Statistical identification of penalizing configurations in high-dimensional thermalhydraulic numerical experiments: The ICSCREAM methodology

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STATISTICAL IDENTIFICATION OF PENALIZING CONFIGURATIONS IN HIGH-DIMENSIONAL THERMAL-HYDRAULIC NUMERICAL EXPERIMENTS: THE ICSCREAM METHODOLOGY

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ABSTRACT

In the framework of risk assessment in nuclear accident analysis, best-estimate computer codes are used to estimate safety margins. Several inputs of the code can be uncertain, due to a lack of knowledge but also to the particular choice of accidental scenario being considered. The objective of this work is to identify the most penalizing (or critical) configurations (corresponding to extreme values of the code output) of several input parameters (called "scenario inputs"), independently of the uncertainty of the other input parameters. However, complex computer codes, as the ones used in thermal-hydraulic accident scenario simulations, are often too CPU-time expensive to be directly used to perform these studies. A solution consists in fitting the code output by a metamodel, built from a reduced number of code simulations. When the number of input parameters is very large (e.g., around a hundred here), the metamodel building remains a challenge. To overcome this, we propose a methodology, called ICSCREAM (Identification of penalizing Configurations using SCREening And Metamodel), based on screening techniques and Gaussian process (Gp) metamodeling. The efficiency of this methodology is illustrated on a thermal-hydraulic industrial case simulating an accident of primary coolant loss in a Pressurized Water Reactor. This use-case includes 97 uncertain inputs, two scenario inputs to be penalized and 500 code simulations for the learning database. The study focuses on the peak cladding temperature (PCT) and critical configurations are defined by exceeding the 90%-quantile of PCT.

For the screening step, statistical tests of independence based on the Hilbert-Schmidt independence criterion are used for global and target sensitivity analyses. They allow a significant reduction of inputs (from 97 to 20) and a ranking of these influential inputs by order of influence. Then, a Gp metamodel is sequentially built to reach a satisfactory predictivity of 82% of explained PTC variance, and a high capacity of identifying PTC critical areas (94% of good ranking rate above the threshold). Finally, the Gp is used to estimate, within a Bayesian framework, the conditional probabilities of exceeding the threshold, according to the two scenario inputs. The analysis reveals the strong interaction of the two scenario inputs in the occurrence of critical configurations, worst cases corresponding to medium values of both inputs.

1. INTRODUCTION

In the framework of risk assessment in nuclear accident analysis, best-estimate computer codes are increasingly used to understand, model and predict physical phenomena and, ultimately, estimate safety margins. These codes, or numerical simulators, take a large number of input parameters characterizing the phenomenon under study or related to its physical and numerical modeling. The available information about some of these parameters is often limited or uncertain. The uncertainties come mainly from the lack of knowledge about the underlying physics and about the characterization of the input parameters of the model (e.g., due to the lack of experimental data) [1]. There are also additional sources of uncertainty arising from the particular choice of the accidental scenario being considered. These input parameters, and consequently the simulator output, are thus uncertain. In this context, it is essential to take into account the uncertainties tainting the results of computer simulations. This constitutes a major step for safety studies and is referred to as uncertainty propagation of numerical models and called BEPU ("Best-Estimate Plus Uncertainty") in nuclear safety analysis [20, 1].

In this work, we focus on the identification of the most penalizing configurations (corresponding to critical values of the output) of specific scenario inputs, regardless of the uncertainty of the other inputs. Our study is motivated and guided by the "Intermediate Break Loss Of Coolant Accident" (IB-LOCA) safety analysis, based on the numerical simulation of an accident of primary coolant loss in a Pressurized Water Reactor [19]. We consider in this paper a realistic and reactor-scale modeling [3, 12] of the accident with a very high number of uncertain parameters (compared to previous simplified studies [11]). The thermal-hydraulic responses are computed using the CATHARE2 code [8]. In order to characterize the limiting scenario in a BEPU approach, [13] has recently proposed the RIPS method which aims at analyzing the higher (or lower) quantiles of the output cumulative distribution function and determining, for each scenario input, the critical zone within its variation interval. A first issue of this method is that it finally relies on a quite subjective visual analysis. However, its most important drawback is due to the intrinsic complexity in the tuning of the method.

Our goal is to provide a more automatic method as well as to reduce the computational cost (in terms of number of code runs) that the standard BEPU approaches often require. To solve the cost issue in uncertainty quantification studies, a widely accepted method consists in replacing the CPU-time expensive computer models by CPU inexpensive mathematical functions (called "metamodels") based, e.g., on polynomials, neural networks, or Gaussian processes [6]. This metamodel is built from a primary set of computer code simulations. Then, it must be as representative as possible of the code in the variation domain of its uncertain parameters together with having good prediction capabilities. The use of metamodels has been extensively applied in engineering issues as it provides a multi-objective tool [7]: once estimated, the metamodel can be used to perform global sensitivity analysis (GSA), as well as uncertainty propagation, optimization, or calibration studies. However, the building process of the metamodel remains complex in the case of high-dimensional numerical experiments (with typically several tens of inputs). In order to efficiently build a metamodel in such cases, [11] has proposed a methodology which combines several advanced statistical tools: an initial space-filling design of experiments, a screening step[1] to identify

[1] In the framework of GSA, screening aims at separating the inputs into two sub-groups: the significant ones and

the non-influential inputs and to reduce the dimension, and a sequential building of a joint Gaussian process (Gp) metamodel. Then, the resulting joint Gp metamodel was used to accurately estimate Sobol' sensitivity indices and high-order quantiles. The efficiency of the methodology to deal with a large number of inputs and reduce the calculation budget was illustrated on a simplified IB-LOCA use-case with $d = 27$ inputs and a total budget of $n = 500$ simulations for the experimental design.

The objectives and constraints of the present study are different than those of [11] and require a new statistical methodology called ICSCREAM (pronounced "ice-cream") for "Identification of penalizing Configurations using SCREening And Metamodel". First, this more complete and realistic simulation of the IB-LOCA case (dataset and modeling at reactor-scale) involves a much larger number of uncertain inputs, namely $d = 96$. Even if the total budget of simulations n is almost doubled compared to that of the simplified study, it remains insufficient to directly perform uncertainty propagation, sensitivity analysis and identification of penalizing values of scenario inputs. The use of a metamodel is once again required. However, the building process with almost a hundred of inputs is a new challenge for our methodology. To meet this, we first perform the screening step via statistical independence tests based on Hilbert-Schmidt Independence Criterion (HSIC) measures, in global and target sensitivity analysis versions. "Target" sensitivity analysis, as described later in this paper, refers here to the area where the output exceeds a given critical value. Then, from the results of independence tests based on HSIC and target HSIC, the significantly influential inputs are identified and ordered by decreasing influence. A Gp metamodel is then efficiently built with the same sequential process as in [11]. Secondly, as the final objective here is to identify the penalizing configurations of two scenario inputs of interest, regardless of the uncertainty of the other inputs, the Gp metamodel is used to estimate within a Bayesian framework the conditional probabilities of exceeding the critical value. The steps of the ICSCREAM methodology are summarized in Figure 1.

Mathematically, the system under study can be modeled as follows:

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

where $g(\cdot)$ is the numerical model (computer code), whose output variable Y (called "output") and input parameters $\mathbf{X} = (X_1, \ldots, X_d)$ (called "inputs") belong to some measurable spaces $\mathscr{Y}$ and $\mathscr{X} \subset \mathbb{R}^d$, respectively. For a given value of the vector of inputs $\mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d$, a simulation run of the code yields an observed value $y = g(\mathbf{x})$. Under the probabilistic framework, the inputs are considered as random variable with probability density functions (pdf) $\mathbb{P}_{\mathbf{X}}$ on $\mathscr{X}$.

After a description of the complete IB-LOCA use-case (Section 2), Sections 3, 4 and 5 are dedicated to each main step of the ICSCREAM methodology (see Fig. 1), supplemented by the results of their implementation on the IB-LOCA use-case. The last section gives some conclusions of this work.

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the non-significant ones.

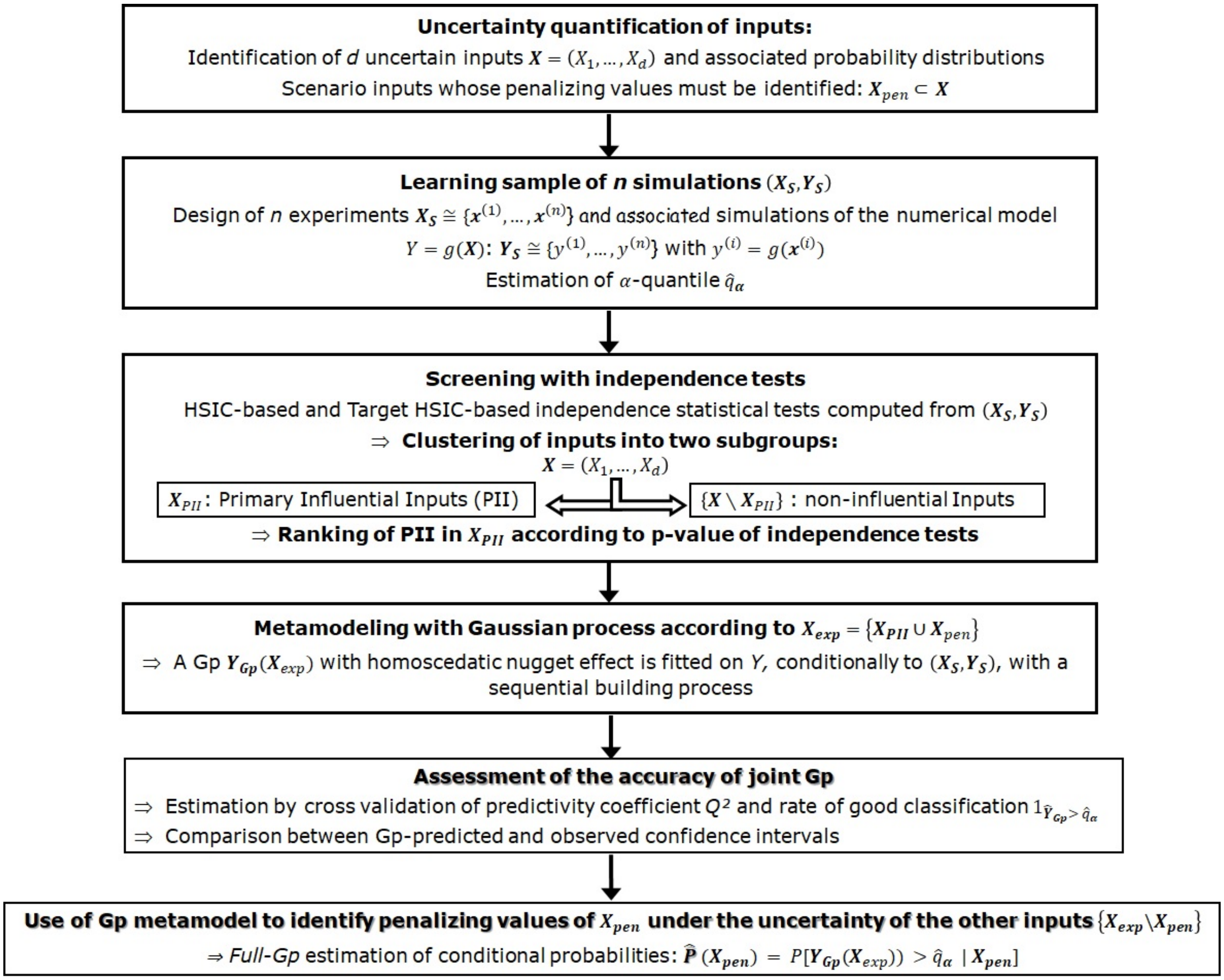

Figure 1: General workflow of the ICSCREAM methodology.

2. DESCRIPTION OF THE THERMAL-HYDRAULIC USE-CASE AND DATASET

Our use-case consists of a set of thermal-hydraulic computer experiments, as those typically used in support of regulatory work and nuclear power plant design and operation. Indeed, some safety analyses consider the IB-LOCA that takes into account a break on the main coolant system. The IB-LOCA transients are simulated using the thermal-hydraulic system code (two phase flow six equations) CATHARE2 [8], developed by CEA, EDF, Framatome and IRSN. During a IB-LOCA, the reactor coolant system minimum mass inventory and the peak cladding temperature (PCT) are obtained shortly after the beginning of the accumulators' injection [3]. $d = 96$ inputs (i.e., in the $\mathbf{X}$ vector) are considered uncertain and can be split into three different types [12]:

1. The boundary and initial conditions whose pdf are easy to specify (as uniform or normal distributions);

2. The model parameters, as the models related to two-phase flow hydraulics, the models associated to heat transfer and the models describing the clad behavior. The pdf of these inputs

can be obtained from data, from expert knowledge or recovered by solving inverse problems on experimental database [1]. This leads to uniform, log-uniform, normal or log-normal distributions;

3. The scenario parameters which cover some variability between minimal and maximal bounds.

All the inputs of the first and second types are independent.

The inputs corresponding to the third type have to be taken at their worst-case values (corresponding to the maximal value that can be reached by the PCT) [3, 13, 12]. These worst-case (or penalizing) values are unknown and a domain of variation of each input is given. In our use-case, these two inputs correspond to the size of the break (denoted X_{127} in the dataset) and the stopping time of the primary pumps (denoted X_{143} in the dataset), which are statistically dependent. The two scenario inputs whose penalizing values must be identified will be denoted $\mathbf{X_{pen}} \subset \mathbf{X}$.

This initial step of sampling consists in defining a design of n experiments for the inputs and performing the corresponding runs with the numerical model $g(\cdot)$. The obtained sample of inputs/outputs will constitute the learning sample on which the screening will be performed and the metamodel fitted. A Monte Carlo sample of $n = 889$ CATHARE2 simulations has been given by the EDF engineering division. All the 96 inputs are drawn according to their prior probability distributions. The histogram of the obtained values for the output of interest, namely the PCT, is given by Figure 2 (temperature is in °C). Note that the number n of simulations is a compromise between the CPU time required for each simulation and the number of inputs. For uncertainty propagation and metamodel-building purpose, some rules of thumb propose to choose n at least as large as 10 times the dimension d of the input vector [14, 17].

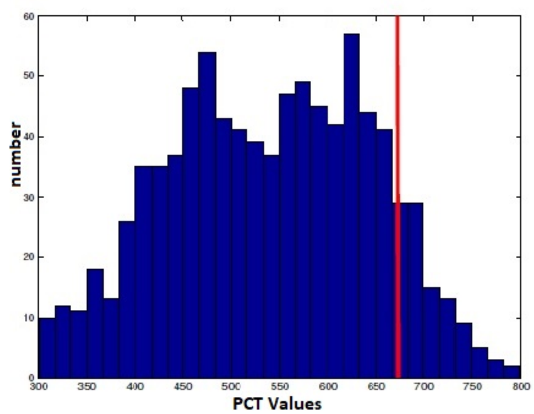

Figure 2: Histogram of the PCT from the learning sample of $n = 889$ simulations. The estimated 90%-quantile is indicated by the red line.

Mathematically, the experimental design corresponds to a n-size sample $\left\{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}\right\}$ which is performed on the code $g(\cdot)$. This yields n model output values denoted $\left\{y^{(1)}, \ldots, y^{(n)}\right\}$ with $y^{(i)} = g(\mathbf{x}^{(i)})$. The obtained learning sample is denoted (X_s, Y_s) with $X_s = \left[\mathbf{x}^{(1)^T}, \ldots, \mathbf{x}^{(n)^T}\right]^T$ and $Y_s = \left[y^{(1)}, \ldots, y^{(n)}\right]^T$. Then, the goal is to build an approximating metamodel of $g(\cdot)$ from the n-sample (X_s, Y_s).

From the learning sample, the empirical 90%-quantile of PCT is estimated to $\hat{q}_{0.9} = 673.18$°C and illustrated by the red line in Figure 2. As aforementioned, the ICSCREAM methodology aims to identify the values of the inputs and more precisely of $\mathbf{X_{pen}} = \{X_{127}, X_{143}\}$ which yield to a high probability of exceeding this quantile.

3. PRELIMINARY SCREENING BASED ON HSIC-INDEPENDENCE TESTS

Before building the metamodel, the dimension of the inputs is reduced by identifying the primary influential inputs (PII), denoted $\mathbf{X_{PII}}$ in Figure 1. These inputs will be the only explanatory inputs of the metamodeling, while the other inputs (screened as non-significantly influential) are considered as global stochastic (i.e., unknown) inputs, denoted $\mathbf{X}_\varepsilon$ in Figure 1 (see [11] for more details). To achieve this selection, a screening technique is directly performed from the learning sample. For this, we use the HSIC importance measures introduced by [10] and built upon kernel-based approaches for detecting dependence, and more particularly on cross-covariance operators in reproducing kernel Hilbert spaces. This amounts to considering covariance between feature functions applied to the two variables (here X_k and Y). This set of functions (possibly nonlinear), which is defined by the space and the kernel, can be of infinite dimension and allow to capture a very broad spectrum of forms of dependency. The HSIC, which is defined as the Hilbert-Schmidt norm of the cross-covariance operator, somehow "summarizes" the set of covariances between features. Furthermore, the kernel trick allows to get rid of an explicit expression of the features: HSIC can be directly expressed with kernels and estimated in a very simple and low cost way (a few hundred simulations against several tens of thousands for the variance-based Sobol' indices). For all these reasons, [4] and then [5] were interested in using the HSIC measures for GSA purposes. Finally, if a characteristic kernel (such as the Gaussian one) is used, the nullity of HSIC is equivalent to independence and statistical independence tests can be built for screening purposes ([5]).

For a given input X_k, statistical HSIC-based tests aim at testing the null hypothesis "$\mathscr{H}_0^{(k)}$: X_k and Y are independent", against its alternative "$\mathscr{H}_1^{(k)}$: X_k and Y are dependent". The significance level[2] of these tests is hereinafter noted α and usually set at 5% or 10%. Several HSIC-based statistical tests are available: asymptotic versions (i.e., for large sample size) based on an approximation with a Gamma law ([9]), spectral extensions and permutation-based versions ([5]) for non-asymptotic case (i.e., case of a small sample size). Beyond the screening task, HSIC sensitivity measures can be quantitatively interpreted for GSA and used to order the PII by decreasing influence, which paves the way for a sequential building of metamodel ([11]). Here, we prefer to use the *p-value*[3] of independence tests for ranking the PII, as it can be viewed as a "margin" from independence. The lower the p-value, the stronger $\mathscr{H}_0^{(k)}$ is rejected and the higher the influence of X_k.

Moreover, as the ICSCREAM final objective is to identify the penalizing configurations and more precisely to accurately fit the critical areas where the PCT exceeds $\hat{q}_{0.9}$ (i.e., $Y > \hat{q}_{0.9}$), we consider an additional *Target* sensitivity analysis based on *Target* HSIC (T-HSIC), recently proposed by [15]. Applied here, target sensitivity analysis aims at measuring the influence of an input X_k over the occurrence of $Y > \hat{q}_{0.9}$. For this, T-HSIC and associated independence tests can be built by

[2]The significance level is the probability of rejecting the null hypothesis $\mathscr{H}_0$ when it is true.
[3]Probability of obtaining HSIC estimates at least as extreme (high value) as the observed HSIC assuming $\mathscr{H}_0$ true.

defining specific kernels. In addition, to cope with the loss of information and to take into account some additional information near the critical domain, a weight function can be relevantly used for relaxation, see [15] for more details. All this step of the ICSCREAM methodology is further detailed in [2].

HSIC-independence tests with a permutation approach for the estimation of p-values are applied on the learning sample of the IB-LOCA use-case. The obtained p-values are given by Figures 3 and 4 for global HSIC and T-HSIC respectively. The level $\alpha = 10\%$ is represented in black dotted line and the inputs with a p-value lower than α (independence hypothesis $\mathscr{H}_0^{(k)}$ rejected) are represented by red bullets. Thus, 18 variables are identified as influential by global HSIC-based tests. The two inputs to penalize are the most influential: X_{142} (stopping time of primary pumps) being the most influential, followed by X_{127} (break size). Then X_{113} (upper plenum interfacial friction), X_{110} (core interfacial friction), X_{11} (hot spot for the hot rod), X_{42} and X_{50} (two inputs relative to accumulators) are identified. A group of 13 other variables of lower influence is also selected by global HSIC-tests. Similar results are obtained with T-HSIC-based tests, except that two additional inputs, namely $X125$ (diphasic degradation law of pumps) and $X83$ (residual power), are selected as very influential. Consequently, a total of 20 inputs are selected by the screening step (denoted by $\mathbf{X_{PII}}$ in the methodology presented in Figure 1) and ordered by influence based on p-value results.

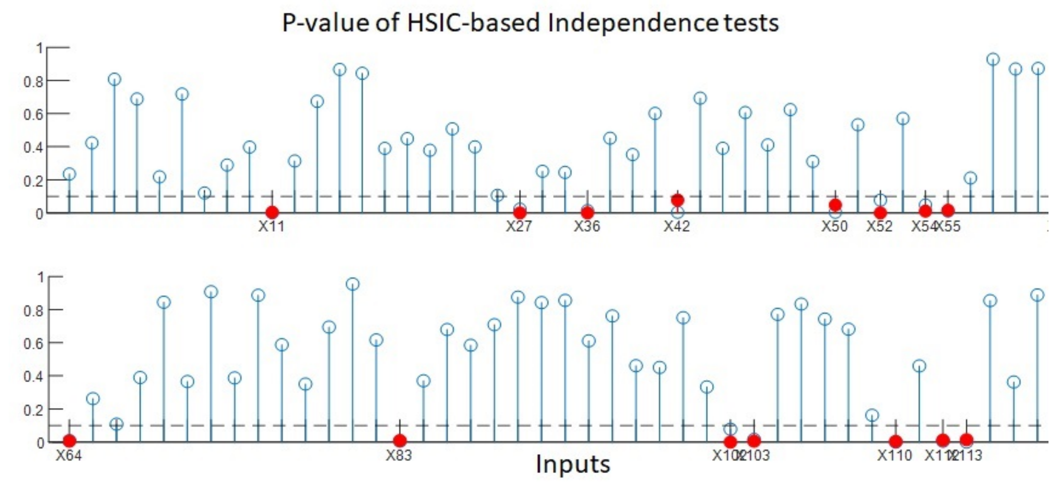

Figure 3: P-values of HSIC-based independence tests from the computed learning sample.

In our case, the inputs of interest to be penalized $\mathbf{X_{pen}}$ are also the two most influential and consequently, $\mathbf{X_{exp}} = \mathbf{X_{PII}} \cup \mathbf{X_{pen}} = \mathbf{X_{PII}}$. The other 76 inputs are merged into the stochastic variable denoted $\mathbf{X}_\varepsilon = \mathbf{X} \setminus \mathbf{X_{exp}}$. Note that, an heuristic choice founded on the objective of the study, not detailed here for the sake of conciseness, is made to aggregate the results of both global and target sensitivity analysis tests for the ranking: priority is given to the target results in the order of inputs. Moreover, if $\mathbf{X_{pen}}$ are not detected as influential by the screening, different choices are possible regarding the order in which they are added in $\mathbf{X_{exp}}$, not discussed here.

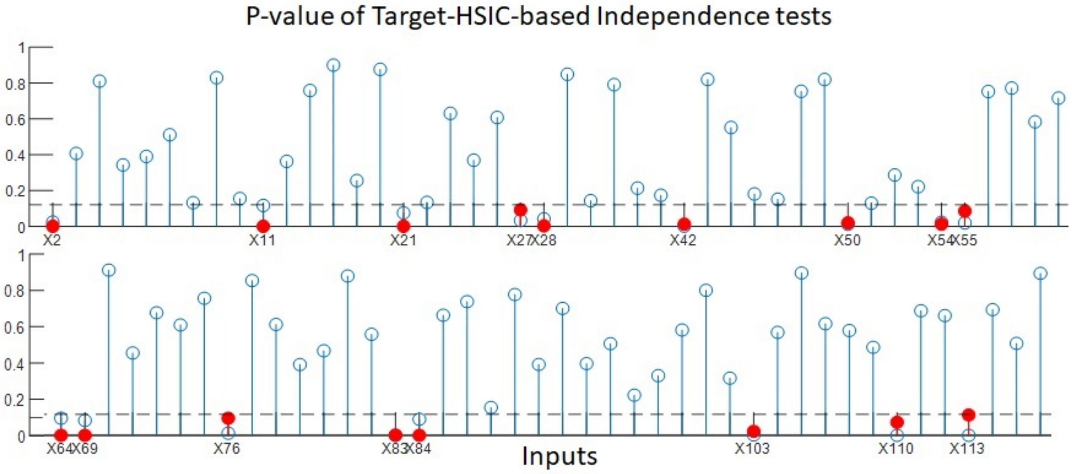

Figure 4: P-values of T-HSIC-based independence tests computed from the learning sample.

4. BUILDING AND VALIDATION OF METAMODEL

The second main step of the ICSCREAM methodology consists in building a metamodel to fit the simulator output Y (here the PCT), from the learning sample. For this, we use the same method than in [11], based on an homoscedastic (non-interpolating) Gaussian process (Gp) metamodel. The reader can refer to [18] for a detailed review on Gp metamodel.

More precisely, the output is here defined by $Y = g(\mathbf{X_{exp}}, \mathbf{X}_\varepsilon)$ and the metamodeling process is focused on fitting the random variable $Y|\mathbf{X_{exp}}$[4]. In other words, only the inputs in $\mathbf{X_{exp}}$ are considered as the explanatory inputs of the Gp. Basically, the Gp is built to approximate the expected value $\mathbb{E}(Y|\mathbf{X_{exp}})$. The residual effect of the other inputs (merged into $\mathbf{X}_\varepsilon$) is captured using an additional nugget effect[5]. Note that contrary to [11], a simple Gp metamodel with an homoscedastic nugget effect is estimated, since fitting a joint Gp with heteroscedastic nugget is neither relevant nor realistic given the high dimensionality of the problem and the low sample size. Finally, concerning the estimation of the Gp according to $\mathbf{X_{exp}}$, a sequential process using the ranking deduced from the screening step is used (see [11] for the detailed sequential building process and parametric choices of Gp metamodel). Note that a Matérn stationary anisotropic covariance and a constant trend are considered here.

Once the Gp hyperparameters (covariance parameters) estimated by maximum likelihood on the learning sample, the Gp is conditioned by the observations of the learning sample to obtain the Gp metamodel. This resulting conditional random process is still a Gaussian process, denoted $Y_{Gp}(\mathbf{X_{exp}})$. For each unobserved point of prediction, it is therefore fully characterized by its mean and variance (see [18] for an explicit expression of mean and covariance). The conditional mean is used as predictor and denoted $\hat{Y}_{Gp}(\mathbf{X_{exp}})$. The conditional variance which is also the mean squared error of predictor is denoted $MSE[\hat{Y}_{Gp}(\mathbf{X_{exp}})]$ and is used to build a confidence interval for the prediction. The accuracy and prediction capabilities of the Gp metamodel are assessed by

[4] $Y|\mathbf{X_{exp}}$ (i.e., Y knowing $\mathbf{X_{exp}}$) is a random variable as its value depends on the uncontrollable random vector $\mathbf{X}_\varepsilon$.

[5] Borrowed from geostatistics, a "nugget effect" assumes an additive white noise effect and relaxes the interpolation property of the Gp metamodel. It can be assumed to be constant (homoscedastic) or depends on x (heteroscedastic).

cross-validation, given the limited budget of simulations.

First, to quantify the accuracy of predictor, we use the predictivity coefficient Q^2:

$$Q^2 = 1 - \frac{\sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}_{Gp,-i}\right)^2}{\sum_{i=1}^{n}\left(y^{(i)} - \frac{1}{n}\sum_{i=1}^{n} y^{(i)}\right)^2} \tag{2}$$

where $y^{(i)}$ and $\hat{y}^{(i)}_{Gp,-i}$ are respectively the i-th observation of the learning sample and the corresponding prediction of the Gp metamodel built without $y^{(i)}$. Q^2 corresponds to the coefficient of determination in prediction, computed by cross-validation on the learning sample. The closer to one the Q^2, the better the accuracy of the metamodel. We use here a K-fold cross-validation with $K = 10$ and obtain $Q^2 = 0.82$. Only 18% of the output variability remains not explained by the Gp metamodel (built with only 20 explanatory inputs): this includes both the inaccuracy of the Gp and the total effect of $\mathbf{X}_\varepsilon$ (group of non-selected inputs). Note that building the Gp directly in dimension $d = 97$, without selection and sequential processes, leads to a poor estimation of the Gp (e.g., with a failure of the optimization in the estimation of the Gp hyperparameters) and yields a Gp with null predictivity. This illustrates the practical interest of our methodology.

In the purpose of identifying the input area yielding to critical configurations, we also compute the rate of good prediction of $Y > \hat{q}_{0.9}$ and obtained, still by cross-validation, a rate of 94%. This testifies to the high capacity of the Gp metamodel to identify critical input areas. This quantitative analysis of predictivity can be supplemented with a plot of predicted values against observed values ($\hat{y}^{(i)}$ versus $y^{(i)}$) or a quantile-quantile plot (not presented here).

Finally, remember that for each point of prediction, the conditional Gp provides a Gaussian distribution of mean $\hat{Y}_{Gp}(\mathbf{X_{exp}})$ and variance $MSE[\hat{Y}_{Gp}(\mathbf{X_{exp}})]$. And, for a set of points of prediction, predictions are correlated with a covariance matrix (given by the covariance of conditional Gp). The Gp metamodel therefore provides confidence intervals (beyond mean squared error) for any prediction. Consequently, it is relevant to evaluate the quality of these confidence intervals using the graphical tool introduced in [16]. For a given Gp metamodel, it consists in evaluating the proportions of observations that lie within the α_{CI}-theoretical confidence intervals predicted by the Gp (the whole Gp structure is used to build this interval and not only the conditional mean). These proportions (i.e., the observed confidence intervals) can be visualized against the α_{CI}-theoretical confidence intervals, for different values of α_{CI}. By definition, the more accurate the confidence intervals, more the points should be located around the $y = x$ line. This plot, obtained still from a cross-validation process, is given for the IB-LOCA use-case by Figure 5. The quality of confidence intervals is on average satisfactory, although they are sometimes too conservative for central values of α_{CI}. This study allows to further validate the whole structure of Gp metamodel, i.e. the predicted probability law for each point of prediction.

Note that convergence studies, not presented here for sake of brevity, have also been performed using a bootstrap-based approach. Results show a stagnation (and therefore convergence) of Gp performance with an average Q^2 equal to 0.8 from $n = 400$. The remaining part of the unexplained variance may come, either from the loss of information conveyed by the inputs not selected in the screening, or from some “chaotic” code behavior (e.g., physical bifurcations, threshold effects, very strong non-linearities or discontinuities). In our case, we think this is the second explanation, since we tried to add non-influential inputs in the Gp without noticing any improvement. To cope with the second case (bifurcation or irregularities), other metamodels could be considered (e.g., Gp trees) but the large dimension remains a problem to apply them.

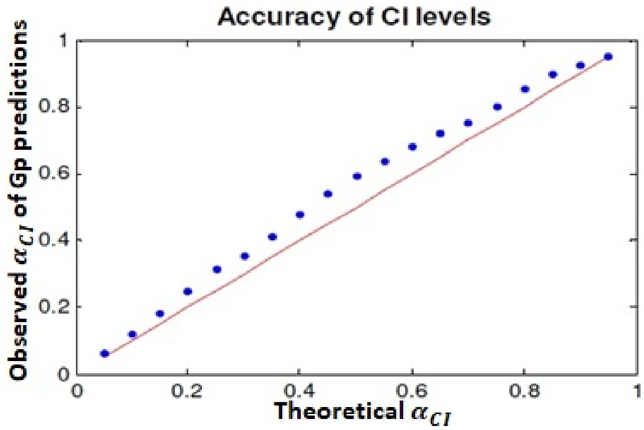

Figure 5: Proportion of PCT observations that lie within the α_{CI}-confidence interval predicted by the Gp according to the theoretical level α_{CI}.

5. IDENTIFICATION OF PENALIZING CONFIGURATIONS

The final goal of the ICSCREAM methodology is to identify the penalizing configurations (corresponding to a maximal PCT) of the two inputs of interest $\mathbf{X_{pen}}$, namely the break size (X_{127}) and the stopping time of the primary pumps (X_{143}), regardless of the uncertainty of the other inputs. For this, we compute for any couple of possible values of $\mathbf{X_{pen}}$ the probability of exceeding the critical value $\hat{q}_{0.9}$. This conditional probability can be estimated with the *full-Gp* metamodel approach by:

$$
\begin{aligned}
\hat{P}(\mathbf{X_{pen}}) &= P[Y_{Gp}(\mathbf{X_{exp}}) > \hat{q}_{0.9} \,|\mathbf{X_{pen}}] \\
&= 1 - \mathbb{E}(1_{Y_{Gp}(\mathbf{X_{exp}}) \leq \hat{q}_{0.9}} |\mathbf{X_{pen}}) \\
&= 1 - \mathbb{E}(1_{Y_{Gp}(\mathbf{\tilde{X}_{exp}}, \mathbf{X_{pen}}) \leq \hat{q}_{0.9}} |\mathbf{X_{pen}}) \\
&= 1 - \mathbb{E}(\mathbb{E}(1_{Y_{Gp}(\mathbf{\tilde{X}_{exp}}, \mathbf{X_{pen}}) \leq \hat{q}_{0.9}} |\mathbf{\tilde{X}_{exp}}) |\mathbf{X_{pen}}) \\
&= 1 - \int_{\tilde{\mathscr{X}}_{exp}} \Phi \left(\frac{\hat{q}_{0.9} - \hat{Y}_{Gp}(\mathbf{\tilde{x}_{exp}}, \mathbf{X_{pen}})}{\sqrt{MSE[\hat{Y}_{Gp}(\mathbf{\tilde{x}_{exp}}, \mathbf{X_{pen}})]}} \right) d\mathbb{P}_{\mathbf{\tilde{X}_{exp}}}(\mathbf{\tilde{x}_{exp}})
\end{aligned} \tag{3}
$$

where $\mathbf{\tilde{X}_{exp}} = \mathbf{X_{exp}} \setminus \mathbf{X_{pen}}$ denotes the explanatory inputs deprived of $\mathbf{X_{pen}}$, $\tilde{\mathscr{X}}_{exp}$ their domain of variation, $d\mathbb{P}_{\mathbf{\tilde{X}_{exp}}}$ their probability density, and $\Phi(\cdot)$ the cumulative distribution function of the standard Gaussian distribution. In order to obtain the fourth line in Eqn. (3) from the third one, one invokes the independence between $\mathbf{\tilde{X}_{exp}}$ and $\mathbf{X_{pen}}$ (let us recall that only the two inputs in $\mathbf{X_{pen}}$ are dependent in our use-case). In practice, this probability (and, more precisely, the 18-dimensional integral) is computed for each possible value of the couple $\mathbf{X_{pen}}$ by intensive Monte Carlo simulations. Results obtained for the IB-LOCA use-case are given in Figure 6.

Remark 1. *This approach is also referred as a "Bayesian approach" since all the Gp structure is used to estimate the quantity of interest, in opposition to the "plug-in" or "kriging believer"* *approach where only the mean of the Gp (predictor $\hat{Y}_{Gp}$) is taken into account. Bayesian approach allows to take into account the prediction error of Gp metamodel in the estimation of $\hat{P}(\mathbf{X_{pen}})$. This limits here the impact of the 18% of unexplained variance, in comparison with simple plug-in approach (with no prediction error taken into account), especially since we have shown the accuracy of prediction variance (cf. Figure 5). However, it might be possible that the unexplained part of the model (which represents 18% of output variance) depends significantly enough on $\mathbf{X_{pen}}$ to impact the true value of $P(\mathbf{X_{pen}})$. To prevent this risk, it is advisable (if possible) to add new CATHARE2 simulations in the critical areas to increase the confidence in the predicted conditional probability. Once again, the Gp metamodel will show all his interest since it can be used (still in a Bayesian approach) for sequential sampling strategies (e.g., goal-oriented sampling to reduce the uncertainty of predicted conditional probability).*

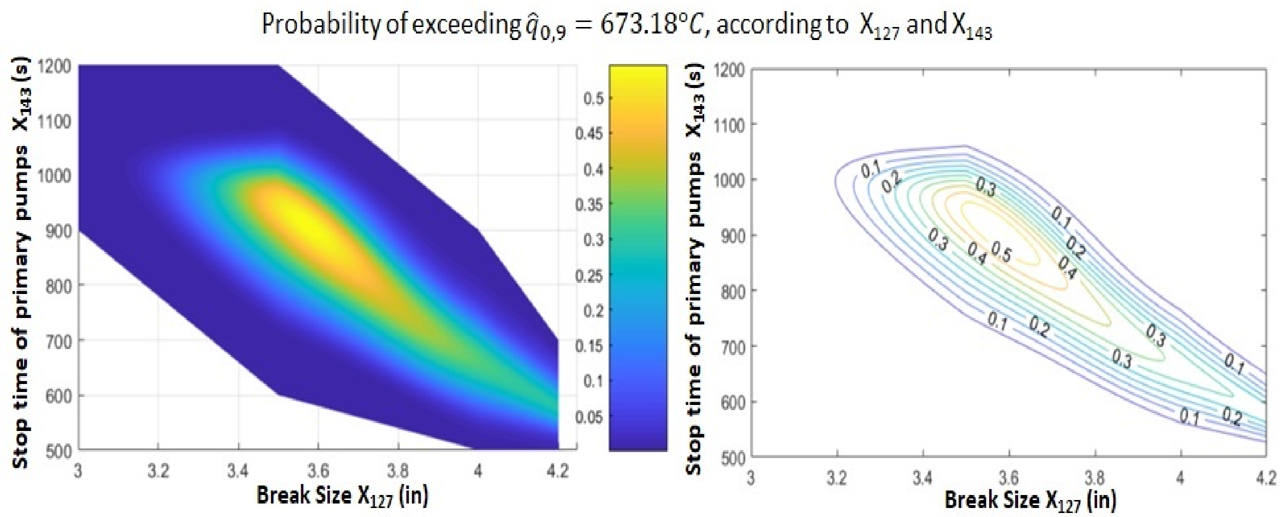

Figure 6: Estimated probability $\hat{P}(X_{127}, X_{143})$ of exceeding $\hat{q}_{0.9}$, with both surface and contour plot representations.

The analysis of the conditional probability reveals the strong interaction of the two scenario inputs in the occurrence of critical configurations. The worst cases correspond to medium values of both inputs. Conditionally to a given break size, the probability function according to the stopping time of primary pumps has a bell shape that reaches its maximum value for a stopping time which decreases linearly as the break size increases. Note that the worst configuration is obtained for a size of break equal to 3.57 inches and a stopping time of the primary pumps of about 907.8 seconds, which leads to an estimated probability of exceeding the quantile $\hat{q}_{0.9}$ of 0.55.

These results can be enlightened by an analysis of the physical phenomenon. In a nutshell, the correlation between these two scenario inputs drives the degradation of the water inventory. The smaller the break size, the longer the pump will have to run for the same inventory degradation. As for the distinct left and right limits on the domain, they can also be explained. On the one hand, if $X_{127} < 3.3$ inches, meaning that the break size is rather small, the water inventory does not degrade too much (whatever the primary pump does). This leads to a slow LOCA which can be contained by the protection systems which have enough time to intervene (hence, the net border). On the other hand, when the break size increases too much, the break tends to be prevailing and reduces the impact of the stop time of the primary pumps (hence, the fading area).

6. CONCLUSION

In the framework of risk assessment in nuclear accident analysis, it is essential to quantitatively assess the uncertainties tainting the results of best-estimate codes. Beyond the usual uncertainty propagation, this paper has been focused on identifying the most penalizing (or critical) configurations of scenario inputs, regardless of the uncertainty of the other inputs. This methodology, called ICSCREAM, was motivated by the study at the reactor-scale of an IB-LOCA scenario in a Pressurized Water Reactor, with the thermal-hydraulic CATHARE2 code. In our use-case, 96 scalar input variables are uncertain and the penalizing values of two of them, the break size and the stopping time of primary pumps, must be identified. The output variable of interest characterizing a critical phenomenon is the PCT during the accident transient.

The high-fidelity of the numerical modeling, the limited budget of simulation and the very large number of uncertain inputs (around a hundred) are real challenges that lead for the development of a sophisticated methodology based on advanced statistical tools. To do this, we relied on our methodology for estimating high-order quantiles in previous studies of a more simplified IB-LOCA use-case. We improved it to fit the new constraints (much larger number of inputs) and objectives (identification of penalizing configurations) required by the reactor-scale IB-LOCA study.

Thus, from a single Monte Carlo sample of CATHARE2 simulations, an initial screening step, based on HSIC independence tests, is used for GSA and target sensitivity analysis. Applied on the IB-LOCA use-case, target sensitivity analysis has highlighted the importance of two inputs on critical values of PCT, while not being detected as influential by GSA. Based on these results, a group of significantly influential inputs is identified and ordered by decreasing influence. The, output PCT is fitted with a Gaussian process (Gp) metamodel. According to the reduced number of influential inputs, the Gp is built from the learning sample with a sequential process. Much effort during the building process of the Gp metamodel is concentrated on the main influential inputs. Consequently, the robustness of the metamodel is enhanced and its building is made possible in such a high-dimensional problem. The non-selected inputs are not completely removed but integrated in the variance of Gp prediction. The predictivity of the Gp as well as the quality of the confidence interval of its predictions are evaluated by cross-validation and provide very satisfying results, considering the complexity of the problem and the reduced number of code simulations.

From this Gp metamodel, the evaluation of penalizing configurations of the two scenario inputs, not directly feasible with the numerical model due to its computational cost, becomes tractable. From the Gp, the probability of exceeding the critical value corresponding to the empirical 90%-quantile is computed for any possible couple of values of the break size and stopping time of primary pumps. For this, all the Gp metamodel is used in a Bayesian framework, to take into account the variance of prediction of the Gp. The analysis of the conditional probability has revealed the strong interaction of the two scenario inputs in the occurrence of critical configurations.

The ICSCREAM methodology would be achieved with its industrial application, as for the RIPS methodology [13]. Before this achievement, some methodological improvements are required. First, the sensitivity of the results according to the considered (and estimated) quantile (which defines the critical output area) has to be studied. Second, a possible larger set of inputs to penalize (e.g., around 10) has to be considered. Finally, a technical perspective is to consider learning samples not drawn from a pure Monte Carlo design of experiments. Indeed, space-filling or quasi-Monte Carlo designs [6] are more adapted to build metamodel, as they ensure a better coverage and distribution of points in the input space. However, the screening step has to be adapted to deal with this kind of samples since some statistical assumptions in the HSIC-based tests (independence of the observations) are not satisfied anymore.

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8. GLOSSARY

Acronym	Definition
Gp	Gaussian process
GSA	Global Sensitivity Analysis
HSIC	Hilbert-Schmidt Independence Criterion
IB-LOCA	Intermediate Break Loss Of Coolant Accident
ICSCREAM	Identification of penalizing Configurations using SCREening And Metamodel
LOCA	Loss Of Coolant Accident
PCT	Peak Cladding Temperature
PII	Primary Influential Inputs
pdf	probability density function

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