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# TOOLS FOR GLOBAL AND TARGET SENSITIVITY ANALYSES IN THE CONTEXT OF HIGH-DIMENSIONAL THERMAL-HYDRAULIC NUMERICAL EXPERIMENTS

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## ABSTRACT

In nuclear engineering, the quantification of the input uncertainties and their propagation through high-fidelity computer models in order to estimate relevant statistical quantities of interest constitute the core phases of the so-called “best-estimate plus uncertainty” (BEPU) methodology. However, several methodological and numerical issues can make the BEPU methodology difficult to execute in practice, and in particular, the large number (e.g., up to one hundred in our case) of uncertain input variables. Recently, an advanced BEPU methodology, called ICSCREAM, has been proposed for the identification of penalizing configurations in high-dimensional framework. The present work aims to detail the first step of the ICSCREAM method which consists in identifying and ranking the primary influential inputs. For this purpose, global and target sensitivity analyses based on dependence measures are performed. Their principles and estimation techniques are explained, as well as their pragmatic implementation. Their use is then illustrated on an industrial use case simulating an intermediate-break loss-of-coolant accident via the CATHARE2 simulator.

## 1. INTRODUCTION

Uncertainty quantification techniques [6] are gaining an increasing attention in the field of nuclear engineering, not only to assess the reliability and safety of nuclear power plants (e.g., for pressurized water reactors), but also to provide robust methodological tools to better identify the safety margins. The “best-estimate plus uncertainty” (BEPU) methodologies [11] are now used to complete and enhance the deterministic analyses already performed. As an example, one can mention the various safety analyses performed for accident scenarios such as the *intermediate-break loss-of-coolant accident* (IBLOCA), requiring best-estimate thermal-hydraulic numerical experiments obtained with validated simulation codes. In France, for IBLOCA studies, the CATHARE2 simulator (developed by CEA, EDF, Framatome and IRSN) is used to simulate the transients and a BEPU methodology, named “CathSBI” (Cathare Statistical Intermediate Break) is then applied to assess the safety margins [2].

Several practical challenges of such a BEPU methodology may arise: firstly, the number of input parameters that have to be treated can be large (e.g., around a hundred parameters); secondly, these parameters can be of different nature (e.g., initial/boundary conditions, model parameters, scenario parameters) and might require different statistical treatment regarding their nature and

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regulatory requirements; thirdly, the uncertainty propagation through the best-estimate computer model can be difficult as the code is often complex, strongly nonlinear and costly-to-evaluate; and fourthly, the *quantity of interest* (QoI) is often a statistical risk measure (e.g., a high-order quantile) estimated from a limited number of output realizations. In such a context, it is widely recognized that *global sensitivity analysis* (GSA) [6] can play a key role in the BEPU methodology to identify the most influential inputs which constitute the effective input dimension as they strongly influence the variability of the model output (see for example [9]). Furthermore, due to the nature of the QoI (i.e., a high-order quantile far in the right tail of the output distribution), dedicated tools have to be used to perform *target sensitivity analysis* (TSA). Finally, the use of metamodeling techniques is another powerful tool to reduce the computational cost and to allow a better management of the numerical experiments in the context of complex and costly-to-evaluate computer models [6].

From this perspective, a new methodology, called “ICSCREAM” (pronounced “ice-cream”, for “Identification of penalizing Configurations using SCREening And Metamodel”) is proposed in [10] to handle several of these issues and to enhance the first part of the CathSBI methodology [2]. The ICSCREAM method relies mainly on two parts: a first one whose aim is to use both GSA and TSA to achieve screening and ranking of the most influential inputs; and a second one whose aim is to build, based on the first part, a Gaussian process metamodel so as to facilitate the uncertainty propagation for finding the penalizing configurations. The present paper aims at detailing the first part only. For more information about the whole methodology, the interested reader is invited to refer to [10].

*Screening* aims at qualitatively separating the inputs into two groups: the significantly influential ones vs. the noninfluential ones. The first group, called here “*primary influential inputs*” (PII), constitute the effective input dimension as they influence the variability of the model output. As for *ranking*, it aims at providing a quantitative measure of this influence, in order to sort the PII by order of influence. Among several GSA methods available in literature, a recent emphasis has been put over the use of the *Hilbert-Schmidt Independence Criterion* (HSIC) which led to define a sensitivity index which measures the statistical dependence between the model output and each input under consideration [3]. The aim of the present paper is to provide more insights about the theoretical tools involved in such an analysis, to describe their practical use and illustrate their application on an industrial use case.

Thus, the main objectives of this paper can be listed as follows:

- (O1) Identify the PII w.r.t. the model output and the QoI using screening;
- (O2) Rank the PII according to their relative importance on the model output and the QoI.

However, these two objectives have to be achieved under the following core constraint:

- (C1) Only a single (finite) Monte Carlo learning sample containing a set of input-output realizations of the complex computer model is available.

This paper is organized as follows: Section 2 aims at presenting the core concepts and algorithms used to perform GSA and TSA using HSIC. Section 3 details the proposed methodology and specifies the novelty of the approach. Section 4 aims at presenting a detailed application to an industrial IBLOCA case. Finally, Section 5 draws a few conclusions and perspectives.

## 2. SENSITIVITY ANALYSIS VIA HILBERT-SCHMIDT INDEPENDENCE CRITERION

### 2.1 Notation

Mathematically, a standard BEPU study can be modelled by assuming a deterministic input-output best-estimate computer model  $\mathcal{M}(\cdot)$  given by:

$$\mathcal{M} : \begin{cases} \mathcal{X} & \longrightarrow \mathcal{Y} \\ \mathbf{X} & \longmapsto Y = \mathcal{M}(\mathbf{X}). \end{cases} \quad (1)$$

It is assumed that the methodology proposed in this paper is non-intrusive w.r.t. the model. The uncertain inputs are supposed to be independent and are treated in a probabilistic framework by assuming, first, a probability space  $(\Omega, \mathcal{A}, \mathbb{P})$ . The inputs are gathered in a  $d$ -dimensional random vector  $\mathbf{X} := (X_1, X_2, \dots, X_d)^\top$  distributed according to a continuous joint probability distribution  $P_{\mathbf{X}} := \prod_{i=1}^d P_{X_i}$  over a measurable space  $\mathcal{X} := \times_{i=1}^d \mathcal{X}_i$  with  $\mathcal{X} \subseteq \mathbb{R}^d$ . For each realization of the input vector  $\mathbf{X}(\omega)$ , denoted by  $\mathbf{x} = (x_1, x_2, \dots, x_d)^\top \in \mathbb{R}^d$ , an observed scalar output value  $y = \mathcal{M}(\mathbf{x})$  is obtained. Thus, by propagating the uncertainties through  $\mathcal{M}(\cdot)$ , one can assume a probabilistic structure for the output which is a random variable characterized by a distribution  $P_Y$  over a measurable space  $\mathcal{Y} \subseteq \mathbb{R}$ .

Finally, to stick with constraint **(C1)**, one supposes that only a limited number of simulations are available for the study. Moreover, these samples are obtained via crude Monte Carlo (CMC) sampling. Thus, the *learning sample* used in the following is a  $n$ -sample of the couple  $(\mathbf{X}, Y)$  given by:

$$\left( \mathbf{X}^{(j)}, Y^{(j)} \right)_{(1 \leq j \leq n)} = \left( X_1^{(j)}, X_2^{(j)}, \dots, X_d^{(j)}, Y^{(j)} \right)_{(1 \leq j \leq n)} \quad (2)$$

with  $P_{\mathbf{X}^{(j)}} = P_{\mathbf{X}}$ , meaning that the realizations are *independent and identically distributed* (i.i.d.) and  $Y^{(j)} = \mathcal{M} \left( X_1^{(j)}, X_2^{(j)}, \dots, X_d^{(j)} \right), \forall j \in \{1, \dots, n\}$ .

### 2.2 Global sensitivity analysis using HSIC-based indices

GSA aims at providing several tools to analyze the behavior of computer models and to track the effects of the inputs on the output variability [6]. Among several indices, one can mention the well-known Sobol indices based on the output variance decomposition. However, Sobol indices suffer from a few drawbacks such as a high computational cost and a lack of relevance for tracking other types of influence than those based on the output variance. Thereafter, various authors investigated the use of “distributional” or “moment-independent” approaches to derive sensitivity indices. However, these indices still suffer from a high computational cost which can be cumbersome for complex computer codes.

Recently, a few authors proposed to adopt another point of view: quantifying the impact of each input  $X_i$  on the output  $Y$  by means of a well-chosen *dependence measure*. This idea, originally proposed in the machine learning community by [8], has been brought to the GSA community with the work from [3]. More specifically, [3] proposed to use the *Hilbert-Schmidt Independence Criterion* (HSIC) to measure and test the dependence between the output  $Y$  and an input  $X_i$ . To do so, one will use a generalization of the notion of covariance between two random variables, by considering the covariance between nonlinear transformations of  $X_i$  and  $Y$ .

Formally, one needs to define a few core mathematical ingredients to properly present the HSIC. Suppose  $\mathcal{X}_i, \forall i \in \{1, \dots, d\}$  and  $\mathcal{Y}$  are measurable spaces. Let  $\mathcal{F}_i : \mathcal{X}_i \rightarrow \mathbb{R}$  and  $\mathcal{G} : \mathcal{Y} \rightarrow \mathbb{R}$  be two universal *reproducing kernel Hilbert spaces* (RKHS) [13]. These functional spaces are equipped with their *characteristic kernels*: respectively,  $\kappa_i(\cdot, \cdot)$  and  $\kappa(\cdot, \cdot)$ . These characteristic kernels (e.g., Gaussian, exponential) present fundamental properties which enable a unique representation in the RKHS embedding [5]. Together with Hilbert spaces come the scalar products given by  $\langle \cdot, \cdot \rangle_{\mathcal{F}_i}$  and  $\langle \cdot, \cdot \rangle_{\mathcal{G}}$ . Under these hypotheses, one can consider the generalized *cross-covariance* operator  $C_{(X_i, Y)}[\cdot]$  given, for any functions  $f \in \mathcal{F}_i$  and  $g \in \mathcal{G}$ , by:

$$\langle f, C_{(X_i, Y)}[g] \rangle_{\mathcal{F}_i} = \text{Cov}(f(X_i), g(Y)) \quad (3)$$

which generalizes the notion of covariance between  $X_i$  and  $Y$ . Therefore, a larger panel of input-output dependency can be captured by this operator.

As a consequence, the HSIC measure can be theoretically defined as follows:

$$\text{HSIC}(X_i, Y)_{\mathcal{F}_i, \mathcal{G}} = \|C_{(X_i, Y)}\|_{\text{HS}}^2 = \sum_{l, m} \langle u_l, C_{(X_i, Y)}[v_m] \rangle_{\mathcal{F}_i} \quad (4)$$

where  $(u_l)_{l \geq 0}$  and  $(v_m)_{m \geq 0}$  are orthonormal bases of, respectively,  $\mathcal{F}_i$  and  $\mathcal{G}$ . However, due to the relevant property of universality of the two underlying RKHSs, this approach exhibits a mathematical trick, known as the “kernel trick” [3], which implies that computing a distance between the two probability distributions only requires to know the kernels  $\kappa_i(\cdot, \cdot)$  and  $\kappa(\cdot, \cdot)$ . Thus, one can show that the HSIC measure can be written, in an equivalent manner, using expected values of kernels:

$$\begin{aligned} \text{HSIC}(X_i, Y)_{\mathcal{F}_i, \mathcal{G}} &= \mathbb{E} \left[ \kappa_i(X_i, X'_i) \kappa(Y, Y') \right] + \mathbb{E} \left[ \kappa_i(X_i, X'_i) \right] \mathbb{E} \left[ \kappa(Y, Y') \right] \\ &\quad - 2 \mathbb{E} \left[ \mathbb{E}[\kappa_i(X_i, X'_i) | X_i] \mathbb{E}[\kappa(Y, Y') | Y] \right] \end{aligned} \quad (5)$$

where  $(X'_i, Y')$  is an i.i.d. copy of  $(X_i, Y)$ . This last equation highlights interesting estimation properties since it only involves expected values which are simpler to estimate than variances of conditional expected values (such as in the Sobol indices). A fundamental property directly arises if and only if one uses characteristic kernels:

$$\text{HSIC}(X_i, Y)_{\mathcal{F}_i, \mathcal{G}} = 0 \Leftrightarrow X_i \perp Y \quad (6)$$

which means that  $X_i$  and  $Y$  are independent. This property makes this measure naturally relevant for GSA purposes as the independence corresponds to the nullity of the measure, which indicates that  $X_i$  does not influence  $Y$  at all. Finally, another fundamental property which makes it relevant for high-dimensional GSA is that it does not depend on the input dimension  $d$ .

A common estimator proposed by [8] (and based on V-statistics, i.e., meaning that it is biased but asymptotically unbiased) is given by:

$$\widehat{\text{HSIC}}(X_i, Y) = \frac{1}{n^2} \text{Tr}(L_i H L H) \quad (7)$$

where  $L_i = \left( \kappa_i \left( X_i^{(j_1)}, X_i^{(j_2)} \right) \right)_{1 \leq j_1, j_2 \leq n}$  and  $L = \left( \kappa \left( Y^{(j_1)}, Y^{(j_2)} \right) \right)_{1 \leq j_1, j_2 \leq n}$  are two Gram matrices, and  $H = \left( \delta_{j_1, j_2} - \frac{1}{n} \right)_{1 \leq j_1, j_2 \leq n}$  a shift matrix, with  $\delta_{j_1, j_2}$  the Kronecker operator (which gives 1 if  $j_1 = j_2$ , 0 otherwise).

A second estimator, cheaper than the first one, adapted from [15] by [4], is given by:

$$\widehat{\text{HSIC}}(X_i, Y) = \frac{1}{n^2} \sum_{j_1, j_2}^n A_{j_1 j_2} B_{j_1 j_2} \quad (8)$$

where  $A_{j_1 j_2} = (L_i)_{j_1 j_2} - (L_i)_{j_1 \cdot} - (L_i)_{\cdot j_2} + (\bar{L}_i)_{\cdot \cdot}$  and  $B_{j_1 j_2} = L_{j_1 j_2} - L_{j_1 \cdot} - L_{\cdot j_2} + (\bar{L})_{\cdot \cdot}$  are linear combinations of Gram matrices such that,  $\forall M \in \mathcal{M}_n(\mathbb{R})$ , one gets  $M_{j_1 \cdot} = n^{-1} \sum_{j_2=1}^n M_{j_1 j_2}$ ,  $M_{\cdot j_2} = n^{-1} \sum_{j_1=1}^n M_{j_1 j_2}$  and  $\bar{M}_{\cdot \cdot} = n^{-2} \sum_{j_1=1}^n \sum_{j_2=1}^n M_{j_1 j_2}$ . In the following, this estimator will be the one used in practice for the numerical experiments.

Finally, [3] proposed to build a plug-in estimator to produce a normalized sensitivity index allowing a better interpretation. This index is given by:

$$\widehat{R}_{\text{HSIC}, i}^2 = \frac{\widehat{\text{HSIC}}(X_i, Y)}{\sqrt{\widehat{\text{HSIC}}(X_i, X_i) \widehat{\text{HSIC}}(Y, Y)}}. \quad (9)$$

As a last remark, one would like to insist on the following technical detail. As stated before, HSIC-based indices rely on an a priori choice of characteristic kernels for the inputs and the output. The most famous characteristic kernel for a real variable is the Gaussian one which is given by (assuming  $x$  and  $x'$  two i.i.d. samples):

$$\kappa(x, x') = \exp \left( -\theta \left\| x - x' \right\|_2^2 \right) \quad (10)$$

with  $\theta = 1/\sigma^2$  ( $\sigma^2$  being the empirical variance of the sample  $x$ ). If the choice of the type of the kernel does not fundamentally influence the results (as soon as they are characteristic kernels), the estimation of  $\theta$  might influence the values of the estimated HSIC measures and the  $\widehat{R}_{\text{HSIC}}^2$  estimates (often used for ranking).

As a conclusion, the HSIC seems to be a relevant tool to achieve GSA, and especially for screening purposes. In the following, one will see how one can provide a robust procedure to perform screening with HSIC measures.

### 2.3 Statistical tests for screening with HSIC-based indices

Using HSIC measures for screening purposes has been proposed by [4]. Screening consists in separating, in a qualitative manner, the inputs between two distinct groups: the noninfluential ones vs. the others (which are influential with various intensities) [6]. HSIC measures seem well dedicated for this task as their fundamental property is the equivalence between independence and the nullity of the measure. Thus, zero-valued HSIC measures indicate independence and correspond to statistically noninfluential inputs.

However, from the estimation point of view, one should keep in mind that, in practice, HSIC measures are computed from a finite set of realizations. The estimates might fluctuate, and get

values which are close to zero, but not properly equal to zero. As shown by [4], this framework can benefit from the theory of statistical hypothesis testing in order to strengthen the decision process. Indeed, starting back from the fundamental property of the HSIC, one can build the following statistical test  $\mathcal{T}$ :

$$\mathcal{T} : \text{Test } "(\mathcal{H}_{0,i}) : \text{HSIC}(X_i, Y) = 0" \quad \text{vs.} \quad "(\mathcal{H}_{1,i}) : \text{HSIC}(X_i, Y) > 0". \quad (11)$$

As a natural *test statistic*, one can choose  $\widehat{S}_{\mathcal{T}} := n \times \widehat{\text{HSIC}}(X_i, Y)$ . Finally, the decision process is driven by the *p-value*, which is the probability, under  $(\mathcal{H}_{0,i})$ , that  $\widehat{S}_{\mathcal{T}}$  becomes greater or equal to the observed  $\widehat{S}_{\mathcal{T},\text{obs}}$  statistic on the learning sample. Formally, one reads:

$$p_{\text{val}} = \mathbb{P} \left( \widehat{S}_{\mathcal{T}} \geq \widehat{S}_{\mathcal{T},\text{obs}} \mid \mathcal{H}_{0,i} \right). \quad (12)$$

To discriminate, one uses the *significance level*  $\alpha$  (also known as ‘‘Type I error’’, corresponding to an error of rejecting the null hypothesis  $(\mathcal{H}_{0,i})$  when it is true). This significance level is often fixed at  $\alpha = 0.05$  (or  $\alpha = 0.10$ ). Finally, the decision rule is given by: if  $p_{\text{val}} < \alpha$ , then  $(\mathcal{H}_{0,i})$  (i.e., the independence) is rejected, which means that the input is influential.

HSIC-based independence statistical tests can be split into two different cases depending on the size of the learning sample (i.e., depending on whether the asymptotic regime is reached or not). Under asymptotic convergence (i.e., when  $n$  is sufficiently large), it can be proved that the asymptotic law of the  $n \times \widehat{\text{HSIC}}(X_i, Y)$  estimator can be reasonably approached by a *Gamma distribution* parametrized by shape and scale parameters  $(\gamma, \beta)$ . The reader can refer to [7] and [4] for more details on  $(\gamma, \beta)$  and their estimation. This asymptotic property can be used to build a class of dedicated tests, called *asymptotic tests*. For an asymptotic test  $\mathcal{T}_{\text{asympt}}$ , the p-value can be approximated as follows:

$$p_{\text{val}} \approx 1 - F_{\text{Ga}} \left( n \times \widehat{\text{HSIC}}(X_i, Y)_{\text{obs}} \right) \quad (13)$$

where  $F_{\text{Ga}}(\cdot)$  is the CDF of the Gamma distribution and  $\widehat{\text{HSIC}}(X_i, Y)_{\text{obs}}$  is the observed value of the random variable  $\widehat{\text{HSIC}}(X_i, Y)$ .

In the non-asymptotic framework (i.e., when  $n$  is rather small), the Gamma approximation cannot be used anymore without introducing a strong bias. Therefore, *permutation-based tests* can be used instead [4]. A permutation-based test  $\mathcal{T}_{\text{perturb}}$  can be summarized by the following procedure:

- Let  $Z_n := \left( X^{(j)}, Y^{(j)} \right)_{(1 \leq j \leq n)}$  be the initial learning sample, and  $\widehat{\text{HSIC}}(Z_n)$  the corresponding HSIC estimator.
- Let  $\{\tau_1, \dots, \tau_B\}$  a set of  $B$  independent random permutations of  $\{1, \dots, n\}$ , uniformly distributed, and independent of  $Z_n$ .
- For each  $\tau_b$  ( $b = 1, \dots, B$ ), consider the permuted sample  $Z_n^{\tau_b} = \left( X^{(j)}, Y^{(\tau_b(j))} \right)_{(1 \leq j \leq n)}$  and estimate the following statistic  $\widehat{H}^{*b} := \widehat{\text{HSIC}}(Z_n^{\tau_b})$ .
- Under  $(\mathcal{H}_{0,i})$ ,  $Z_n^{\tau_b}$  ( $\forall b \in \{1, \dots, B\}$ ) and  $Z_n$  are identically distributed. Thus,  $\widehat{H}^{*b}$  ( $\forall b \in \{1, \dots, B\}$ ) and  $\widehat{\text{HSIC}}(X, Y)$  are also identically distributed. Consequently, one can consider

the order statistic associated to the sample  $\{\widehat{H}^{*1}, \widehat{H}^{*2}, \dots, \widehat{H}^{*B}\}$  :

$$\widehat{H}^{*(1)} \leq \widehat{H}^{*(2)} \leq \dots \leq \widehat{H}^{*(B)} \quad (14)$$

where brackets for the exponents denotes the order.

- Therefore, the p-value can be approximated as follows:

$$p_{\text{val}} \approx \frac{1}{B} \sum_{b=1}^B \mathbb{1}_{\widehat{H}^{*b} > \widehat{\text{HSIC}}(X, Y)}. \quad (15)$$

As a conclusion, one can keep in mind that two distinct statistical tests (asymptotic vs. permutation-based) are available to perform a robust screening with HSIC measures. However, some variables which could have a very localized impact over some specific region of the output space, might not be detected by the test (corresponding to a ‘‘Type II error’’). Therefore, in the context of safety analysis, complementary tools have to be considered to ensure the robustness of the screening phase.

## 2.4 Target sensitivity analysis using HSIC-based indices

If the word ‘‘*target*’’ in TSA has been first introduced by [12], one can consider that a large panel of TSA methods have already been proposed before, especially in the structural reliability community (see, e.g., [1] for a recent review about these methods). The basic idea of TSA is to measure the influence of the inputs on a *critical domain* of the model output (typically, in the tail of the distribution). In particular, one could be interested in analyzing the most influential inputs that lead to the occurrence of the critical phenomenon [12]. Thus, TSA focuses on specific QoIs such as rare event probabilities, quantiles or any other risk measures.

Formally, a critical domain of interest can be modeled as a subset  $\mathcal{C} \subset \mathcal{Y}$  such that  $\mathbb{P}(Y \in \mathcal{C})$  is small. Let  $Y \rightarrow \mathcal{R}(Y)$  be a generic risk measure. Then, for a risk analysis, one can consider that the critical event corresponds to getting an output value beyond, e.g., the 90%-order quantile of  $Y$  denoted  $q_{0.9}(Y)$ . Finally, one has  $\mathcal{C} = \{y \in \mathcal{Y} \mid y \geq \mathcal{R}(y)\}$  with  $\mathcal{R}(Y) = q_{0.9}(Y)$ . To perform TSA, one needs to get a measure of occurrence of such a critical event. A first possible measure is the indicator function  $\mathbb{1}_{\mathcal{C}} : \mathcal{Y} \rightarrow \{0, 1\}, y \mapsto 1$  if  $y \in \mathcal{C}$ , 0 otherwise.

In the specific context of HSIC measures, the idea is to apply a ‘‘thresholding transformation’’ to the output. Several transformations can be considered, from indicator-thresholding in [3, 14] to smoother thresholding transformations. The choice of the transformation might impact the choice of the kernel (e.g., for indicator-thresholding, one should use the linear kernel since the output becomes a binary variable [14]). However, when focusing on a high-order quantile, only a few samples of  $Y$  might be relevant regarding a binary thresholding, leading to a significant loss of information, especially for samples which are close to the threshold. In the context of risk analysis, one would prefer to improve conservatism of the statistical procedures. Thus, in the following, one uses a weighted thresholding transformation proposed by [12]. The weight function is defined as follows:

$$w_{\mathcal{C}} : \begin{cases} \mathcal{Y} & \longrightarrow [0, 1] \\ y & \longmapsto w_{\mathcal{C}}(y) = \exp\left(-\frac{\max(q_{0.9}(Y) - y, 0)}{s \sigma_Y}\right) \end{cases} \quad (16)$$



with  $s = \frac{1}{5}$  a smoothness parameter which can be tuned [12] and  $\sigma_Y$  the empirical estimation of the standard deviation of  $Y$ . The underlying idea of such a function is to provide a measure that preserves the contribution of the samples which are close to the critical domain and makes the other vanish smoothly. Finally, the target HSIC measure (named “T-HSIC” in the following) is defined such that:

$$\text{T-HSIC}_i := \text{HSIC}(X_i, w_{\mathcal{E}}(Y)). \quad (17)$$

In the following, T-HSIC measures will be estimated with the same type of estimator as the HSIC.

### 3. COUPLING GSA AND TSA FOR BOTH SCREENING AND RANKING USING INDEPENDENCE STATISTICAL TESTS

This section aims at highlighting the core contribution of this work: extending the statistical hypothesis testing framework to T-HSIC and, jointly, extending the screening phase with a ranking one.

One can first recall the two objectives of this paper: **(O1)** – *Identify the PII w.r.t. the model output and the QoI using screening* and **(O2)** – *Rank the PII according to their relative importance on the model output and the QoI*. However, one has to deal with the constraint which is **(C1)** – *Require a single CMC learning sample of input-output realizations*.

As a preliminary remark, one should keep in mind that both screening and ranking phases here do not imply any final dimension reduction. Indeed, this paper deals with the first step of the ICSCREAM methodology [10] which only aims at identifying and ranking the PII. These inputs will be the ones that will drive the metamodeling building phase. As for the other inputs (the noninfluential ones), they will be used as a residual in the metamodeling but they will not be fixed at deterministic values such as it could be in more standard GSA studies. Consequently, both screening and ranking are not crucial phases that could lead to dramatic consequences in terms of model bias.

Regarding **(O1)**, identifying the PII w.r.t. to the model output can be achieved using HSIC-based screening coupled with statistical hypothesis testing. The extension to the specific QoI such as a high-order quantile can be achieved by extending the statistical tests to the T-HSIC measure, which constitute the first contribution of this paper.

Regarding **(O2)**, i.e., the qualitative ranking of the influential inputs, one needs to extend the previous tools established for screening. It is proposed here to use the p-values as a tool for ranking since they provide a sort of “distance” to the independence.

Finally, concerning **(C1)**, one should notice that both HSIC and T-HSIC measures are perfectly dedicated to deal with such a finite CMC input-output sample. Moreover, such a constraint arises in many industrial applications for which only a few number of model evaluations are available, or for which only pure Monte Carlo analyses can be performed for technical and/or regulatory reasons.

The proposed methodology can be summarized into three steps:

- **Step #1:** Apply a {GSA + Independence Tests} strategy to perform a GSA-oriented screening using HSIC measures.

- **Step #2:** Extend the use of statistical tests to T-HSIC estimators to apply a {TSA + Independence Tests} strategy. Thus, perform a TSA-oriented screening.
- **Step #3:** Aggregate GSA and TSA results by considering the union of results with priority given to the TSA results for conservatism reasons.

In practice, this methodology relies on a few set of rules for screening and ranking which are detailed hereafter:

- **About the nature of the test:** if  $n$  is large ( $n > n_{th}$ ), use an asymptotic test; if not ( $n \leq n_{th}$ ), use a permutation-based test.
- **About the p-values:** the lower  $p_{val}$ , the stronger ( $\mathcal{H}_{0,i}$ ) is rejected and the higher the influence of  $X_i$ .
- **About screening:** the influential inputs are those associated to a p-value such that  $p_{val} < \alpha$ .
- **About ranking:** the most influential inputs have the lowest p-values. If p-values are equal, the inputs are ordered using their  $R_{HSIC}^2$  indices.
- **About aggregating:** finally, the PII correspond to the union of the influential inputs kept from both GSA- and TSA-oriented screening phases. Their ranking correspond to the previous rule applied to this set of PII.

As a final remark, one should notice that this methodology only depends on three tuning parameters which have to be set: the sample size threshold  $n_{th}$  which determines whether the asymptotic regime is reached or not; if not, the number of permutations  $B$  has to be chosen; and the significance level of the test  $\alpha$ .

In the following section, this whole methodology is applied to a realistic industrial use case concerning thermal-hydraulic simulations in nuclear accident simulation context.

## 4. APPLICATION TO A THERMAL-HYDRAULIC USE CASE

### 4.1 Presentation of the use case

This use case consists in simulating a loss-of-coolant accident appearing in the primary circuit of a pressurized water reactor. The break in the piping structure is supposed to be of intermediate size. Due to this accident, a thermal-hydraulic transient happens, leading to an increase of the temperature into the core, especially, at the cladding level. During this process, several uncertainty sources can be identified. Thus, a dedicated BEPU methodology has been defined for this specific IBLOCA scenario [2]. Note that the present use case differs from the one presented in [10].

Numerically, the CATHARE2 (V2.5\_3mod3.1) simulator, which is a thermal-hydraulic system code, is used to generate high-fidelity thermal-hydraulic transients. The physical inputs of this best-estimate code are, typically, critical flowrates, interfacial friction coefficients, condensation and heat transfer coefficients, but also some initial/boundary conditions. The dimension of the input vector is  $d = 97$  here. A set of marginal probability distributions are assumed for the uncertain inputs (mainly, uniform, log-uniform, normal and log-normal distributions). These distributions

are either estimated from industrial/experimental datasets, calibrated from inverse problems, or elicited from expert judgment.

Basically, the study consists first to propagate the uncertainties through the CATHARE2 simulator so as to get a learning sample. This input-output dataset consists in a CMC experimental design of  $n_{\text{tot}} = 2988$  simulations drawn according to the marginal distributions. The empirical distribution of the output variable of interest, which is here the 2<sup>nd</sup> *peak of cladding temperature* (PCT), is plotted in Figure 1a. From a risk analysis perspective, one is interested in estimating the 90%-order quantile of the PCT. Here, the empirical quantile estimated from the whole dataset is  $\hat{q}_{0.9} = 668^\circ\text{C}$ . Figure 1b illustrates the convergence of the empirical estimation (together with bootstrap to get confidence intervals) through the first  $n = 500$  simulations. It can be seen that only a few hundred of samples are sufficient to estimate  $\hat{q}_{0.9}$  with enough accuracy.

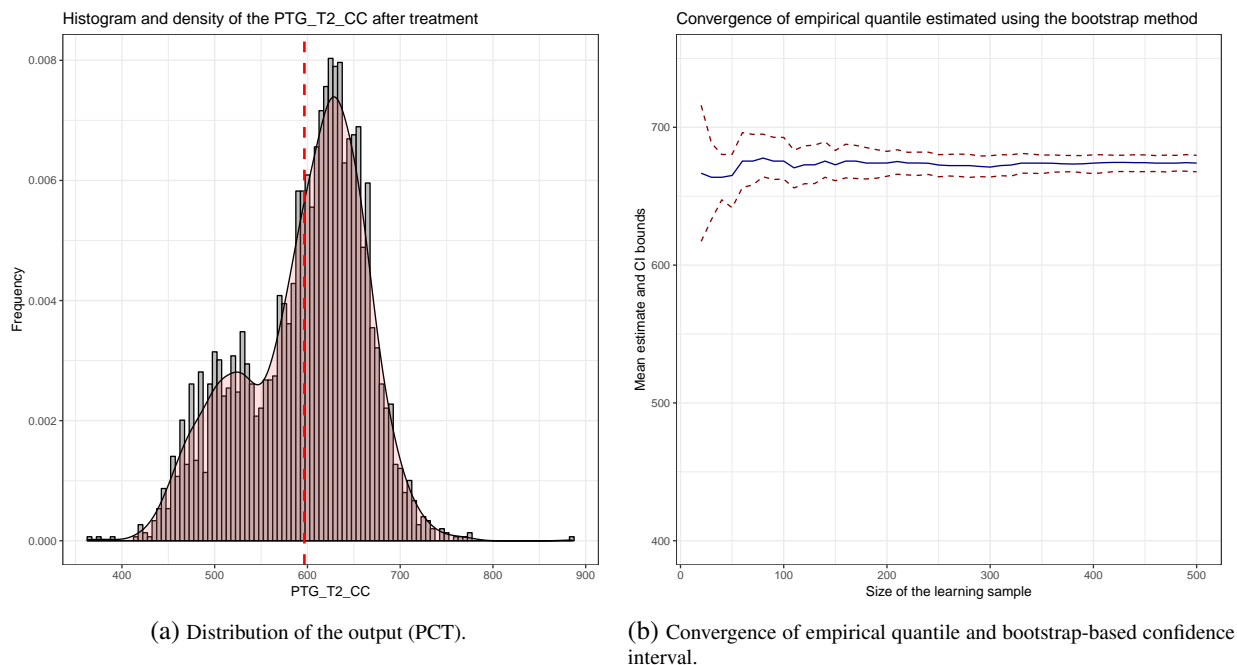


Figure 1 – Output statistics of interest.

## 4.2 Numerical results

Before presenting the HSIC-based results, one can first investigate basic relationships between a few inputs and the model output with the help of *scatter plots*. As an illustration, Figure 2a highlights the significant and nonlinear influence of input  $X_{15}$  while the scatterplot according to  $X_{47}$ , given by Figure 2b, seems to indicate that this latter input has little influence on the model output.

The methodology detailed in Section 3 is now applied to this 97-dimensional IBLOCA use case. Again, the goal here is to perform both screening and ranking. Two analyses are considered: a GSA-oriented one and a TSA-oriented one. For TSA, the critical event to be characterized is the occurrence of very large values of the PCT. Thus, with  $Y := \text{PCT}$ , one is interested in the specific event of the type  $Y > \hat{q}_{0.9}(Y)$ .

For the sake of conciseness, only a single study is presented here. Indeed, with  $n_{\text{tot}} = 2988$  sim-

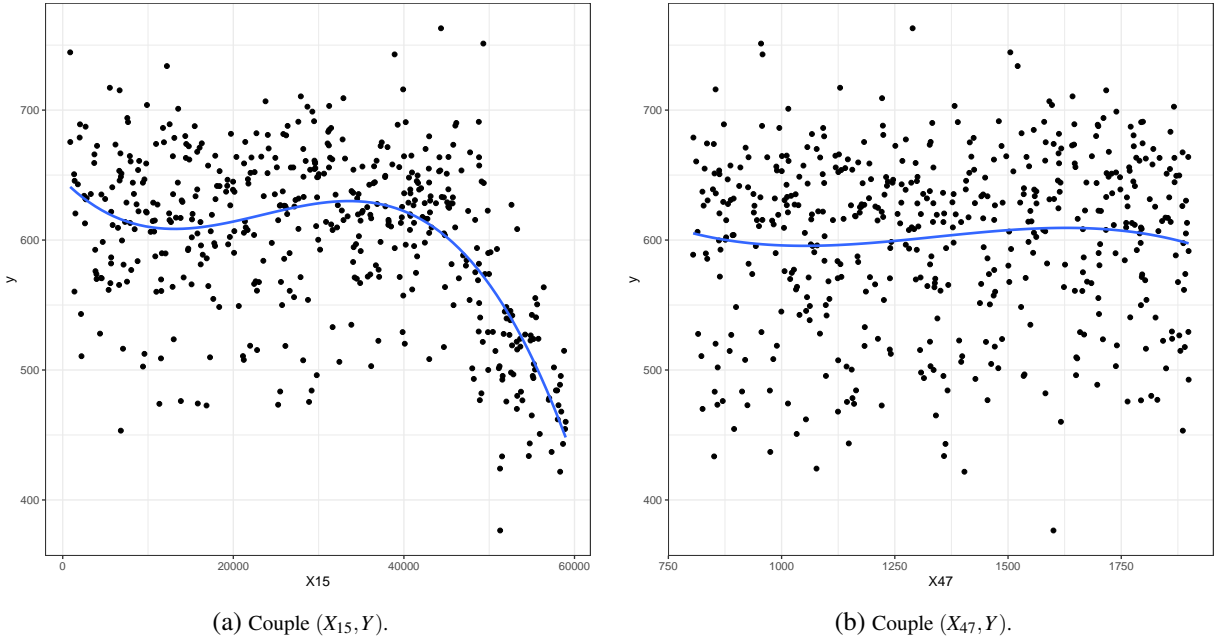


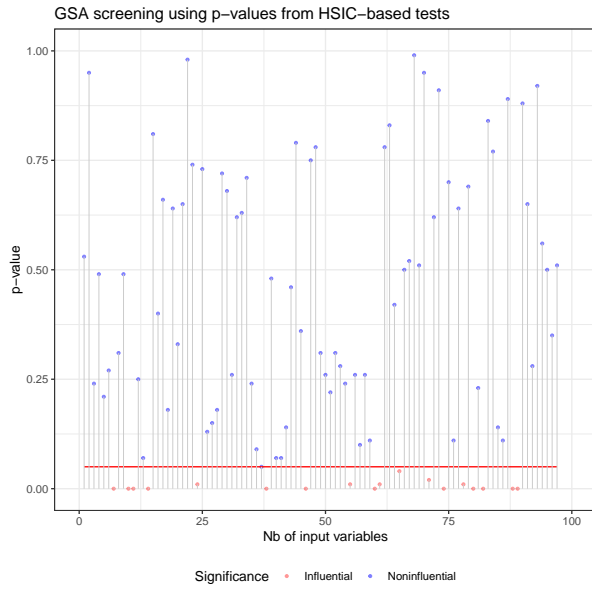
Figure 2 – Scatter plots with splines.

ulations, it has been chosen to illustrate the methodology here with a reduced dataset made of only  $n = 500$  samples. The idea is to illustrate the potential of the methodology under very limited simulation budget. In such a context, one will consider that the asymptotic regime is not valid. Therefore, the use of permutation-based tests is a necessity. In the following, the tuning parameters are set to  $B = 200$  permutations and  $\alpha = 0.05$  for the significance level.

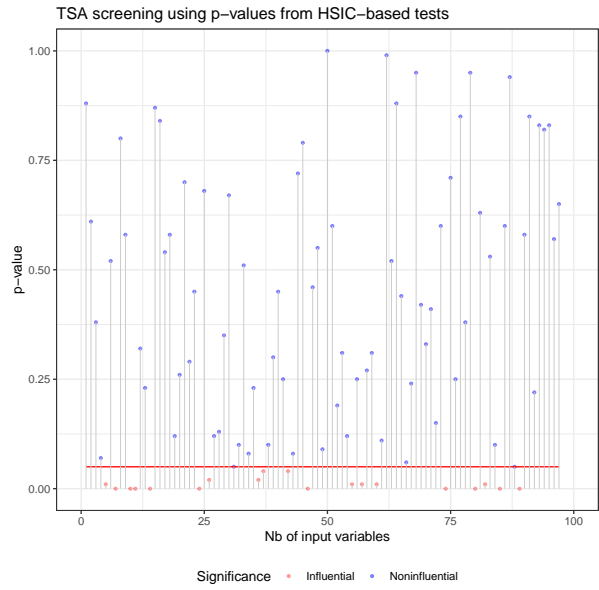
The GSA-oriented screening shown in Figure 3a illustrates the basic principles of the decision process based on p-values. The lower the p-value, the stronger  $(\mathcal{H}_{0,i})$  (i.e., the independence) is rejected. Thus, variables that are below the redline (corresponding to  $\alpha = 0.05$ ) correspond to influential variables. By comparing this plot to the one shown in Figure 3b, one can notice that the influential variables differ from the previous ones. This clearly highlights the necessity of dedicated tools to achieve TSA. As for the choice of the significance level, it is clear that choosing  $\alpha = 0.10$  would change the threshold, and thus, the number of “influential” variables. However, one should insist here on the core problem of this study: detecting the noninfluential variables, not to remove them, but just to help for the metamodel building phase. Again, these results are relative and do not imply any model simplification. As a remark, one should notice that, for the sake of conciseness, a deeper study about the sensitivity of such a methodology to the prior choice of various parameters (e.g., the quality of the quantile estimation, the choice of the significance level, the kernel parameters for HSIC measures and the weight function for TSA) is not achieved here and is left for future work.

Considering ranking purposes, Figure 4a provides a relative ranking of the most influential inputs w.r.t. to their p-values. Similarly, Figure 4b provides another insight about the most influential variables w.r.t. to the critical event  $Y > \hat{q}_{0.9}(Y)$ .

Finally, by aggregating and ranking, with priority given to TSA results, the variables detected, one



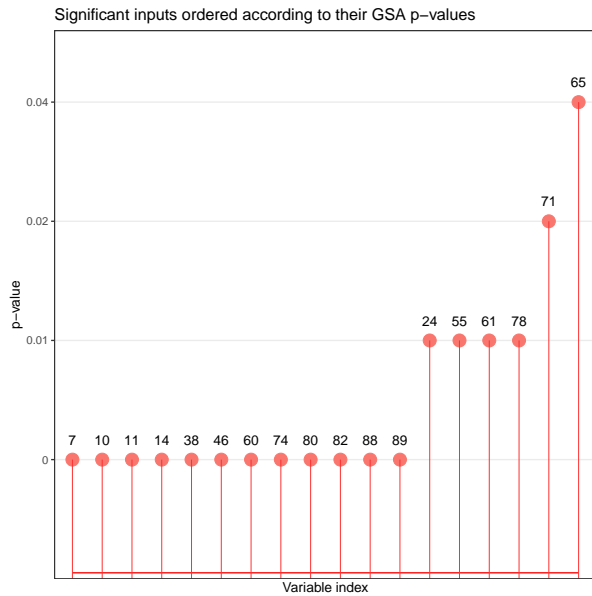
(a) GSA-oriented screening.



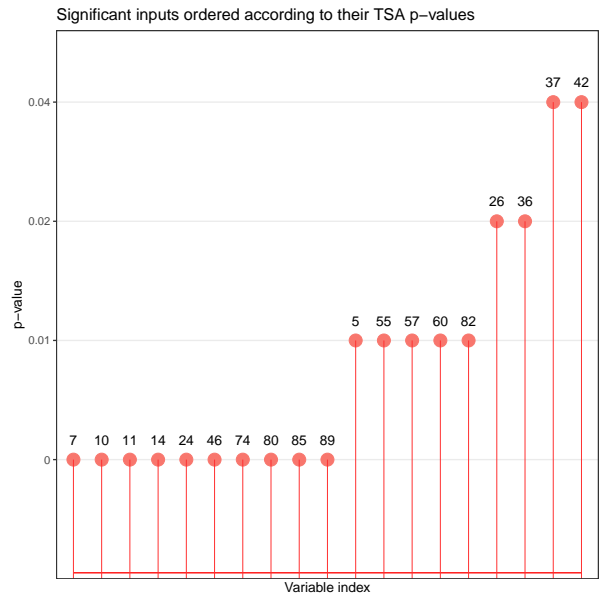
(b) TSA-oriented screening.

Figure 3 – Screening based on GSA and TSA using p-values.

gets a final pool of influential variables which drive, not only the global behavior of the output variability, but also and more importantly, the occurrence of the critical event.



(a) GSA-oriented ranking.



(b) TSA-oriented ranking.

Figure 4 – Ranking based on GSA and TSA using p-values and  $R_{HSIC}^2$ .

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## 5. CONCLUSION

Assessing risk and reliability of nuclear reactors through accident analysis requires to develop advanced BEPU methodologies in order to make robust the current deterministic approaches. However, the key challenges of those analyses remain the limited number of simulations available (due to the computational cost of high-fidelity computer models), and a large input dimension.

Recently, a new methodology, called ICSCREAM, has been proposed to provide probabilistic and statistical tools to overcome these methodological challenges and to enable the identification of penalizing configurations regarding some inputs of interest. The first step of this methodology consists in identifying the most influential inputs driving both the output variability and the variability of a risk measure estimated from this output.

In this paper, this first step of ICSCREAM methodology has been fully presented and has been put into practice through an industrial thermal-hydraulic IBLOCA use case. The statistical tools used here mostly focus on HSIC dependence measures (and variants of them to take specific QoIs into account) and statistical hypothesis tests. Minimal theoretical arguments have been provided to demonstrate the strong mathematical properties that make these tools relevant for the target purposes (identifying the most influential inputs among a large number of variables) and constraints (a single and limited CMC learning sample).

Finally, this paper also aimed at illustrating that the ICSCREAM methodology is based, at least for this first step, on fully open source statistical tools. This study has been realized using the ‘*sensitivity*’ package of the R statistical software. Moreover, most of these tools (HSIC, T-HSIC and tests) are or will be soon available in the open source uncertainty quantification platforms URANIE (CEA) and OpenTURNS (EDF, Airbus, IMACS, Phimeca and ONERA).

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