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DETECTING OUTLYING SIMULATIONS IN BEPU APPROACHES

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ABSTRACT

Nuclear safety studies, based on the so-called BEPU (Best Estimate Plus Uncertainty) approaches, aim to calculate not only the possible values of a physical variable of interest, but also to quantify its associated uncertainty. From the results of a BEPU study, statistical analysis tools aim to improve the understanding of the physical phenomena simulated by the computer codes. The data outputs generated by these codes typically possess a functional nature, i.e. they represent the temporal evolution of a physical parameter throughout a transient. However, this functional nature is not always taken into account, in spite of the fact that it may provide relevant information regarding nuclear safety. On top of that, the functional analysis of data is even more relevant for transients where the safety criteria is directly associated to the dynamic behavior of a physical parameter, as it is in the case of the pressurized thermal shock. This work addresses the automatic identification of atypical transients (called "outliers") in sets of time-dependent simulations that can help to better detect the physical phenomena that influence the safety margins, to find penalizing scenarios, or to verify the physical consistency of industrial simulators. A new functional outlier detection technique is then presented, as well as the eventual statistical link between the outlying simulations and the inputs of the computer code. The relevance of this methodology is illustrated on pressurized thermal shock simulations.

1 INTRODUCTION

In the context of the nuclear industry, Best Estimate (BE) codes are increasingly used [1] to better estimate the safety margins provided by the analysis of accidental transients, as well as to better understand the complex underlying physics that exist in these simulations. This kind of codes can also provide some insight about the degree of conservatism that is typically adopted in order to ensure the safety of the nuclear power plant.

However, there is an uncertainty intrinsically associated to the results that are provided by BE codes, which typically comes from a lack of knowledge of the real phenomena that occur in complex nuclear transients (epistemic uncertainty). This is one of the reasons that justify the employment of statistical tools capable of quantifying the uncertainty associated to the conclusions that

are extracted thanks to the information given by the BE codes. The employment of this kind of codes is in general expensive in time (the simulations may take several hours or days), which considerably hinders their usefulness when taken alone and without making use of complementary tools such as BEPU approaches.

Classically, this problem is solved by generating a limited number of expensive but accurate BE simulations of the target transient through a design of numerical experiments. Once all the simulations are performed the output data are treated in order to obtain the statistics of interest for nuclear safety, such as extreme values, quantiles, superquantiles [2]. This procedure may eventually make use of surrogate (less expensive) models of the code if a larger number of simulations is required, for instance in the context of global sensitivity analysis [3, 4, 5]. However, this methodology has several downsides. First of all, for an essentially physical or an engineering problem, the considered approach is entirely mathematical, which may overlook potentially useful physical information. In addition, it usually only takes into account scalar input and output variables, even though the output information is usually richer (not only a scalar, but a temporal evolution of physical parameters of interest, like cladding temperature, pressures or flow rates).

Indeed, the data outputs generated by these codes typically possess a functional nature, i.e. they represent the temporal evolution of a physical parameter throughout a transient. However, this functional nature is not always taken into account, in spite of the fact that they may provide relevant information regarding nuclear safety. On top of that, the functional analysis of data is even more relevant for transients where the safety criteria is directly associated to the dynamic behavior of a physical parameter, as it is in the case of the pressurized thermal shock. This work addresses the automatic identification of atypical transients (called "outliers") in sets of time-dependent simulations that can help to better detect the physical phenomena that influence the safety margins, to find penalizing scenarios, or to verify the physical consistency of industrial simulators. A new functional outlier detection technique is then presented, as well as the eventual statistical link between the outlying simulations and the inputs of the computer code.

In this context, the general objective of the present work is to develop tools that help improve the current black-box approaches, making use of all the information provided by the BE codes. In order to do so, the industrial context and application case is first presented in section 2, followed by a brief explanation of the modeling in section 3. The new functional outlier detection technique is exposed in section 4, allowing the identification of atypical transients. Then, a score (probability) is associated to each transient, and the link between the input variables and the outlyingness of the curves can be quantified by means of the evolution of the original density functions of the input variables in section 5 (illustration on a simulated pressurized thermal shock). Finally, the main conclusions are explained in section 6.

2 THE INDUSTRIAL CONTEXT

The analyzed transient of interest is the Pressurized Thermal Shock (PTS) that can occur on Pressurized Water Reactors (PWR). This accidental transient is a multidisciplinary problem related to thermal-hydraulics, fracture dynamics, material resistance and risk analysis that carries a high

level of importance since it involves the integrity of one of the most essential components in a nuclear power plant: the vessel. The possible rupture of the vessel in this type of transient is the consequence of three essential factors [6]: The embrittlement of the steel of the vessel due to the long-term exposure to high energy neutrons, the existence of an initiating flaw, and an overcooling of the component (rapid drop in temperature). Under these conditions, a fracture may appear in the material that constitutes the second confinement barrier in PWR.

Due to these reasons, this is an event to take into consideration mostly in older nuclear power plants, where the vessel has been exposed to high levels of radiation flux for a significant period of time, inducing an embrittlement of the steel. Regarding the overcooling, a typical scenario to take into consideration is the case of an already existing Loss of Coolant Accident (LOCA), which triggers the activation of the injection systems, inducing a fast decrease in the temperature of the vessel through low temperature water. Examples of such temperature evolution are given in Fig. 1.

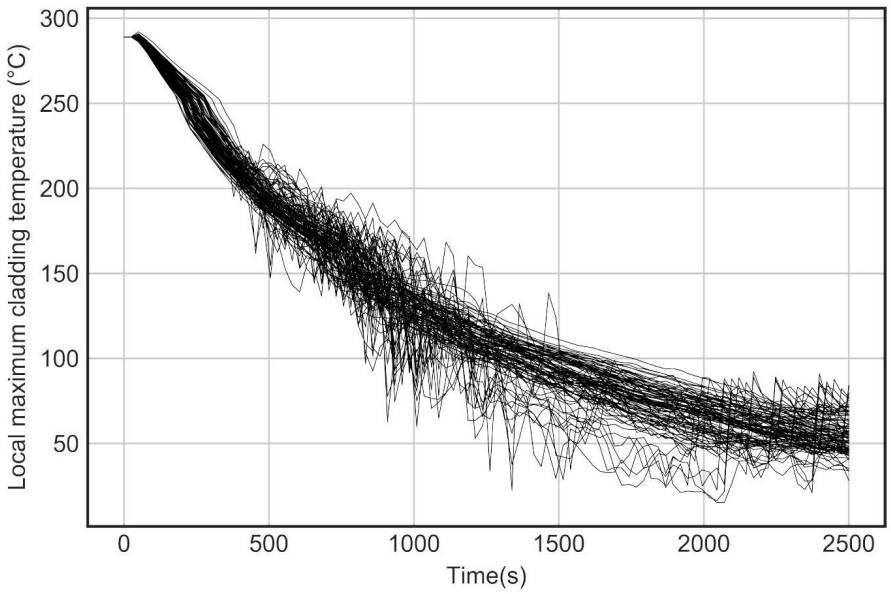

Figure 1: Example of evolutions of the maximum cladding temperature for several PTS transients.

In this case, the safety margin is more difficult to estimate than in the case of a LOCA accident, since the safety criteria is not only dependent on the maximum cladding temperature of the nuclear fuel, but also on others such as the water injection flows at all times in the transients. This is one of the motivating reasons of this work, since in this case, focusing on the scalar inputs and one scalar output is not sufficient to assess the safety of the installation, the whole transient must be analyzed. In order to do so, the works presented in the following sections that are based on the analysis of functional data have been developed.

3 THE STATISTICAL MODEL

In this section the setting of the problem is clarified. We suppose that a certain number of input variables, with known probability laws that allow their sampling, is available. These variables are the input of a (usually expensive to evaluate) BE computer code, CATHARE2 [7], a two-phase thermal-hydraulic simulator system code, capable of simulating the physical behaviour of a PWR power plant in thermal-hydraulic transients. The outputs of the code can typically be the temporal evolution of some physical variables of interest, and they will constitute the core of the analysis.

More formally, the mathematical formulation of this setting is the following:

$$X \in \mathbb{R}^P \longrightarrow \text{CATHARE2: } z \longrightarrow z(X) = (z(X,u))_{u\in\mathscr{U}} \in \mathscr{F} \tag{1}$$

where:

- (X,z) forms a couple of vectors where the components are random variables (real and functional),
- P is the dimension of the vector X,
- $\mathscr{F}$ is a functional space that appropriately models the Q outputs of the code,
- (X,z) has a known joint probability distribution, which models the sources of uncertainty, i.e., $(X(\omega),(z(\omega)) \in \mathbb{R}^P \times \mathscr{F}$ for each event $\omega \in \Omega$,
- For any realization $x \in \mathbb{R}^P$ of X, there are Q variables $z(x)$ functions of the variable u,
- u is the coordinate variable (of dimension $L \leq 4$) of the studied spatio-temporal domain $\mathscr{U} \in \mathbb{R}^L$,
- the domain $\mathscr{U}$ is defined as the cartesian product of a real domain $\mathscr{S} \subset \mathbb{R}^{L-1}$ in the physical space, and a time interval $[0,T]$ such that $\mathscr{U} = \mathscr{S} \times [0,T] : z(x,u) = (z(x))(u) \in \mathscr{F}, \forall u \in \mathscr{U}$.

The previously mentioned variables $z(x)$ are functional [8], i.e, they are data taking their values in an infinite dimensional vector space [9]. This is the case for the aforementioned outputs of the CATHARE2 code, where the variables of interest take the form of one-dimensional curves. Naturally, when working with them, data are only registered in finite grids of time.

The general framework of functional data analysis can be formalised in the context of these works through the notion of functional random variable [10]. Given a probability space $(\Omega,\mathscr{A},\mathbb{P})$, where Ω is the sample space, $\mathscr{A}$ is the event space, and $\mathbb{P}$ is a probability measure, as well as a certain functional space $\mathscr{F}$, then a random variable is called *functional*, if it takes its values in a vector space of infinite dimension $(\mathscr{F},\mathscr{B}_{\mathscr{F}})$, where $\mathscr{B}_{\mathscr{F}}$ is the Borel σ-algebra of the space. It is then a measurable application $X : \Omega \to \mathscr{F}$. If the function space is defined in a certain interval $\mathscr{T}$, which is frequently the case, as well as of real values, we can see the functional variable X as an application: $X : \Omega \times \mathscr{T} \to \mathbb{R}$ such that:

- For all $\omega \in \Omega$ fixed, the function $X(\omega,\cdot) : \mathscr{T} \to \mathbb{R}$ is a *trajectory* of X;

- For all $t \in \mathscr{T}$ fixed, the function $X(\cdot,t) : \Omega \to \mathbb{R}$ is a real-valued random variable.

This modeling is not arbitrary. It comes from the fact that the input values of the BE code have an intrinsically random nature, with their associated probability distributions.

4 THE FUNCTIONAL OUTLIER DETECTION PROCEDURE

The methodology presented in this paper consists of several different stages:

- Design of experiments for the input variables in order to get the output functional data of the temperature for each set of inputs;
- Functional outlier detection on the output curves with the objective of identifying the simulations having an atypical nature;
- Estimation for each simulation of the probability of being an outlier through a bootstrap method;
- Quantification of the difference in the probability laws of the input variables conditioned to high outlying probability curves.

4.1 Design of experiments

The first stage is the generation of a design of experiments in the input variable space. For this PTS application, the number of input variables of CATHARE2 is fixed at $P = 10$, so the vector of inputs takes the form: $\{X_1, X_2, ..., X_P\}$, where every $X_p, p \in \{1, ..., P\}$ is a real-valued random variable. For every set of input parameters there is a functional output z_i, where $i \in \{1, ..., N\}$ indexes the simulation in the original design of experiments.

These P random variables model the most relevant input parameters for the simulation, and they are sampled accordingly to their estimated probability laws, given mostly by expert judgement and experimental results. In this case, the ten inputs of the code are modelled by uniform probability laws in their respective domains of variation.

The space-filling design algorithm that will be followed is a Latin Hypercube (LHS) design of experiments (see, e.g., [5]), and the total number of simulations is a compromise between the required simulation time and the dimension of the input space. In our case, the total number of simulations is established at $N = 100$, so for each simulated transient a set of ten realizations of the real-valued input random variables with its respective functional output is available: $\{X_{i1}, X_{i2}, ..., X_{iP}, z_i\}_{i=1}^{N}$.

4.2 Functional outlier detection

When a set of data is considered, regardless of its nature (multivariate or functional), certain objects of the set may have been produced by a different distribution than the vast majority of them. In other cases, even if the underlying distribution is shared by all the data, some of them can constitute extreme values of said distribution, i.e., they have a low probability of appearance. These data are usually called outliers. However, there is no formal definition of this concept, and outliers are

mostly defined as data within the studied set that behave in an abnormal way when compared to the majority of the data [11] [12]. Other authors, such as in [13], while staying general in the definition of outliers, make a distinction between magnitude (those which deviate from the normal set by a certain distance criterion), and shape (those which form is significantly different from most of the curves of a set) functional outliers.

In the context of nuclear transient simulations, an abnormal or atypical behaviour of a reduced number of simulations can be symptomatic of several relevant things. For instance, an atypical behaviour of a simulation can be representative of a severe transient, since in general, accidental transients may happen, but severe ones are supposed to have a very low probability of occurrence. Another important aspect is the validation of the simulators, since an abnormal simulation can be produced due to a failure in the simulation, and this may expose the existence of bugs, singularities or numerical and convergence problems in the code itself. These arguments justify the interest in functional outlier detection techniques applied to nuclear transients.

Since as we said, most functional outliers can be classified into the categories of magnitude and shape outliers, the usage of some functional descriptors specifically sensitive to the detection of these types of outliers would be a logical approach. In this work, two functional measures are retained thanks to their sensitivity to magnitude and shape differences, although the second is not a measure from a strict mathematical point of view. They are the *h-modal* depth [14] (also called *h-mode* depth) and the Dynamic Time Warping (DTW) [15] which is a measure of correspondence between temporal sequences that allows the comparison of their shapes.

4.2.1 The h-mode depth and the DTW

The *h-mode* depth is a definition of local depth due to the fact that it does not take into account the whole empirical sample of functional data, but only a slightly smaller window in order to guarantee to a certain degree that multimodality distributions can be detected. The *h-mode* depth of a realization $z \in \mathscr{C}([0,1])$ with respect to $Z \sim P \in \mathscr{P}(\mathscr{C}([0,1]))$ is defined as

$$h_M(z,P) = \mathbb{E}\Big(\frac{1}{h(P)} K\Big(\frac{\|z-Z\|}{h(P)}\Big)\Big), \tag{2}$$

where h is the bandwith and $K : \mathbb{R} \to \mathbb{R}$ is a kernel function. There are several kernel functions available, the Gaussian one being the most used:

$$K(t) = \frac{2}{\sqrt{2\pi}} \exp\Big(-\frac{t^2}{2}\Big),\ t > 0. \tag{3}$$

The other measure, the DTW, will be used mainly for shape outlier detection. It comes from the time series domain, and provides a measure of similarity and correspondence between two sequences of data. Given two sequences $X := (x_1, x_2, ..., x_N)$; $N \in \mathbb{N}$ and $Y := (y_1, y_2, ..., y_M)$; $M \in \mathbb{N}$, as well as a feature space $\mathscr{S}$ such that $x_n, y_m \in \mathscr{S}$ for $n \in [1:N]$ and $m \in [1:M]$, we can define a local cost measure (sometimes also called local distance measure) as the function:

$$c : \mathscr{S} \times \mathscr{S} \to \mathbb{R}_{\geq 0}. \tag{4}$$

An (N,M)-warping path is a sequence $p = (p_1, ..., p_L)$ with $p_l = (n_l, m_l) \in [1:N] \times [1:M]\ \forall l \in [1:L]$ which also satisfies the following conditions:

- Boundary condition: $p_1 = (1,1)$ and $p_L = (N,M)$;
- Monotonicity condition: $n_1 \leq n_2 \leq ... \leq n_L$ and $m_1 \leq m_2 \leq ... \leq m_L$;
- Step size condition: $p_{l+1} - p_l \in \{(1,0),(0,1),(1,1)\}$ for $l \in [1:L-1]$.

The total cost $c_p(X,Y)$ of a given warping path is:

$$c_p(X,Y) := \sum_{l=1}^{L} c(x_{n_l}, y_{n_l}). \tag{5}$$

Finally, an *optimal warping path* between X and Y is a warping path p^* having minimal total cost among all possible warping paths. Having defined this path, *DTW distance* $DTW(X,Y)$ between X and Y is defined as the total cost of the optimal warping path.

This way, if two curves are normalised, it is possible to compare the shape of curves by making use of modified versions of this DTW measure. In order to simplify the notation, from here onward both notions are expressed as:

$$h_M(z,P) \equiv d_{i,1}(z_i), \forall z \in (\mathbb{R}^Q)^{\mathscr{U}}, \tag{6}$$

$$DTW(z_i,z_j) \equiv d_{i,j,2}(z_i,z_j), \forall z_i, z_j \in (\mathbb{R}^Q)^{\mathscr{U}}, \tag{7}$$

$$\overline{DTW(z_i)} = d_{i,2} = \frac{1}{N}\sum_{j=1}^{N} d_{i,j,2}(z_i,z_j). \tag{8}$$

4.2.2 The Gaussian mixture model

The association of a value of depth for each functional datum z_i and of DTW for each pair of data z_i, z_j is the basis of our functional outlier detection technique. Since the outputs of the BE code will be considered functional random variables due to the probabilistic nature of its inputs, any measure applied to them shall be treated as a real-valued random variable. In this case, the h-mode depth and the DTW shall be denoted $\{D_1, D_2\}$.

The main idea of the algorithm is to fit a probabilistic model such as the Gaussian Mixture Model (GMM) to the two real-valued random variables that are supposed to quantify the degree of outlyingness in the magnitude and shape sense, i.e., the variables D_1, D_2, which will have a set of realizations depending on the original data: $\{d_{i,1}, d_{i,2}\}_{i=1}^{N}$.

Following this logic, a joint bivariate parametric probabilistic model to the pair of data $\{d_{i,1}, d_{i,2}\}$ for every functional datum z_i is fit. By proceeding this way, a particular curve can be considered as an outlier even if it does not have an extreme value with regard to both measures if they are looked upon independently, but the combination of its depth and DTW values can make it have an outlying nature.

The form of the GMM model is:

$$\hat{f}(d_1,d_2) = \sum_{k=1}^{K} \hat{\alpha}_k \mathcal{N}(\hat{\mu}_k, \hat{\Sigma}_k), \tag{9}$$

where $k \in \{1,..,K\}$ is the number of bivariate Gaussian probability functions of mean vector $\hat{\mu}_k$ and covariance matrix $\hat{\Sigma}_k$ with weight vector $\{\hat{\alpha}_1,\ldots,\hat{\alpha}_K\}$ such that $\sum_{k=1}^{K}\hat{\alpha}_k = 1$ and $\hat{\alpha}_k \geq 0$. The function $\hat{f}(d_1,d_2)$ is the joint probability density function (PDF) of the random variables D_1, D_2, which associates a depth and a DTW value to each functional realization. The estimation of all these parameters can be done through the Expectation Maximization (EM) algorithm [17].

4.2.3 Algorithm of outlier detection

Once the joint PDF is adjusted, it is possible to extract probabilistic conclusions on the random variables that are modelled. For instance, if a certain set of pairs of values of $\{d_{i,1}, d_{i,2}\}$ defines a closed region such that a certain percentage of probability mass of the PDF is kept, there is a notion of multivariate quantile that can be interpreted. More formally, if there exists a value q such that:

$$\int_{\mathbb{R}\times\mathbb{R}} \mathbb{1}_{\{\hat{f}(d_1,d_2)\leq q\}} = Q, \tag{10}$$

then the identity $\hat{f}(d_1,d_2) = Q$ defines a (closed, due to the convex nature of the GMM) curve that can be written as $\gamma = g(d_1,d_2) \equiv \partial D$, where D is the open domain in $\mathbb{R}\times\mathbb{R}$ with frontier defined by ∂D, and such that $\forall (d_{i,1}, d_{i,2}) \notin D$, z_i is considered to be an outlier.

Naturally, the estimation of the joint PDF is dependent on the estimated set of parameters $\{\hat{\alpha}_k, \hat{\mu}_k, \hat{\Sigma}_k\}_{k=1}^{K}$, which is dependent on the quantity of available functional data.

4.3 Estimation of the probability of being an outlier

In order to associate to each curve a probability of being an outlier, a practical way is to generate a bootstrap sample from the original curves and perform an estimation of $\gamma, \hat{\gamma}(d_1,d_2) = \gamma_{\{\hat{\alpha}_k,\hat{\mu}_k,\hat{\Sigma}_k\}_{k=1}^{K}}$ for each group. By proceeding this way, it could be possible to estimate confidence intervals for the estimated curve, or to associate a score to the likelihood of being an outlier. In summary, and taking the original curves $\{z_i\}_{i=1}^{N}$ as starting point, several bootstrap (sampling from the curves with replacement) groups are obtained, each one with the same number of samples from $\{z_i\}_{i=1}^{N}$. Then an independent GMM model is fitted to the data of each group through the EM algorithm, and the desired quantile curve γ is estimated for every group. By doing this, it is possible to quantify if every curve is considered an outlier by fulfilling the criterion of each bootstrap group.

More formally, if we have defined a certain number of groups B, indexed by b such that $b \in \{1,...,B\}$, then for each functional datum $z_i, i \in \{1,...,N\}$ it is possible to define a binary random variable W such that:

$$W = \begin{cases} 1 & if \quad z_i \notin D_b, \\ 0 & if \quad z_i \in D_b, \end{cases} \tag{11}$$

where D_b is the previously mentioned acceptance region (open domain) in $\mathbb{R}\times\mathbb{R}$ for the bootstrap group b. By doing this, there will be a realization of the random variable $w_{i,b}$ for each functional

datum z_i according to the criterion of each group b. Then, by computing the expectation of the random variable W_i for each z_i, it is possible to quantify a score that will be equivalent to the probability of being considered an outlier according to the aforementioned measures $\{d_{i,1}, d_{i,2}\}$. As an example, the value $\mathbb{P}(W_i = 1)$ quantifies the probability that the functional datum z_i is an outlier according to our criteria.

4.4 Link between input and output variables

Once a random variable (or probability measure) has been associated with every functional datum, it is possible to make an association between the input variables of the first model and the functional outputs (z_i) in order to quantify the degree of independence between them, which is interesting under the hypothesis that there can be a direct link between the anomalous behaviour of a simulation and nuclear safety.

One way of quantifying this dependence could be to measure the discrepancy between the original probability law of each input ($X \in \mathbb{R}^P$) and their conditional laws when some restrictions are imposed over the analyzed output curves. As an example, a magnitude of interest can be:

- Law of $(X_p|\mathbb{P}(W_i) > 0.9), \forall i \in \{1, ..., n\}$ compared to the law of (X_p).

By measuring some kind of distance between both distributions, we can quantify the influence of a certain input over the behaviour of the responses of the first model (the one that produces functional outputs) in the chain. A way of doing this is by using the Wasserstein measure [18], which is defined by:

$$W_p(\mu, \nu) = \Big(\inf_{\pi \in \Pi(\mu,\nu)} d(x,y)^p d\pi(x,y) \Big)^{1/p}, \tag{12}$$

where μ, ν are probability measures on the considered metric space , $\mathscr{X}$, and $\Pi(\mu, \nu)$ is the set of all joint probability measures on $\mathscr{X} \times \mathscr{X}$ whose marginals are μ and ν.

5 APPLICATION

The application of this methodology on our application case (see section 2) provides an ordering of the degree of outlyingness of the simulations of the PTS transient and was able to establish the link between the input variables of the expensive code CATHARE and its functional outputs. Through the use of $B = 50$ bootstrap groups, the probabilities of being an outlier (falling outside of the previously defined acceptance region) were estimated. The following step was the calculation of the Wasserstein distances of the laws of $X_p, \forall p \in \{1, ..., 10\}$, the input variables of the simulator (i.e., the prior probability law) and $(X_p|\mathbb{P}(W_i) > 0.5)$ (i.e., the conditioned law).

Now that the probabilities of being an outlier have been estimated for every curve, it is possible to represent in a histogram the values of the associated probabilities for the $N = 100$ curves (see Fig. 2). There is only a small number of curves that have a high probability of being considered as outliers.

The Figures 3 and 4 illustrate the prior and conditioned laws of two input variables. For X_6, the laws remain almost unchanged, while for X_4, the influence of the conditioning is made more obvious,

suggesting a certain importance of that particular variable when atypical behaviour is manifested in the functional outputs. In X_4, it is easy to appreciate the multimodality of the conditioned distribution when a certain level of outlyingness is demanded. This may suggest that there exists a relationship between the values that this variable takes and the distance of a transient (curve) to the zone where most data are located, the dynamics of the transient with respect to the others, or a combination of both.

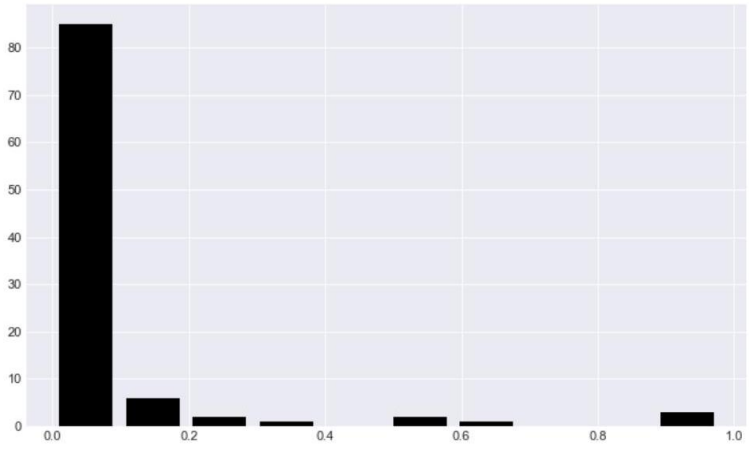

Figure 2: Histogram of the estimated probabilities of being an outlier for 100 simulated transients.

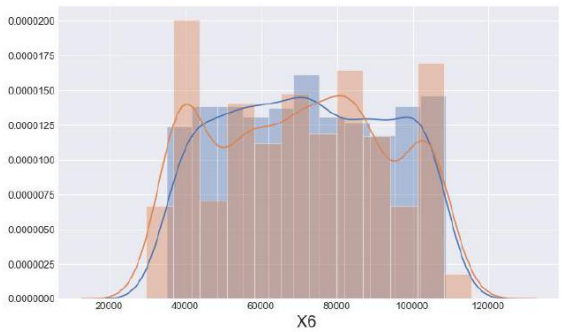

Figure 3: Prior (Blue) and conditioned (orange) density functions for the input variable X_6

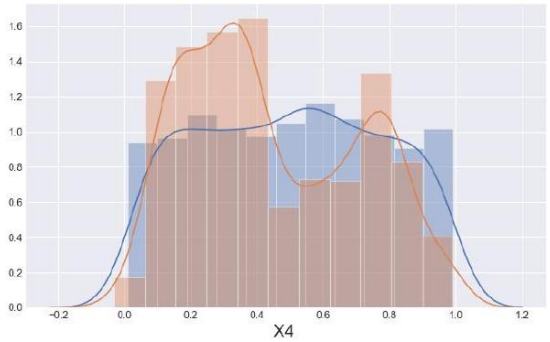

Figure 4: Prior (Blue) and conditioned (orange) density functions for the input variable X_4

Table 1 gives the scaled values of the Wasserstein differences between the prior and conditioned densities of the input variables can be generated, which provides an ordering of their importance with respect to the level of outlyingness of transients. Finally, an ilustration of the outlying curves according to this criterion is shown in Fig. 5.

Table 1: Wasserstein distances between the laws of every variable.

Variables	X_1	X_2	X_3	$\mathbf{X_4}$	X_5	$\mathbf{X_6}$	X_7	X_8	X_9	X_{10}
Distances	0.031	0.028	0.032	**0.074**	0.053	**0.020**	0.029	0.043	0.032	0.047

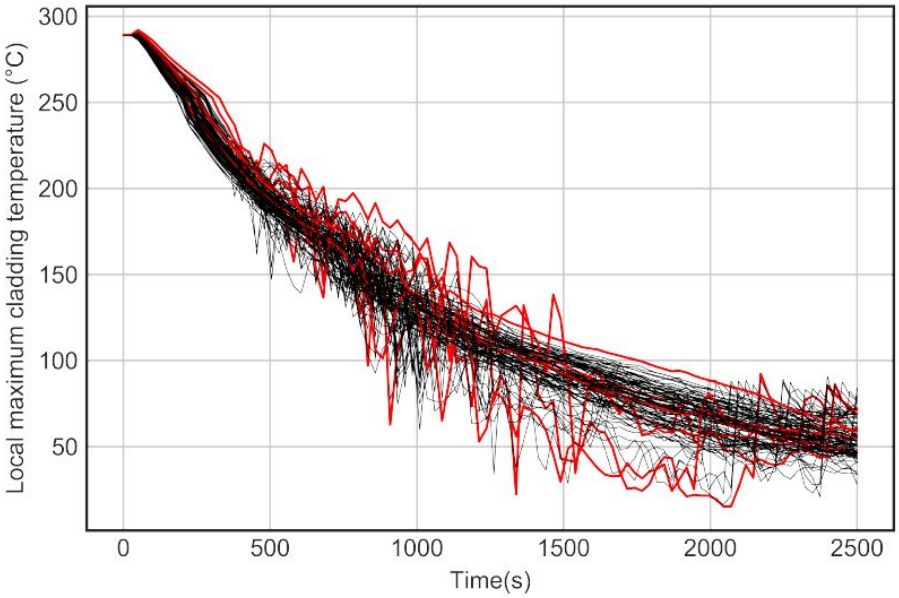

Figure 5: Outliers found (in red), according to the established criterion, amongst the 100 temperature curves.

The outliers have been found due to statistical criteria. The two measures that have been considered, the h-mode depth and the DTW have been particularly adapted to the detection of magnitude and shape outliers respectively, but the curves might have been chosen due to their outlying nature in any of those senses, or due to the combination of both criteria.

It is also possible to relate the input variables and the interactions between them to the outlying nature of the curves. We present the scatter plot in Fig. 6 as an example.

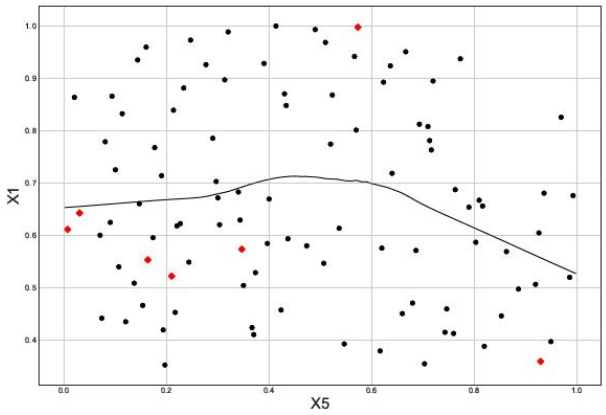

Figure 6: Outliers found according to the established criterion.

In this case, the plot presents the corresponding values of the input variables X_5 and X_1 in each simulation of the design of experiments. X_1 represents the jet condensation, whereas X_5 represents the friction coefficient of the water injected by the safety injection system. This variable is the second one presenting the highest distance between the prior and posterior distributions and, as it can be seen, most of the outliers are located in the region where both variables present low values. Both of the parameters are related to the maximum heat exchange that can be produced within the primary circuit during the transient, and so their low values influence the analyzed variable of interest (the Local Maximum Cladding Temperature), making it more extreme. However, these are obviously not the only parameters that intervene, and the non-linear interactions that result in the simulation of the transient can be of higher order and not appreciated in a two-dimensional graph. Therefore, a more in depth physical analysis is necessary in order to really quantify the link between outliers in the set of simulations and all the intervening parameters, for example by using interactive parallel coordinate plot diagrams as in [19].

6 CONCLUSIONS

This paper has shown a new functional outlier identification methodology suitable to be applied to nuclear thermal-hydraulic transients. This identification tool can be used for the automatic identification of penalising scenarios, and most of all, for the identification of the transients presenting atypical behaviours which might be associated with non expected physical phenomena. The main contributions of that can be noted are:

1. Definition of descriptors that allow the probabilistic quantification of the degree of outlyingness of every object in a set of functional data;

2. Establishment of a measure of the influence of the input variables of a simulator over the degree of outlyingness of its outputs.

More details and numerical tests about this functional outlier detection technique are given in [20].

The usefulness of the identification of outlying simulations in the context of nuclear safety is twofold. First of all, and taking into consideration the fact that nuclear power plants are supposed to be robust against severe accidents, it is logical to assume that those simulations where the safety margin becomes too small or it is even surpassed will likely have an outlying nature. The precise physical analysis of the simulations whose the outlyingness is considered to be high should provide more useful insight regarding nuclear safety than the others. The second main advantage is the validation aspect of the system codes that are used to simulate nuclear transients. Since the underlying physics of these transients are considerably complex (high influence of non linearities), it is not possible to verify every single aspect of every simulation in order to validate the code. The use of of functional outlier detection techniques can help improve this process by automatically targeting simulations with an anomalous behaviour that should be primarily analysed.

An important perspective of this work is the association of the criteria that have been presented with the nuclear safety criteria and margins, studying how the outlying nature of some simulations might be related to these margins from a quantitative point of view. The other main branch of improvement of the work is related to the physical side of the problem, and concerns the detailed analysis of the physical phenomena that occur in the outlying simulations when they are compared with the *normal* ones, see some first attempts in [21, 22] on other nuclear transients.

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