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A SELF-LEARNING DIGITAL TWIN FOR PROCESS CONTROL OF FAST PROCESSES UNDER UNCERTAINTY

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Abstract. *With the recent developments of sensor technologies appear new opportunities for conducting increasingly efficient and close control of industrial processes. This paper proposes a new scheme for near real-time process control of extremely fast complex processes using the framework of digital twins and an adaptively calibrating grey-box model. It focuses specifically on processes for which first-principle based numerical simulation is computationally expensive, and orders of magnitude slower than the physical process itself (e.g., spot welding). In this context, the goal is to adjust the process parameters based on a digital twin in order to maintain satisfying performance under non-deterministic process drift. In order to alleviate the time discrepancy between the process and its numerical simulation, the control scheme is coupled with a Kriging surrogate providing faster approximated performance evaluations. The surrogate is associated with an adaptive refinement scheme to reduce the computational burden associated with its calibration and actively maintain satisfying accuracy in any state of the process drift. To do so, a dedicated learning function is developed to guide the refinement as well as criteria to detect when process adjustment, surrogate refinement and refinement termination are necessary. The performance of the proposed approach is studied on three benchmark analytical cases through confusion matrices of the control decisions.*

Keywords: Digital Twin, Process control, Kriging, Surrogate modelling, Learning function.

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1 INTRODUCTION

The development of sensor technologies and modelling techniques enable continuous monitoring in many industrial fields, e.g., structural health monitoring for civil engineering [1]. In the context of production processes, they provide opportunities to asses the current state of the process with increasing frequencies thus allowing finer process control [2]. The principle is, based on frequent quality assessment, to adjust the process through control input parameters to maintain satisfying quality and reduce the occurrence of faulty products. This can improve the product quality and reliability, potentially extending the lifetime of the product while reducing maintenance and production costs [3]. The goal of automatic process control is to develop efficient schemes performing such a task automatically. Process control problems generally consider two sets of variables affecting the system. The control parameters can be adjusted within acceptable limits and represent the user-defined parameters. The state variables represent the current state of the system. Their current values can only be known or estimated from monitoring. Furthermore, some of these often evolve in a way that cannot be deterministically predicted, especially when they are related to non-controllable or environment induced effects, e.g., wear and tear of material or dust accumulation over time.

Automated process control necessitates the prediction of the influence of the control parameters on the product quality considering the current state of the system. While this influence is unknown for closed-loop systems [4] it can be estimated through a numerical model. In this context the popular framework of digital twins [3] is extremely relevant. Its principle is to couple a numerical model of the system with the monitoring feedback to continuously update the model parameters to the current state of the system. The digital model can in turn change the physical state, e.g., by adjusting the input parameter [5]. In addition to the accuracy of the model used in the digital twin, the computation time associated with its evaluation is of critical importance for process control. The quality assessment, prediction as well as control decision need to be obtained faster than one process cycle in order to reach so-called real-time control. This real-time process control is of high importance in manufacturing, as it enables the early detection and correction of any deviations from the desired product quality. This becomes more challenging the faster the process cycle gets, and usually makes the problem intractable for extremely fast and complex processes. Near real-time control consists in performing adjustment for several process cycles in advance and can be an efficient solution for these cases. However, the spot welding process considered in this study is an extreme example with a process cycle in the order of milliseconds while the computation of the dynamical multi-physics model requires several hours, making also classical near real-time approaches unachievable based on such a model.

Recent work proposes the use of grey-box models [6] coupled with an active learning-scheme as a fast digital twin. Grey-box models aim at efficiently combining white-box physical models with black-box data-driven ones. This work adopts this approach, under the assumption that an accurate physical model of the process is available but requires a computation time that is orders of magnitude larger than the physical process cycle itself. The proposed strategy is to associate the physical model with a calibrated surrogate model that emulates its behaviour without simulating the physics and thus requiring only a fraction of the computation time. Surrogates however induce an extra approximation error related to the quality of their calibration. Moreover, while the evaluation of a surrogate is very fast, its calibration is done based on a number evaluations of the physical model which induces significant computational burden. Many types of regression models have been proposed as surrogates such as Gaussian processes (also known

as Kriging) [7, 8], Neural Networks [9],polynomial chaos expansion [10], response surface models [11] or support vector machines [12]).

The first type provides, in addition to an estimation of the model response, a localized estimation of the uncertainty related to this prediction. This information allows the development of so-called adaptive learning schemes [13, 14] aiming at building a near-optimal calibration data base tailored to the predictive accuracy of the surrogate. Assuming the surrogate evaluation is used to monitor a problem-dependent quantity of interest (QOI), one can expect that the influence of surrogate inaccuracies on the QOI predictions are not homogeneous through the input space. The idea is then to adjust the accuracy of the surrogate such that areas of great importance are finely calibrated. Adaptive-calibration schemes iteratively build a calibration data-base by identifying the samples that have the highest expected contribution to the uncertainty reduction of the QOI. The readers are referred to section3 for more details. This calibration scheme is used in this work as a way to actively ensure that the surrogate stays accurate despite the evolution of the state parameters due to process drift. As such, this surrogate can be seen as a self-improving digital twin [5, 3], able to continuously evaluate and update itself based on the state of the physical process.

The ability of such a model to predict the quality of future processes relies, apart from the accuracy of the model, also on an estimation of the state parameters evolution. As previously stated, this process drift usually cannot be extrapolated deterministically. Yet, non-deterministic approaches allow us to obtain estimations within uncertainty bounds. While often critical, this particular problem is not addressed in this work. We simply consider process drift as a stochastic process calibrated from past monitoring data which, while remaining a simple approach, preserves the main properties we can expect from such a model.

The focus of this work is rather on the grey-box surrogate based digital twin methodology. More specifically, the process control scheme requires several criteria to decide which action to take in any given situation. Three main criteria are presented and discussed in this paper. The first one aims at identifying when the quality of the next few processes is at risk. Based on this criterion the algorithm can identify if adjustment of the process control parameters is necessary. When no satisfying solution can be found, the algorithm will attempt to refine the calibration of the surrogate. The active calibration relies on a so-called learning function that can be seen as a criterion to define which sample should be selected to refine the calibration. Finally a stopping criterion is needed to indicate when the calibration loop should stop.

In the following section, the methodology of the proposed digital twin is detailed. In section 3, the adaptive Kriging scheme and its principal components, the learning function and its stopping criterion, are presented, followed by an application on a benchmark problem and its results in section 4. Here the convergence of the learning function and the choice of an appropriate stopping criterion are discussed in further detail. Lastly, the paper concludes with the conclusions and future outlook.

2 METHODOLOGY

2.1 Process definition and variables

In the methodology development, we simplify the problem to a process affected by two types of time dependent variables: the state variables $\mathbf{x}$ and the control variables $\mathbf{v}$. We assume that the process output represented by $y(\mathbf{x}, \mathbf{v})$ is completely determined by these variables. In this, the state variables $\mathbf{x}$ represent the uncontrollable process variations. We consider those to be affected by process drift and as such unpredictable in a deterministic sense. While the evolution

of $\mathbf{x}$ is not known beforehand and also cannot be influenced, its past instances can be measured. Based on those measurements, a stochastic estimation for the evolution of $\mathbf{x}$ can be made. In this work it is proposed to fit a Gaussian process from the previous time-series and predict the amplitude of possible next values considering confidence intervals (see section 4). The second set of parameters $\mathbf{v}$ represents the input or control variables, which are used to counter the process drift through control actions.

We associate a function $y(\mathbf{x}, \mathbf{v})$ with the process. The time is assumed to be discrete where one time step equals to one process. As such, time is not directly included as an input of the model. Each process cycle therefore is associated with the coordinates of the input space corresponding to its state and control parameters. The function output represents the physical output QOI of the process reflecting the process performance as a function of the state and control variables. In practice, this represents a product quality measure, like e.g., the nugget diameter in spot welding. It is assumed that the first-principle based evaluation of this function for a given parameter set (e.g., using a multi-physical finite element model) is extremely hard, and requires a computational effort several orders of magnitude larger than the physical process itself. Therefore, we propose to use a surrogate model as digital twin.

2.2 Grey-box digital twin

The proposed surrogate is a grey-box model consisting of a white-box physical model as well as a black-box Kriging meta-model [15], trained on evaluations of the first. The Kriging model is based on a Gaussian process, calibrated using a design of experiments (DoE) of realisations over an input $(\mathbf{x}, \mathbf{v})$-domain using the white-box model. After calibration, this Kriging model provides a prediction of the system behaviour at untrained parameter combinations in the shape of a Gaussian random variable, which can be described by its localised mean $\hat{\mu}$ and variance $\hat{\sigma}^2$. The hat symbol is used to indicate estimated results as compared to true ones. The mean can be considered as the surrogate's best guess and the variance as an indicator of the confidence with regards to this estimation [14]. The ability to assess its own local accuracy is the biggest advantage of Kriging over other surrogate techniques and makes it well suited for adaptive refinement, which aims at reducing the number of necessary full model evaluations by trying to find a near-optimal DoE. Adaptive refinement means that the black-box model is initially trained on only a limited number of white-box model evaluations, limiting the precision of its predictions. Next, new samples will be added to the DoE in order to refine the model for the most effective parameter combinations only. The key-idea of the proposed method is that this adaptive refinement is performed on-line. That is, the adaptive refinement can be performed during the process control and does not have to be performed beforehand. This allows to refine only if required from the process drift observations or predictions, and only in the area of interest to limit time-consuming evaluations of the physical model. This is also referred to as an adaptive Kriging meta-model [13, 16, 14]. The active refinement process is described in more details in section 3. This section now first introduces the reliability based control strategy.

2.3 Reliability based control strategy

Due to the assumed time discrepancy between simulation and effective process cycle, real-time process control is difficult to achieve, even associated with a surrogate. Process control is therefore assumed to be performed over multiple processes at once. The ambition of this work is to propose a method adaptable enough to accommodate a wide range of time discrepancies between the computation times of the physical model, the surrogate and the process cycle. Such

a method would then adapt to any given situation by adjusting the number of cycles that have to be predicted at once.

Consider an arbitrary step i of process control. The goal before the next cycles occur is to find the input v_{opt} that guarantees maximal reliability (i.e. probability of satisfactory process quality) over the next t_n steps. The reliability is in general assessed using a performance function $g(\mathbf{X})$, which is formulated so that $g(\mathbf{X}) < 0$ corresponds to system failure. Hence, the input space can be divided into a safe and a failure domain and the actual value of $g(\mathbf{X})$ is of little interest as long as the sign is known. In the specific case of this work, the problem can be seen as a classification problem where the so-called limit state function $g(\mathbf{x}, \mathbf{v}) = 0$ defines the boundary between the failure and safe domains. Given a critical lower bound value y_{crit} for the QOI (e.g., minimal acceptabel nugget diameter), this limit state function would be defined by

$$g(\mathbf{x}, \mathbf{v}) = y(\mathbf{x}, \mathbf{v}) - y_{crit}. \tag{1}$$

The limit-state as well as the performance function are not known analytically and each evaluation requires the evaluation of the physical model. In the context of the surrogate-assisted process control, the Kriging model is trained to emulate the performance function g and provides Gaussian predictions $\hat{g} \sim N(\hat{\mu}(\mathbf{x}, \mathbf{v}), \hat{\sigma}(\mathbf{x}, \mathbf{v}))$. The anticipated reliability of a process should then be understood in the sense of the probability, according to the surrogate uncertainty, that the process will produce satisfactory output.

Generating the initial Kriging model with n_{ini} samples, is the first step within the control loop. In the second step, the effect of the process drift is assessed and the evolution of the state variable x for the next t_n processes is extrapolated. Only confidence bounds are extracted from this extrapolation, and no distribution is assumed. These bounds then define the interval $\hat{\mathrm{I}}_x^i$ of possible x of the next t_n time steps.
In the third step, it is estimated, whether adjustment of the input v for the next t_n time steps is necessary, by calculating the estimated reliability $\hat{R}$ defined as follows:

$$\hat{R} = 1 - \Phi\left(\frac{-\hat{\mu}(\mathbf{x}, \mathbf{v})}{\hat{\sigma}(\mathbf{x}, \mathbf{v})}\right) \tag{2}$$

with Φ the standard Gaussian cumulative distribution function and $\hat{\mu}$ and $\hat{\sigma}$ the mean and standard deviation of the Kriging model at the $(\mathbf{x}, \mathbf{v})$ coordinates of the input space. This quantity corresponds to the probability given by the Kriging model, that $\hat{g}(\mathbf{x}, \mathbf{v})$ is positive and thus that the performance is in the safe domain. This reliability metric is associated with a user defined threshold R_{min} such that the anticipated reliability of a process is unacceptable if the reliability value is smaller than R_{min}.
To avoid needless adjustments of the process parameters it is proposed to first test the reliability of the next processes considerng the current set of process parameters v_{i-1}. To do so an optimization problem is solved to find the minimal reliability value $\hat{R}_i$ (i.e., worst-case scenario) within the interval of state parameters I_x^i:

$$\hat{R}_i = \min_{x \in \hat{\mathrm{I}}_x^i} \left(\hat{R}(y(x, v_{i-1}))\right) \tag{3}$$

If $\hat{R}_i > R_{min}$ then the current process parameters are sufficient and kept unchanged for the next processes and $v_i = v_{i-1}$. Otherwise, a nested optimization problem is solved in order to find the set of process parameters associated with the highest $\hat{R}_i$. These process parameters have the maximal worst-case reliability and can be seen as the most reliable parameters according to

our current knowledge of the system. This "maximal worst-case reliability" values $\hat{R}_{opt}$ is then evaluated as follows:

$$\hat{R}_{opt} = \max_{v \in \mathrm{I}_v} \min_{x \in \hat{\mathrm{I}}_x^i} \left(\hat{R}(y(x,v)) \right) \tag{4}$$

If $\hat{R}_{opt}$ satisfies the reliability criterion the process parameters are changed to the optimal value and the process continues. In the case the reliability criterion is still not met and $\hat{R}_{opt} < R_{min}$, it needs to be assessed whether that is due to a badly trained Kriging model or if no solution exists. Indeed, the reliability is related to the Kriging surrogate uncertainty and so the lack of satisfactory process parameters could be only due to insufficient calibration of the surrogate. Or in other words a solution could exist outside of the well-calibrated domain. The details about the refinement of the surrogate are provided in section 3. If the refinement yields satisfying results, the newly optimised control variable v_i can be used for the next processes. If however, the requirement is not met even after refinement, it is assumed that no satisfactory v_i can be found and the process is expected to fail. Depending on the application, either a warning can be given or the process can be halted and operator action requested. Through this procedure, the process parameters are only changed and the Kriging surrogate only refined when needed.

3 KRIGING MODEL

The Kriging model was chosen as a black-box model due to its ability to assess its own uncertainty. This feature makes it well suitable to adaptive refinement. It is a well established surrogate modelling technique, that originated in global optimisation by Jones et al. [13] and became popular for reliability analysis through adaptive Kriging Monte Carlo Simulation (AK-MCS) by Echard et al. [14]. Here the Kriging model is used to emulate the performance function $g(\mathbf{X})$ with $\mathbf{X} = [x, v]$ a Gaussian random variable with mean $\hat{\mu}$ and standard deviation $\hat{\sigma}$. The Kriging model assumes that its samples are a realisation of a Gaussian process where $\hat{\mu}$ indicates its estimated performance. Its standard deviation $\hat{\sigma}$ indicates the model's local accuracy.
The latter has allowed the development of adaptive sampling approaches in order to minimise the effect the modelling error has on the quantity of interest [13, 14]. Here, a near optimal design of experiments (DoE) is formed over time by starting with a rough initial model and adding new samples to the DoE over time and only if necessary. The samples of the DoE are evaluated on the full white-box model and as such require a relatively high computational effort. Each added sample should hence be valuable for reducing the modelling error. This value is estimated through the learning function. The model is refined until a stopping criterion is met. While adaptive surrogate techniques are of general interest, they are more so in an on-line monitoring and control aspect, as the process drift might push the process into a previously unknown area. Through refinement, the control can still be performed adequately. A more detailed introduction to Kriging is provided by Moustapha et al. [17].

3.1 Learning function

The goal of the learning function is to guide the calibration of the surrogate to build a near-optimal DoE. Optimality can be seen in this context as the compromise between the extent of the DoE (i.e., the computation effort required for the calibration) and the uncertainty related to the quantity of interest evaluated with the surrogate. The learning function highly depends on the quantity of interest (e.g., the reliability of the system) and the way it is estimated (e.g., sampling, optimization, ...). However, learning functions usually aim at estimating the contribution of a

sample to the (surrogate induced) uncertainty of the quantity of interest, or in other terms, the expected reduction of this uncertainty from evaluating the sample.

In the context of the proposed process control scheme, the goal of such a refinement is to find a set of process parameters satisfying the reliability constraint as defined in section 2. This goal can also be seen as trying to find, by refinement of the Kriging model, a set of process parameters v^* such that the entirety of the state interval $\hat{\mathrm{I}}_x^i$ falls in the safe domain. The proposed learning function bears some similarity with the learning function of the EGO algorithm called the expected improvement. Being an algorithm for global optimization, EGO defines the learning function as the expected improvement of the current optimum associated with the sample's Kriging prediction. In the context of the process control algorithm the same concept could be seen as the expected expansion of the safe domain within the bounds of the state parameters interval. The proposed learning function is a first approach aiming at approximating this quantity and can be defined as follows. Consider a sample with process parameter coordinates v and within the bounds of the state parameter interval $x \in \hat{\mathrm{I}}_x^i$. The proposed learning function is the product of the probability that the sample falls in the safe domain multiplied by the Euclidean distance between this sample and the closest one belonging to the safe domain and sharing the same parameter coordinates v and reads as follows:

$$L = \Phi\left(\frac{\hat{\mu}}{\hat{\sigma}}\right) \cdot \mathbf{L}^{\mathbf{E}} \quad \forall x \in \hat{\mathrm{I}}_x^i,\, \forall v \tag{5}$$

with the first term being the probability of safety and L_j^E the Euclidean distance of the closest sample, sharing the same process coordinates and belonging to the safe domain:

$$\begin{aligned} L_j^E &= \min\left|(x_j, v_j) - (x_k, v_k)\right| \\ \text{for } x_j \in \hat{\mathrm{I}}_x^i,\; v_j &= v_k \text{ and } \hat{g}(x_k, v_k) > 0. \end{aligned} \tag{6}$$

The sample chosen for enrichment of the DoE X_{DoE}^i is then the sample having the highest learning function value.

$$X_{DoE}^i = \max_{x_j, v_j \in [\hat{\mathrm{I}}_x^i, \mathrm{I}_v^i]} L(x_j, v_j)$$

While this quantity is not directly related to the expected expansion of the safe domain within the bounds of state parameters it proposes a trade-off between exploration and exploitation that shares the same purpose. Adding a new sample that is very close to the known safe domain is more reaffirming the expectation than adding new and usable information. For samples far away from the safe domain however, the probability that they are within the safe domain and as such expand the safe domain greatly, is diminishing low. The domain of search is also limited to the interval $\hat{\mathrm{I}}_x^i$ since the rest of the input space has little effect of the reliability prediction of the next processes.

3.2 Stopping criterion

The development of a stopping criterion is essential to achieve a near-optimal, cost-efficient adaptive Kriging model. If the refinement stops too soon, the process control will be non-optimal and its reliability is less trustworthy. In order to have an efficient algorithm, the refinement should stop as soon as the information gain is negligible. As a first stopping criterion it is then proposed to consider a thresholds C_L for the learning function value of X_{DoE}^i such that

if the optimal sample provides an expected improvement smaller than the threshold the refinement stops. In addition, since the learning function values tend to be quite noisy between the different calibration loops, it is proposed to couple the first criterion with a second one aiming it indicating convergence. This second criterion consist in a threshold for the variation of selected learning function values such that the algorithm stops if the variation is smaller than the threshold twice in a row:

$$\Delta L_i \leq C_{\Delta L} \quad \text{and} \quad \Delta L_{i-1} \leq C_{\Delta L} \tag{7}$$

with

$$\Delta L_i = \frac{L_i}{L_{i-1}}. \tag{8}$$

4 CASE STUDY

In this section, the convergence and appropriate stopping criteria C_L and $C_{\Delta L}$ are discussed based on a case study with three analytical limit state functions in dimension two.

A) Four branch limit state function [14, 18, 19] (Figure):

$$g(x,v) = \min[g_1(x,v), g_2(x,v), g_3(x,v), g_4(x,v)] \tag{9}$$

with

$$\begin{aligned} g_1(x,v) &= k_1 + \tfrac{(x-v)^2}{10} - \tfrac{x-v}{\sqrt{2}} \\ g_2(x,v) &= k_1 + \tfrac{(x-v)^2}{10} + \tfrac{x-v}{\sqrt{2}} \\ g_3(x,v) &= x + v + \tfrac{k_2}{\sqrt{2}} \\ g_4(x,v) &= -x + v + \tfrac{k_2}{\sqrt{2}} \end{aligned}$$

ant $k_1 = 3$ and $k_2 = 7$.

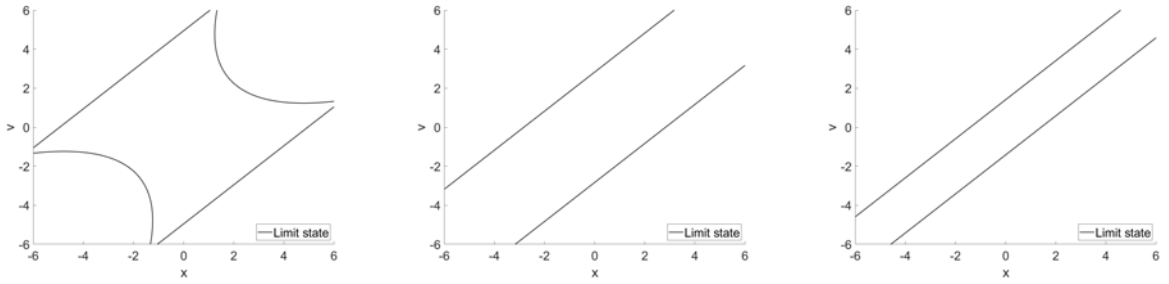
B) and C) Limit state functions consisting of two linear parallel limit states

$$g(x,v) = \min[g_1(x,v), g_2(x,v)] \tag{10}$$

with

$$\begin{aligned} g_1(x,v) &= 0.5 \cdot (x+v) + \tfrac{k_1}{\sqrt{2}} \\ g_2(x,v) &= 0.5 \cdot (-x+v) + \tfrac{k_1}{\sqrt{2}} \end{aligned}$$

with $k_1 = 2$ for a wide safe domain and $k_1 = 1$ for a more narrow safe domain.
While the edge cases of the four branch limit state function are a challenge, v is often times not forces to change, as there is a large safe domain for less extreme x-values. The linear limit state functions were chosen in order to force the change of v over the course of the process drift regularly. The wide one is the simpler to solve case, as it allows to find a v_opt for which $\hat{\mathrm{I}}_x^i$ lies completely inside the safe domain, whereas the narrow one induces multiple cases with no v that can guarantee all processes lie in the safe domain.



(a) Four branch limit state function (b) Wide linear limit state function (c) Narrow linear limit state function

Figure 1: Illustration of the three considered limit-state functions

In these applications it is assumed that the time discrepancy between the process cycle and the control cycle imposes us to conduct control over four processes at a time for a total of 100 processes. As introduced in section 2 an arbitrary process drift function is considered as follows:

$$x = -\sin\left(\frac{\pi \cdot t}{10}\right) - 2\sin\left(\frac{\pi \cdot t}{45}\right) - 3\sin\left(\frac{3\pi \cdot t}{50}\right) \tag{11}$$

This function represents an extreme case with a very fast and non-monotonic evolution of the state variable. The process-drift function is used to generate the successive coordinates of state parameters but is assumed unknown to the process control scheme. Based on the previous values of the state parameters a Gaussian regression model is calibrated and a confidence interval is extracted for the values of the state parameters of the following four processes. For each following process the $[\mu \pm 2\sigma]$ is extracted and the global confidence interval is considered as the lowest, respectively highest of the four lower (resp. upper) bounds. The true process drift and its estimation intervals per 4 processes is displayed in figure 2 for the sake of illustration. It is noted, that this example is a toy example meant as a first illustration of the approach. It is neither a representative example of expected process drift, nor is Gaussian process regression recommended for most real process drifts.

The black-box model was initially trained on 10 Latin hypercube (LH) samples with four different seeds. The Kriging model was evaluated on a set of $2,000,000$ samples drawn from the Latin-hypercube sampling scheme. The required reliability R_{min} was chosen to 0.1. In addition, in order to study the sensitivity of the method to the stopping criteria C_L and $C_{\Delta L}$ defined in section 3.2, respectively four and two values were tested: $C_L = [0.1, 0.01, 0.005, 0.001]$ and $C_{\Delta L} = [0.1, 0.2]$. In total, 32 different settings were tested for each limit state function.

An example of the process control result of the linear, wide limit state function is given in figure 3a and figure 3b. The crosses indicate the selected optimal v and the corresponding actual values of x. While red crosses indicate that the process set was estimated to fail by the algorithm, the colour gradient displayed for the processes estimated to be safe, indicates the order of the processes to show the process drift.

It can be seen, that the optimisation works satisfyingly and the majority of processes lie within the safe domain and are classified as such. For the other two limit state functions, which were more challenging, similar results can be seen (Figure 3c and 3d), although the accuracy

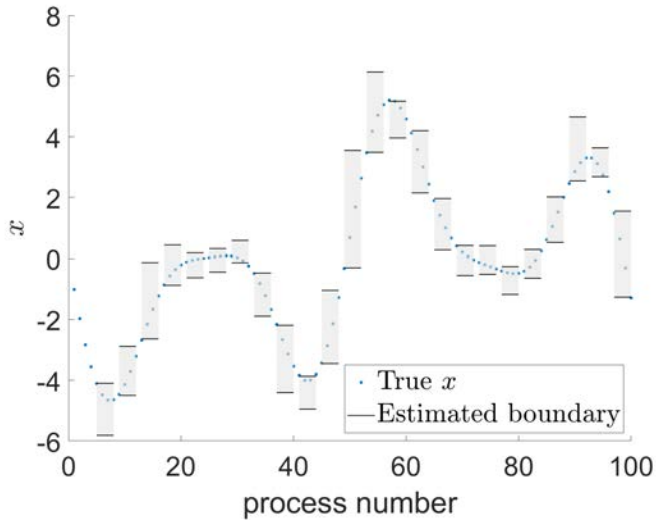
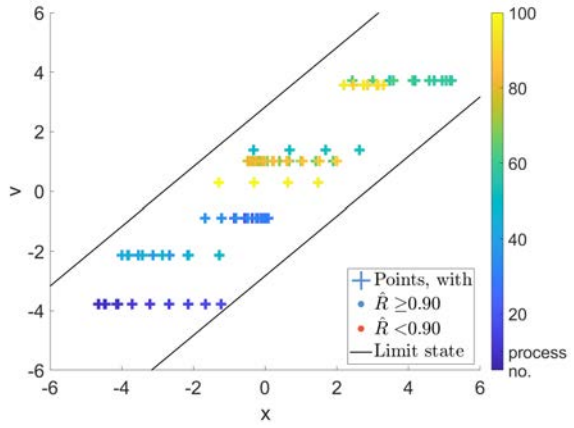


Figure 2: The true process drift and the estimated intervals $\hat{\mathrm{I}}_x^i$ used for the control parameter estimation.

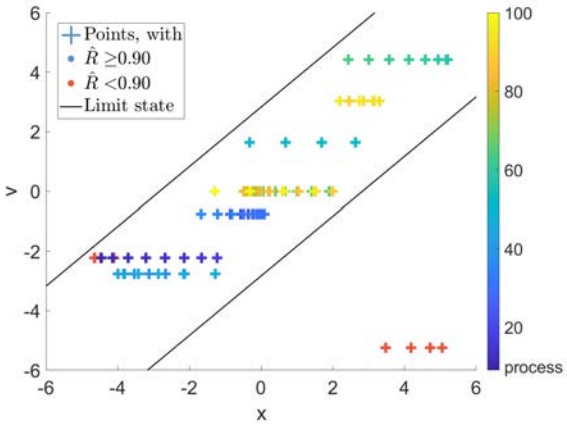
decreased. As a reminder, the narrow linear limit state function was designed in way that interval of possible next x-values is larger than the safe domain, which unavoidably leads to processes in the failure domain and through which misclassification is increased as well. As expected, the optimisation results are less accurate and misclassification occurs more often, although they are still fairly satisfying.
In figure 3b and figure 3c it can be observed that for a set of processes, the optimisation result is very far from the safe domain and the optimisation result does also not comply with what was expected based on the Kriging model at that state. A problem in the global optimisation scheme rather than the refinement of the Kriging is suspected. It is possible, that the global optimisation remains stuck in a local maximum. The origin of those issues is till unclear at this early stage of development but several leads will be explored such as the global optimization algorithm used, the reliability and stopping criteria as well as the learning function.

The Kriging model was enriched between 10 to 30 times, although a larger effect from the initial Kriging model was seen than from the variation in stopping criterion. Previously, a different stopping criterion was tested as well, where $\Delta C_L i$ of the current process was the only criterion. Here, larger differences between $\Delta C = 0.1$ and $\Delta C = 0.2$ were observed.

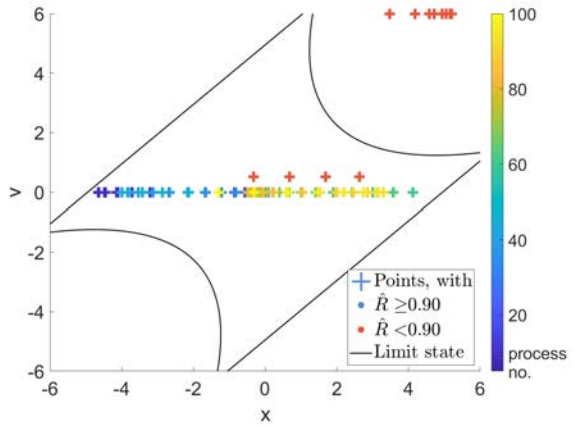
The performances of such a process control scheme are difficult to study quantitatively since what is expected form the method is to make accurate process control decision depending the current state. It then proposed as an illustrative result to draw the confusion matrices of the process control associated with the three limite-state functions considered. The control decisions are divided into four different groups: true positive (tp), true negative (tn), false positive (fp) and false negative (fn). True positive means that the process lies within the safe domain and was correctly classified as well. Similarly for the true negative classification the process failed but it was properly detected. The false classifications are more problematic, especially the false positive. In the case of the false negative more production effort is excerted, e.i. material is thrown away and reproduced, which can have a monetary impact. In the case of false positive classification however, a faulty product is trusted, which can lead to unexpected failure impacting human lifes in the worst case. An illustrative example of the four cases i given in Figure 4 for the sake of clarity.



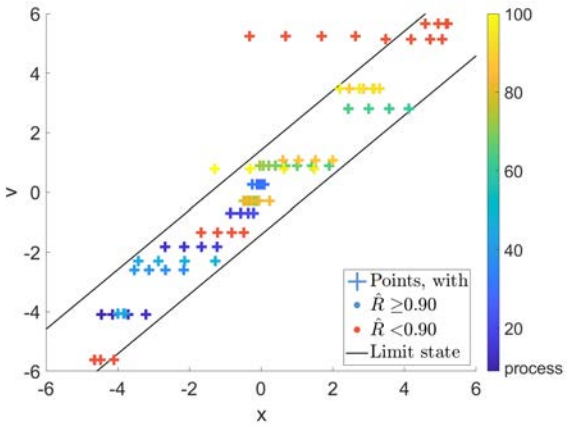
(a) Linear limit state function (B): no misclassification, no failed processes.



(b) Linear limit state function (B): two misclassified samples



(c) Four-branch limit state function (A): No misclassification, one set of failed processes.



(d) Linear limit state function (C): Multiple failed processes and misclassification.

Figure 3: Four illustrative example results of process control over 100 processes

In terms of the classification, identifying the true state is the optimal outcome and false positive values need to be avoided by all means possible. Table 1 shows the total classification for each of the 32 cases of each limit state function. The classification for the four branch limit state function is very good without any false positive classifications. While the classification of the wide linear limit state function has false positive classifications the amount of misclassification is significantly less. It was observed that while for both limit state functions the misclassification was little and relatively consistent, there were very few cases with significantly more misclassification. For the narrow linear limit state function the misclassification is significant.

The seed had a larger effect on both the confusion matrix and the number of refinement steps, which could indicate that the initial design of experiment has a significant impact on the performances. It is therefore difficult to draw sharp conclusions on the influence of the stopping criterion and further investigations are necessary. Based on previous results, it was expected that $\Delta C = 0.2$ and $C = 0.005$ would provide a good ratio between added samples to the DoE and thus computational effort and accuracy of the results.

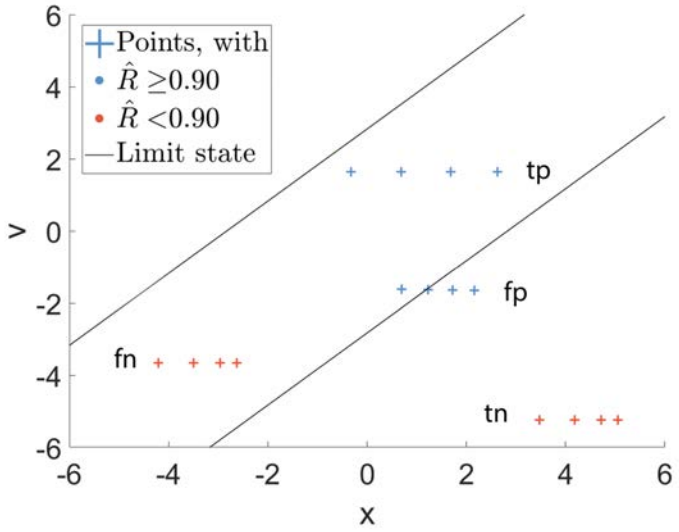


Figure 4: Example to show the meaning of the items of the confusion matrix: true positive (tp), true negative (tn), false positive (fp) and false negative (fn).

Example		LSF (A)		LSF (B)		LSF (C)	
tn	fn	13	5	0.01	0.07	18	7
fp	tp	0	82	1.43	98	8	67

Table 1: confusion matrix for total sum of the each limit state function. Values in %.

5 CONCLUSION

In this paper, a digital twin to perform reliable and robust process control for highly dynamic processes is presented, that is able to address the time discrepancy between process and simulation time as well as effectively cope with unexpected process drift. It makes use of the advantages of grey-box modelling by utilising an adaptive Kriging black-box model, that is trained on white-box evaluations of a numerical model of the process. Cost efficiency can be achieved, by generating a near-optimal DoE that is reliable only in the areas of interest. While it was surprising to see the large effect the initial Kriging model can have, the experimentation set these results come from is rather small and should be extended in order to draw significant conclusions. In order to improve this, different Latin-hypercube sets should be used as well as multiple process drift functions. Furthermore, in order to test the robustness, the sensitivity to the initial control variable v_0 should be tested as well. The sensibility of the method to other parameters is also part of further research. Regardless of the immaturity of the method, the authors were able to show, that the performance is satisfying and promising. Extending on that in the future, detecting the available time to refine the Kriging model based on the evolution of the process drift and adjusting the number of processes that share an optimisation result based on the local size of the safe domain, are promising adjustments to improve the methodology in a real application context.

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