of Υ_i and Υ_i^* (computed at the stopping criterion sample sizes $n = 67$ and $n = 43$) are reported. Note that the values of the indices $S_{T_{11}}, \ldots, S_{T_{20}}$ are smaller than 0.005 and therefore, the

corresponding inputs are considered to be non-influential.

It can be seen that for this test case both indices (Υ_i and Υ_i^*) are able to identify the influential inputs correctly at the stopping criterion (29). Furthermore, even if at $n = 67$ the Υ_i indices are underestimated they are almost for all inputs greater than but close to the total effect indices. To conclude on this numerical test, we can say that for the Morris function the developed

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TABLE 2

Estimated sensitivity indices for the Morris function

Input	Total effect	Υ_i ($n = 67$)	Υ_i^* ($n = 43$)
$X^{(1)}$	0.240	0.249	0.114
$X^{(2)}$	0.241	0.244	0.164
$X^{(3)}$	0.095	0.127	0.088
$X^{(4)}$	0.245	0.252	0.137
$X^{(5)}$	0.098	0.137	0.083
$X^{(6)}$	0.082	0.081	0.048
$X^{(7)}$	0.050	0.078	0.053
$X^{(8)}$	0.105	0.133	0.091
$X^{(9)}$	0.099	0.123	0.084
$X^{(10)}$	0.106	0.173	0.118

TABLE 3

Analytical total effect indices and estimated DGSM indices for the g-Sobol function

Input	Total effect	Υ_i ($n = 59$)	Υ_i^* ($n = 41$)
$X^{(1)}$	0.396	3.671	0.338
$X^{(2)}$	0.279	3.111	0.266
$X^{(3)}$	0.205	1.781	0.144
$X^{(4)}$	0.156	1.383	0.088
$X^{(5)}$	0.122	0.911	0.072
$X^{(6)}$	0.057	0.397	0.031
$X^{(7)}$	0.032	0.234	0.017
$X^{(8)}$	0.021	0.169	0.011
$X^{(9)}$	0.015	0.106	0.008
$X^{(10)}$	0.011	0.078	0.005
$X^{(11)}$	0.009	0.061	0.004

screening method based on Υ_i^* is efficient and not consuming in terms of model evaluations. However, estimating Υ_i indices provides more information since they are very close as an upper bound to the total effect indices, but the drawback is the additional model evaluation cost.

4.2 The G-Sobol Function

Consider the g-Sobol function, which is strongly nonlinear and is described by a non-monotonic relationship. Because of its complexity and the availability of analytical sensitivity indices, this function is a well-known test case in the studies of GSA. Let us define the g-Sobol function for 200 input parameters as follows:

$$g_{\text{Sobol}}(X^{(1)}, \ldots, X^{(8)}) = \prod_{k=1}^{8} g_k(X^{(k)})$$

with:

$$g_k(X^{(k)}) = \frac{\left|4X^{(k)} - 2\right| + a_k}{1 + a_k}$$

where $\{a_1, \ldots, a_{20}\} = \{0, 0.25, 0.5, 0.75, 1, 2, \ldots, 16\}$ and $\{a_{21}, \ldots, a_{200}\} = 99$. The contribution of each input $X^{(k)}$ to the variability of the model output is represented by the weighting coefficient a_k. The lower this coefficient a_k, the more significant the variable $X^{(k)}$.

The analytical values of Sobol's indices are given by:
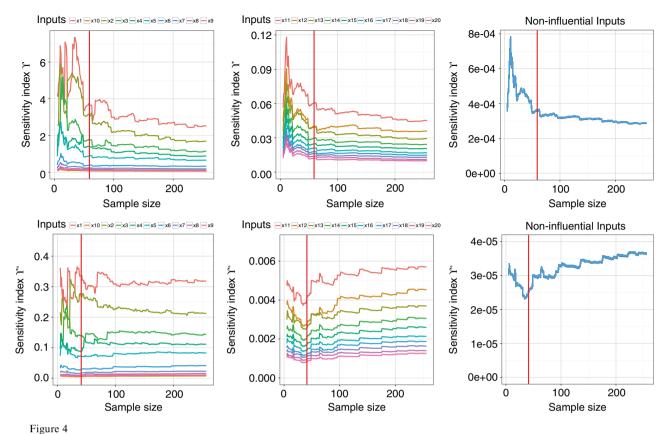
$$V_j = \frac{1}{3(1 + a_j)^2}$$

$$V = \prod_{k=1}^{d} (V_k + 1) - 1$$

$$S_{j_1, \ldots, j_s} = \frac{1}{V} \prod_{k=1}^{s} V_k$$

where $1 \leq j_1 < \ldots < j_s \leq d$ and $s = 1, \ldots, d$. The analytical values of the total effect indices are shown in Table 3. Figure 4 shows the sequential estimation of Υ_i^* and Υ_i indices with a QMC design ranging from $n = 5$ to $n = 256$. As for the previous test example, the estimations of Υ_i^* indices converge faster than those Υ_i. In this test case, the stopping criterion (29) is reached at $n = 41$ for Υ_i^* and $n = 59$ for Υ_i. The analytical values of the total effect indices as well as the values of Υ_i and Υ_i^* (estimated at the sample sizes $n = 59$ and $n = 41$) for the inputs which are identified as influential by the screening method are reported in Table 3. Note that the values of the indices $S_{T_{12}}, \ldots, S_{T_{200}}$ are smaller than 0.007 and therefore, the corresponding inputs are considered to be non-influential. One can see that the information provided by the indices $\Upsilon_1, \cdots, \Upsilon_4$ is difficult to interpret. Indeed, for the g-Sobol function the values of Υ_is provide only qualitative information, because for some inputs $\Upsilon_i > 1$, which is higher than the maximal value for the total effect indices. These results may due to the model non-linearity with respect to the inputs. On the other hand, despite the non-linearity and non-monotonicity of the model, the Υ_i^* measures perform very well in terms of quantitative interpretability.

Figure 4

Convergence of the Υ_i and Υ_i^* indices estimates *versus* the sample size for the g-Sobol function. The red vertical line corresponds to the sample size when the stopping criterion (29) is reached.

The above two numerical tests show us that both DGSM indices are adapted to identify the non-influential inputs. Moreover, the property (27) of Υ_i^* indices allows one to use an automatic screening method regardless of the complexity of the studied model.

5 RESERVOIR FORECASTING APPLICATION

In this section, the proposed screening method is applied to a reservoir simulator. As the goal here is to apply the method to a high-dimensional case, we chose to use horizontal and vertical permeability as input parameters. However, since the number of grid blocks in the considered reservoir simulation model is large, we applied the most basic parametrization technique, which is zonation, to reduce the dimension of the problem. This technique consists of dividing the reservoir into a relatively small number of zones (subregions) and assuming that each zone is homogeneous. In other words, one fixes the permeability (horizontal or vertical) over all the grid blocks of the considered zone.

5.1 Reservoir Model Description

The PUNQS case is a synthetic reservoir model taken from a real field located in the North Sea. The PUNQS test case, which is qualified as a small-size model, is frequently used as a benchmark reservoir engineering model for uncertainty analysis and for history-matching studies [24].

The geological model contains $19 \times 28 \times 5$ grid blocks, 1 761 of which are active. The reservoir is surrounded by a strong aquifer in the North and the West, and is bounded to the East and South by a fault (*Fig. 5*). A small gas cap is located in the center of the dome-shaped structure. The geological model consists of five independent layers, where the porosity distribution in each layer was modeled by geostatistical simulation. The layers 1, 3, 4 and 5 are assumed to be of good quality, while the layer 2 is of poorer quality. The field contains six production wells located around the gas-oil contact. Due to the strong aquifer, no injection wells are required. For more detailed description of the PUNQS model, see [25].

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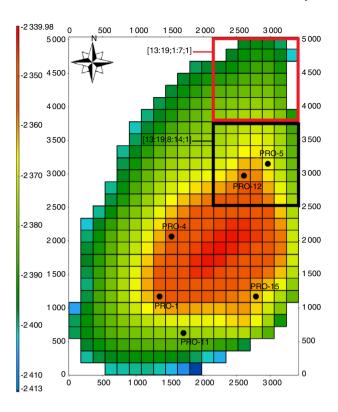Derivative-based Global Sensitivity Indices with Application to Reservoir Simulator
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Figure 5

Top structure map of the PUNQS reservoir field (layer 1); the red square corresponds to the area of the grid position [13:19;1(27)7;1] and the blue square corresponds to the area [13:19;8:14;1].

As input parameters, we considered the horizontal and vertical permeability of 60 zones (12 for each layer). Thus, we have a model of 180 inputs, which are supposed to be independent and defined as follows:

– $Z1, \cdots, Z60$: horizontal permeability in X direction,
– $Z61, \cdots, Z120$: horizontal permeability in Y direction,
– $Z121, \cdots, Z180$: vertical permeability.

The values of the permeability in each zone are distributed uniformly over $[PZ_i - 0.2PZ_i, PZ_i + 0.2PZ_i]$, where PZ_i is the arithmetic mean of the permeability values of the grid blocks which compose the ith zone.

The analyzed output is the production watercut data (the proportion of water in the produced oil) after 20 years of production of the well 5, for which the perforation location correspond to the grid blocks [17;11;3:4], where the notation $3:4$ means that there is a perforation at layer 3 and at layer 4. The reservoir test model was run using the PumaFlow^{TM} [26] simulator, which allows one to compute gradients using a gradient simulator method [27, 28] with an additional $\approx 33\%$ of the simulation time per each calculated gradient.

5.2 Screening

For this reservoir model, we first performed a convergence study of the DGSM indices. Υ_i and Υ_i^* are computed sequentially with a QMC design ranging from $n = 5$ to $n = 200$. From Figure 6, one can see that Υ_i^* indices converge much faster than Υ_i indices. The stopping criterion (29) was reached at $n = 18$ for Υ_i^* and at $n = 42$ for Υ_i^* indices estimation.

The screening method identifies 13 zones as influential. The DGSM sensitivity measures of these 14 parameters are reported in Table 4. We can see that these zones correspond to the region where the studied well is located and the closest north region. This result demonstrates the relevance of application of the developed screening methodology to a reservoir simulator.

To corroborate these screening results, we built a metamodel using a standard implementation of the Gaussian Process method (GP). The GP code used here is a commercial version implemented in the Cougar-Flow^{TM} software [29]. For more detail on the technical aspect of the used GP, we refer to Section 3 of Busby et al. [6]. The GP metamodel is built using the results obtained in the QMC design of the size $n = 200$. However, instead of using the full design of 180 inputs we just selected the 13 inputs identified as influential by the screening method. Thus, rather than building a metamodel that approximates a reservoir model of 180 inputs we built a metamodel $\hat{f}$ which involves only the parameters that are supposed to be influential on the output. To assess the prediction accuracy of the metamodel, we performed an extra 100 random evaluations of the PUNQS simulator (with 180 inputs) and compared the simulator results with the metamodel ones. The measure of the accuracy is given by the Q_2 criterion defined by:

$$Q_2 = 1 - \frac{\sum_{i=1}^{n_{test}} (y_i - \hat{f}(\mathbf{x}_i))^2}{\sum_{i=1}^{n_{test}} (y_i - \bar{y})^2}, \text{with } n_{test} = 100 \quad (30)$$

where y_i denotes the ith simulator evaluation on the test set, $\bar{y}$ is their empirical mean and $\hat{f}(\mathbf{x}_i)$ is the predicted value at the design point $\mathbf{x}_i = (x_i^{(1)}, \ldots, x_i^{(180)})$. The empirical Q_2 criterion of the considered metamodel $\hat{f}$ is equal to 0.94, which means that the metamodel explains 94% of the output variance. Thus, the obtained metamodel is sufficiently accurate to perform a global sensitivity analysis. In the second column of Table 4, the reported total effect indices were computed through the metamodel $\hat{f}$ and using the extended FAST method [2]. From Table 4, one can say that the developed screening method permits the detection of the
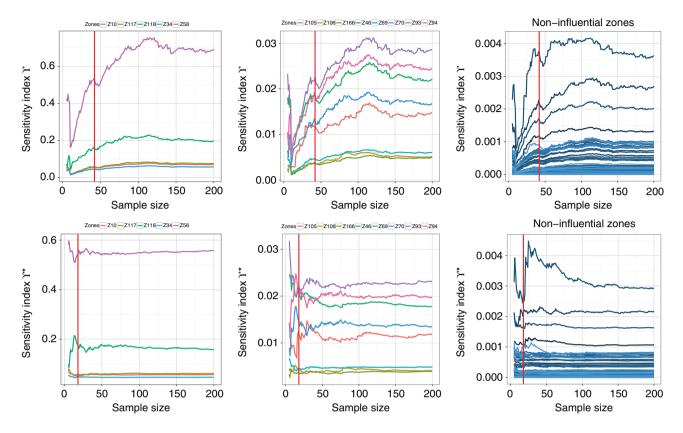
Figure 6

Convergence of the Υ_i and Υ_i^* indices estimates *versus* the sample size for the production watercut output after 20 years of production of the well 5. The red vertical line corresponds to the sample size when the stopping criterion (29) is reached.

TABLE 4

Estimated sensitivity indices for the production watercut output after 20 years of production of the well 5

Input	Total effect	Υ_i ($n = 42$)	Υ_i^* ($n = 18$)	Grid block position
Z58	0.625	0.528	0.542	[13:19;8:14;5]
Z118	0.133	0.158	0.176	[13:19;8:14;5]
Z117	0.066	0.059	0.051	[13:19;1:7;5]
Z10	0.058	0.055	0.058	[13:19;8:14;1]
Z34	0.035	0.045	0.047	[13:19;8:14;3]
Z93	0.022	0.022	0.022	[13:19;1:7;3]
Z94	0.014	0.019	0.021	[13:19;8:14;3]
Z46	0.021	0.018	0.021	[13:19;8:14;4]
Z70	0.014	0.013	0.015	[13:19;8:14;1]
Z105	0.005	0.012	0.012	[13:19;1:7;4]
Z69	0.009	0.005	0.004	[13:19;1:7;1]
Z106	0	0.004	0.004	[13:19;8:14;4]
Z166	0.009	0.004	0.004	[13:19;8:14;4]

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most important inputs. Concerning the input Z106, we notice a difference between the metamodel and the DGSM approach; it is not possible to conclude if this difference is due to an error in the metamodel or in the DGSM; however, the two approaches provide the same conclusions that the parameter Z106 can be considered as not influential. We can notice that for this reservoir model the values of Υ_i and Υ_i^* indices have the same magnitude for all selected inputs at the stopping criterion and the values of Υ_i are smaller than the estimated total effect, which is due to the underestimation of Υ_i indices at $n = 42$.

CONCLUSIONS AND DISCUSSIONS

In this work, we presented a new sequential screening method which is based on DGSM indices. We defined a new DGSM index Υ_i^* in order to have a stronger quantitative measure to define the non-influential inputs. We also used the QMC Sobol sequence sampling method, which allows an intelligent sequential estimation of the DGSM indices in order to reduce the number of model evaluations. We empirically showed, by applying to two analytical models and a reservoir synthetic test case, that the proposed screening method is efficient in detecting the non-influential inputs for an acceptable computational cost.

Computing DGSM indices requires model gradient estimation. A classical way to compute the derivatives is to use the finite-difference approximation method. However, this method suffers from the fact that the required number of model evaluations is equal to $n(d + 1)$, where d is the number of inputs and n the number of points where derivatives are estimated. Since a reservoir simulator evaluation is generally time-consuming, the finite-difference method is infeasible for models with a high number of inputs (roughly more than 20).

Therefore, it is clear that the ability to calculate derivatives efficiently is important for estimating DGSM indices within an acceptable computational cost. In the framework of reservoir simulation, different methods have been developed for more or less computationally efficient gradient calculation. In this paper, we utilized a reservoir simulator, which allows one to compute gradients using the direct method, also called in reservoir engineering the gradient simulator [27, 28]. This method is based on the solution of the governing analytical finite difference equations of flow, which automatically calculate the gradients during the simulation with an additional $\approx 33\%$ of the simulation time per each calculated gradient. Thus, the required number of model evaluations to estimate DGSM indices is $\approx n(d + 1)/3$. However, the

most efficient method to calculate the gradient of a functional with respect to the reservoir simulator parameters is the adjoint state method when this functional depends on those model parameters through state variables, which are the solution of the differential equations that define the problem. The advantage of this method compared with the gradient simulator method is that it consists of the computation of one unique extra linear system and the computation of the gradient with respect to the model parameters is equivalent to one evaluation of the simulator. In other words, it means that the computational cost of gradient calculation is independent of the number of model parameters. So, the required number of model evaluations to estimate DGSM indices is equal to $2n$. For more details on the mathematical aspect of the adjoint state method and its applications in reservoir simulation, we refer to [30-32].

In addition to further testing on reservoir models, using a reservoir simulator which allows one to compute gradients using the adjoint state method is a topic of future work.

ACKNOWLEDGMENTS

REFERENCES

1 Saltelli A., Sobol I. (1995) About the use of rank transformation in sensitivity of model output, *Reliability Engineering and System Safety* **50**, 225-239.

2 Saltelli A., Sobol I. (1999) A quantitative, model independent method for global sensitivity analysis of model output, *Reliability Engineering and System Safety* **41**, 1, 39-56.

3 Saltelli A., Chan K., Scott M. (2000) *Sensitivity analysis*, Wiley.

4 Sobol I.M. (1993) Sensitivity estimates for nonlinear mathematical models, *Mathematical Modelling and Computational Experiments* **1**, 407-414.

5 Blatman G., Sudret B. (2010) Efficient computation of global sensitivity indices using sparse polynomial chaos expansions, *Reliability Engineering and System Safety* **95**, 1216-1229.

6 Busby D., Farmer C.L., Iske A. (2007) Hierarchical nonlinear approximation for experimental design and statistical data fitting, *SIAM Journal on Scientific Computing* **29**, 1, 49-69.

7 Marrel A., Iooss B., Van Dorpe F., Volkova E. (2008) An efficient methodology for modeling complex computer codes with gaussian processes, *Computational Statistics and Data Analysis* **52**, 4731-4744.

8 Sacks J., Welch W.J., Mitchell T.J., Wynn H.P. (1989) Design and analysis of computer experiments, *Statistical Science* **4**, 409-435.

9 Santner T.J., Williams B.J., Notz W.I. (2003) *The design and analysis of computer experiments*, Springer.

10 Storlie C.B., Helton J.C. (2008) Multiple predictor smoothing methods for sensitivity analysis: Description of techniques, *Reliability Engineering and System Safety* **93**, 28-54.

11 Storlie C.B., Helton J.C. (2008) Multiple predictor smoothing methods for sensitivity analysis: examples results, *Reliability Engineering and System Safety* **93**, 57-77.

12 Storlie C.B., Swiler L.P., Helton J.C., Sallaberry C.J. (2009) Implementation and evaluation of nonparametric regression procedures for sensitivity analysis of computationally demanding models, *Reliability Engineering and Systems Safety* **94**, 11, 1735-1763.

13 Touzani S., Busby D. (2013) Smoothing spline analysis of variance approach for global sensitivity analysis of computer codes, *Reliability Engineering and System Safety* **112**, 67-81.

14 Morris M.D. (1991) Factorial sampling plans for preliminary computational experiments, *Technometrics* **33**, 161-174.

15 Sobol I.M., Kucherenko S. (2009) Derivative based global sensitivity measures and the link with global sensitivity indices, *Mathematics and Computers in Simulation* **79**, 3009-3017.

16 Sobol I.M., Kucherenko S. (2010) A new derivative based importance criterion for groups of variables and its link with global sensitivity indices, *Computer Physics Communications* **181**, 7, 1212-1217.

17 Campolongo F., Cariboni J., Saltelli A. (2007) An effective screening design for sensitivity analysis of large models, *Environmental Modelling and Software* **22**, 1509-1518.

18 Sobol I., Gresham A. (1995) On an alternative global sensitivity estimators, *Proceedings of SAMO 1995*, pp. 40-42.

19 Kucherenko S., Rodriguez-Fernandez M., Pantelides C., Shah N. (2009) Monte carlo evaluation of derivative-based global sensitivity measures, *Reliability Engineering and System Safety* **94**, 1135-1148.

20 Lamboni M., Iooss B., Popelin A.-L., Gamboa F. (2013) Derivative-based global sensitivity measures: General links with Sobol' indices and numerical tests, *Mathematics and Computers in Simulation* **87**, 45-54.

21 Sobol I.M. (1976) Uniformly distributed sequences with an additional uniform property, *USSR Computational Mathematics and Mathematical Physics* **16**, 5, 236-242.

22 Sobol I.M., Kucherenko S. (1998) On quasi-Monte Carlo integrations, *Mathematics and Computers in Simulation* **47**, 103-112.

23 McKay M.D., Beckman R.J., Conover W.J. (1979) Conover. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code, *Technometrics* **21**, 239-245.

24 Floris F.J.T., Bush M.D., Cuypers M., Roggero F., Syversveen A.R. (2001) Methods for quantifying the uncertainty of production forecasts-a comparative study, *Petroleum Geoscience* **7**, S87-S96.

25 PUNQS (1996) Production forecasting with uncertainty quantification, Website, URL http://www.fault-analysis-group. ucd.ie/Projects/PUNQ.html.

26 PumaFlow (2011) IFP Energies nouvelles reservoir simulator, URL http://www.openflowsuite.com/software/pumaflow.

27 Anterion F., Eymard R., Karcher B. (1989) Use of parameter gradients for reservoir history matching, *SPE Symposium on Reservoir Simulation*, Houston, Tx, 6-8 Feb., SPE 18433.

28 Killough J.E., Sharma Y., Dupuy A., Bissell R., Wallis J. (1995) A multiple right hand side iterative solver for history matching, *SPE Symposium on Reservoir Simulation*, San Antonio, Tx, 12-15 Feb., SPE 29119.

29 CougarFlow (2011) IFP Energies nouvelles uncertainty analysis software, URL http://www.openflowsuite.com/software/ cougarflow.

30 Eydinov D., Aanonsen S., Haukas J., Aavatsmark I. (2008) A method for automatic history matching of a compositional reservoir simulator with multipoint flux approximation, *Computational Geosciences* **12**, 2, 209-225.

31 Plessix R.-E. (2006) A review of the adjoint-state method for computing the gradient of a functional with geophysical applications, *Geophysical Journal International* **167**, 2, 495-503.

32 Rama Rao B., Mishra S. (1996) Adjoint sensitivity analysis for mathematical models of coupled nonlinear physical processes, *ModelCARE 96, International Conference on Calibration and Reliability in Groundwater Modelling*, Golden, 24-26 Sept.