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SURROGATE MODELING CONSIDERING MEASURING DATA AND THEIR MEASUREMENT UNCERTAINTY

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Abstract. *Virtual approaches to manufacturing processes are a common tool in developing components today. Simulations are always containing uncertainties like simplifying assumptions in computer aided modelling, material deviations, fluctuating external loads or other known and unknown influences. To integrate such uncertainties in an early design stage, the input parameters should be defined as intervals, because insufficient data may be available at this stage to provide probability distributions. To consider such epistemic uncertainties, a large number of intervals can be merged into a fuzzy number. For each interval a membership value is assigned which depends on the interval limits and an expert estimation. However, this interval modelling leads to a very high number of expensive evaluations, which is not feasible for a high number of uncertain input parameters. To reduce the calculation time, surrogate models are used. Here, the full model is evaluated only at some grid points and the system response is approximated by mathematical approaches. Design and Analysis of Computer Experiments (DACE) offers a suitable surrogate model based on the Kriging method. The system model substituted in this way can be evaluated in an efficient way, but in addition to the uncertain simulation results, the approximation error dependent on the surrogate model has to be considered. Investigations of first prototypes lead to new knowledge that can be used to improve the surrogate model. Measurements, however, also include errors that are composed of systematic and random errors. The systematic measurement errors are specific errors for each measuring system and task, which are usually corrected during the measurement. However, an estimation of the random measurement error, which represents the precision of the measurement can be taken into account. Two methods are presented. Either an additional constant term is implemented in the standard Kriging or a superposition of two standard Kriging models, which are based on the simulation data and the measurement data, is used. As an application example a cold forging process of a steel gearwheel is employed.*

1 Introduction

The tasks of developing components and defining their tolerances are part of the design process. Due to increased requirements and shorter development times, the manufacturing processes are designed using computer aided simulations These simulations play an important role in manufacturing processes and are therefore often used [1]. While simulations are reproducible, real processes are subject to fluctuations, such that a virtual model can never reproduce a real-world setting and tolerance limits are necessarily needed, to ensure the functions of the developed components.

The origin of the fluctuations are caused by epistemic uncertainties as well as aleatoric uncertainties [2]. Epistemic uncertainties result from insufficient information and can be eliminated by additional effort. Aleatoric uncertainties are systemdependent deviations that cannot be prevented. These uncertainties have to be taken into account in the process design. Varying parameters are a common way of doing this. Therefore, many evaluations are needed to calculate a simulation for different parameter combinations. The system used in this manuscript is a cold forging process to build gearwheels [3].

Due to the complexity of the simulation and the frequently required evaluations, the system is approximated using a surrogate model. This is done in section 2 using Design and Analysis of Computer Experiments (DACE). The surrogate model should reproduce the computer simulation with sufficient accuracy. Subsequent measurements of real parts in section 3 provide verification of the surrogate model. It can be seen that the surrogate model approximates the simulation well, but the simulation does not match with the results of the real measurements. In section 4, the measurement data is then used to discuss two methods to optimize the simulation results. Considering the measurement method and its measurement uncertainty, the possibility of optimization is limited, which is shown in section 4.3 discussing an exclusively measurement based surrogate model. A first approach to integrate the measurement uncertainty into the discussed surrogate models is shown in section 4.4. At the end there is a short summary and an outlook in section 5.

2 Surrogate model

In general, a surrogate model is an approximation to the output function $\hat{f}(\mathbf{p}) \approx f(\mathbf{p})$ at the parameter combination $\mathbf{p}$. Each vector $\mathbf{p} = \{p_1, p_2, ..., p_k\}^T$ consists of k entries. The number of entries k results from the number of input parameters. In order to create a surrogate model, the system is approximated by using a few sampling points

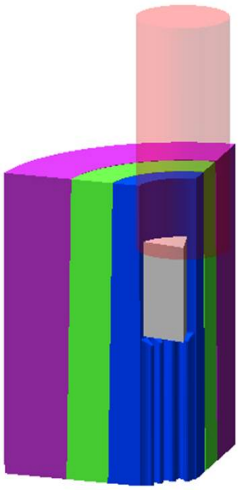
$$\mathbf{P} = \{\mathbf{p_1}, \mathbf{p_2}, ..., \mathbf{p_n}\}^T. \tag{1}$$

Here we use an interpolation, such that the relationship $\hat{f}(\mathbf{p}_i) = f(\mathbf{p}_i)$ applies to the sampling points $\mathbf{p}_i$.

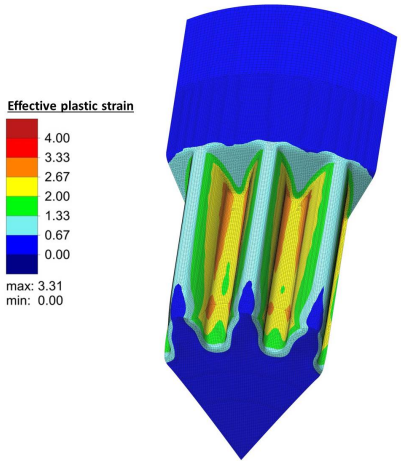
2.1 Cold forging process simulation

In the following, the function f represents a finite element simulation of a cold forging process. In this process, a cylindrical blank with diameter d is extruded forward into a gear die by a punch. The process runs at room temperature (the blank is also not heated, therefore cold forming) and using suitable lubricants, which have a significant influence on the friction force between the blank and the die [4]. Two parameters, the diameter $d = p_1 \in [0.019169\ \text{m}, 0.019589\ \text{m}]$ and friction coefficient $\mu = p_2 \in [0.08, 0.18]$ are considered as uncertain. This setup is simulated in the commercial software Simufact Forming. This tool is

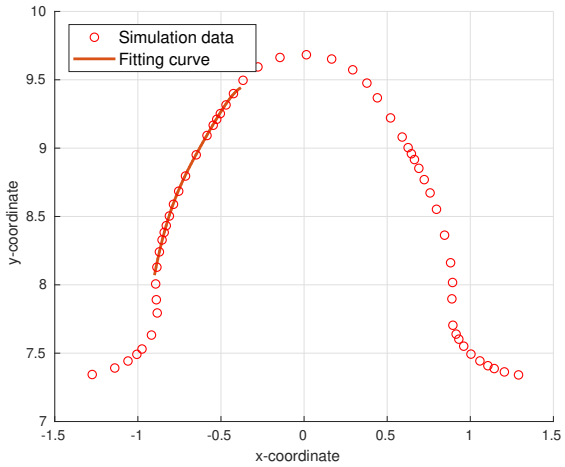
well suited for massive forming processes [5, 6]. Fig. 1 (a) shows the experimental setup in the simulation environment. Because of symmetry it is sufficient to simulate only a quarter of the whole model.



(a) finite element setup for cold forging process



(b) result plot for the effective plastic strain



(c) 2D cut of the result plot for one cog with a fitting curve for the left involute

Figure 1: Simulation data from the cold forging process simulation

The simulation results, as can be seen in Fig. 1 (b) for the effective plastic strain, were explained in [3]. The quantity of interest for a tolerance analysis in gear meshing is the cog involute (see Fig. 1 (c)). To obtain the involute, the STL file of the formed blank is exported from the simulation and a cut is made in the middle of the blank, perpendicular to the flow direction. The nodes located in the immediate vicinity of the cut then describe the 2D shape of the deformed blank, the cogs. The involute can be determined using the standard in [7]. The finite element mesh is designed such that about 16 points are located on the involute.

2.2 DACE model

For the surrogate model $\hat{f}$ exist different approaches, see e.g. [8]. The surrogate model used here is the DACE model. This form of surrogate model is based on the Kriging model developed

by D.G. Krige [9]. It contains a random process $\mathbf{Z}(\mathbf{p})$, which influences the surrogate model depending on the distance of the evaluation point to the sampling points [10]. This random process $\mathbf{Z}(\mathbf{p})$ is assumed to have zero mean and covariance between $\mathbf{Z}(\mathbf{p_i})$ and $\mathbf{Z}(\mathbf{p})$, which results in

$$E[\mathbf{Z}(\mathbf{p_i}), \mathbf{Z}(\mathbf{p})] = \sigma^2 R(\theta, \mathbf{p_i}, \mathbf{p}), \tag{2}$$

with σ^2 as process variance and $R(\theta, \mathbf{p_i}, \mathbf{p})$ as correlation function. For the point correlation

$$R(\theta, \mathbf{p_i}, \mathbf{p}) = \prod_{j=1}^{n_c} R_j(\theta, p_j^{(i)} - p_j) \tag{3}$$

holds and a correlation matrix and a covariance matrix can be obtained. For the correlation function the cubic approach,

$$R_j(\theta, p_j^{(i)}, p_j) = 1 - 3\xi^2 + 2\xi^3 \quad \textit{with} \quad \xi = min\{1, \theta|p_j^{(i)} - p_j|\} \tag{4}$$

is used, which contains a weighting factor θ, defining the importance of the parameters. Calculation of optimal values for θ corresponds to a maximum likelihood estimation, for more details see [11].

In addition to the correlation context, the DACE method consists of a regressions model. It is a linear combination of n_c functions $r_1(\mathbf{p})...r_{n_c}(\mathbf{p})$ with regression parameters β_i. Regression model and random process results in the DACE approach

$$\hat{\mathbf{F}}(\mathbf{p}) = \sum_{i=1}^{n_c} \beta_i r_i(\mathbf{p}) + \mathbf{Z}(\mathbf{p}). \tag{5}$$

This model is applied using the MATLAB toolbox following [11, 12]. In the upcoming chapters a first degree polynomial is used as regression model and the weighting factor $\theta \in [0.001, 10]$.

The model is build with a three-level full factorial design for the two parameters (diameter d, friction coefficient μ), resulting in $n = 3^2$ sampling points. The influence of other sampling strategies is not considered in this document, but will be the topic of future research.

2.3 Model for the involute

As already mentioned in section 2.1, the involute is the quantity of interest. More precisely the left involute of the first cog serves as result function $y(x)$. The first cog is defined as the upper cog intersected by the y-axis of the coordinate system (coordinates $y > 0$, $x_{min} < 0 < x_{max}$).

Due to high numerical costs of the finite element simulations, a surrogate model for the involute is needed for parameter studies. If the discrete representation of the involute as given by the finite element result is directly approximated, a large number of parallel surrogate models are required for each individual point. Moreover, a comparison of two involutes is then difficult because the points lie not necessarily in the normal direction of the underlying cog surface and do not allow a determination of the distance between the two involutes. For this reason, the points of the finite element mesh from the simulation are approximated by a polynomial of the form

$$y(x) = c_4 x^4 + c_3 x^3 + c_2 x^2 + c_1 x + c_0 \tag{6}$$

and a surrogate model $\hat{y}(\mathbf{p}, x)$ is build, where the coefficient c_{0-4} of the polynomial are directly approximated by individual DACE models $\hat{c}_i(\mathbf{p})$, as presented in section 2.2. Thus, the involutes from the surrogate model can be compared with the mesh points of the simulation and later also with the measurement points of the real measurement. The root mean squared error (RMSE), which is generally defined by

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n}} \tag{7}$$

is used for that comparison, where $y_i = y(x_i)$.

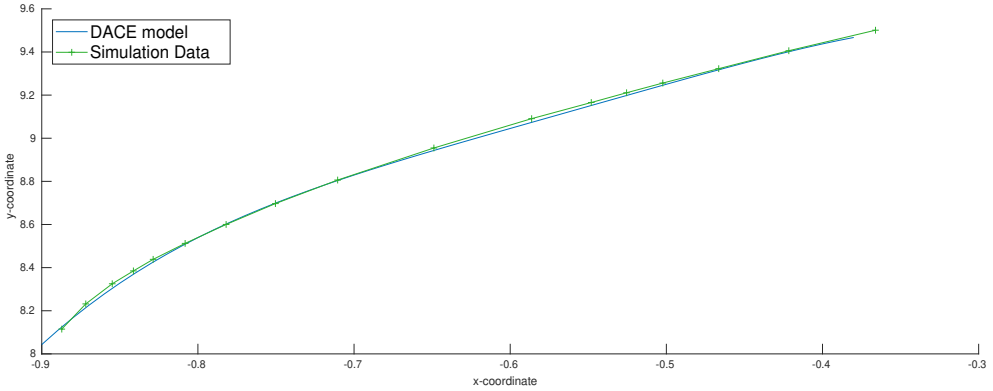


Figure 2: Comparison of involute from surrogate model and simulation

The number of points n in Eq. 7 is for the simulations about 16. Each parameter combination $\mathbf{p}$ has its own involute and thus its own RMSE value. The mean value is then calculated from these RMSE values to determine the global error of the surrogate model over all parameter combinations. Fig. 2 shows one configuration of an involute from the surrogate model and the associated simulation. An evaluation of the RMSE results in a value of 0.004, which is satisfactory. Before we discuss the results of the measurements in comparison to the surrogate model, the next chapter will show how measurement data originate.

3 Measuring Data

Every real measurement is associated with a positive, non-zero measurement error. That means that any measurand can only be determined up to a certain limitation regarding accuracy and precision. Measurement errors are categorized into systematic and random error contributions, which are described as *"component of measurement error that in replicate measurements remains constant or varies in a predicable manner"* and *"component of measurement error that in replicate measurements varies in an unpredictable manner"*, respectively [13].

The measurement uncertainty of a measurement can be calculated by the determination of those mentioned contributions. The application of different measurement methods and measurement objects in combination with numerous environmental influencing factors usually have an effect on the achieved measurement uncertainties. Usually, the measurement uncertainty is determined and associated with a certain standard geometry element (e.g. plane, cylinder). At the Institute of Manufacturing Metrology, the instrument "single point uncertainty" was introduced and used to locally determine the measurement uncertainty with regard to a geometrically

finely resolved reference measurement [14, 15]. The uncertainty contributes are obtained by statistical evaluation of the local distances of repeated measurements to numerous sampling points on the reference geometry.

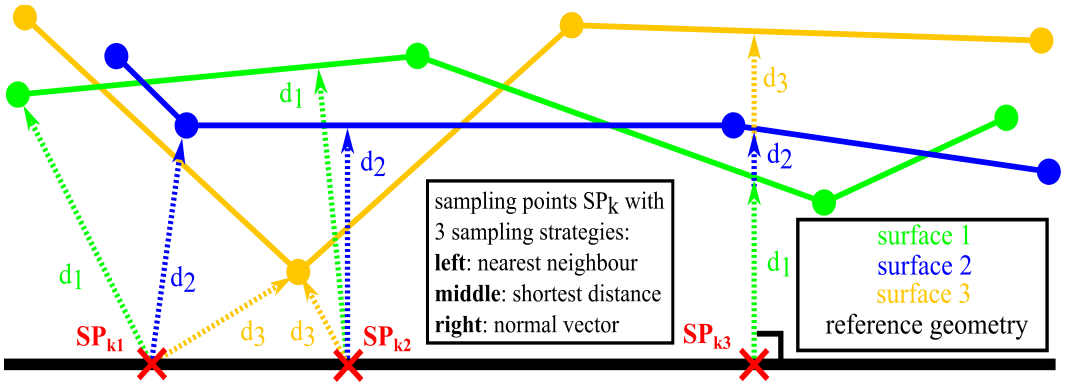


Figure 3: Different sampling strategies to determine the single point uncertainty from repeated measurements [15]

Different sampling strategies are possible to obtain the distances d_n, this contribution uses the "shortest distance" sampling method, see Fig. 3. The mean intersection distances for each sampling point SP_k represent the systematic measurement error, while the random measurement error is represented by the standard deviation of the intersection distances. If no reference (*"quantity value used as a basis for comparison with values of quantities of the same kind"* [13]) geometry is available, the precision of a measurement can be estimated nonetheless by using the nominal geometry (e.g. CAD) instead. That means that the calculated mean intersection distances then represent the combination of the systematic measurement error and the work piece deviations. The "single point uncertainty" framework allows the determination of the components of the measurement uncertainty with respect to numerous single points on a geometry, which is well suited for numerous application scenarios [16], including the supply of parameterized descriptions of the local measurement uncertainty [17].

In order to achieve the random measurement error several repeated measurements (n = 20) of a very precisely manufactured steel gear wheel were performed using the tactile coordinate measurement machine (CMM) "Zeiss UPMC 1200 CARAT S-ACC" in scanning mode in combination with a rotatory stage. The measurements took place in a controlled environment with a constant air temperature of $20\ °C \pm 0.2\ K$ and relative air humidity of $45\ \% \pm 10\ \%$. The operating software "Zeiss GEAR PRO" was utilized to define and evaluate the measurement task. Because of the repeated measurement of the same measurement object under constant conditions, the scatter of the measurement system traversing the complete measurement chain can be observed in the measurement results.

At the beginning of the measurement, the CMM is defining the work piece coordinate system by the determination of the rotation axis of the gear wheel in combination with a centring operation at a single tooth root, in order to resolve the rotation symmetry. After that, two perpendicular line scans are performed for each tooth flank. The line scans representing a complete gear wheel measurement (2 line scans for each gear wheel flank of each tooth) were geometrically registered against the nominal geometry of the gear wheel (CAD) in order to obtain a stable and convenient coordinate system for the subsequent measurement data evaluations. This step was repeated for each of the repeated measurements (n = 20). For each repeated line scan, the mean starting contour (tactile measurement coordiantes are given in combination with the

associated machine probing vector and the distance from the CAD starting contour to the measurement coordiante in the direction of that associated probing vector) was calculated using a least squares procedure, from which the measurements were then sampled. Because of the fact, that the work piece was manufactured very accurately and no superior measurement device was available to determine a reference measurement for the CMM system, the subsequent uncertainty evaluations only consider the random measurement errors, thus the observed ”systematic measurement errors” are regarded as work piece deviations.

4 Measuring Data included in DACE

A comparison of the data determined in section 3 from the measurements with the simulations shows significantly greater deviation than the comparison of surrogate models and simulations in section 2.3, which can be seen exemplary in Fig. 4.

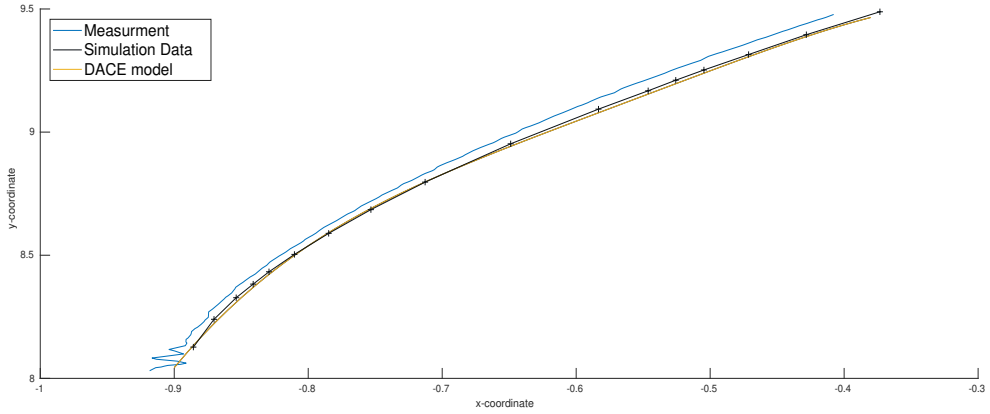


Figure 4: Comparison of involute from surrogate model, simulation and measurement

At first, the evaluation of single gear wheel measurements is discussed without taking the measurement precision (random measurement error) into account. The RMSE between the surrogate model and the simulation is, as we already know, about 0.004, while the RMSE between measurement and simulation is in the order of 0.029. With regard to Fig. 4 it is obvious, that the deviation between measurement and simulation is systematic and not a stochastic error, which leads to the conclusion, that the simulation model is not perfectly fitted. One possibility for optimization would be to improve the simulation, but it would be very time-consuming to further optimize the finite element model. Two alternatives, discussed in the following, are either to integrate the measurement results into the simulation based surrogate model or to construct a separate surrogate model based on measurement data.

4.1 Concept of constant error

The fastest and therefore cheapest approach is extending the DACE model. Eq. 5 is supplemented by a further factor Δ_{Measure}. This factor contains information about the absolute distance of the result variables between surrogate model and measurement values. Assuming that the simulation correctly reproduces the tendency of the parameter variations and thus the surrogate model deviates at each parameter constellation by approximately the same amount, it is sufficient to determine a constant value for Δ_{Measure}. With

$$\Delta_{\text{Measure}} = \mathbf{F}_{\text{Measure}}(\mathbf{p_m}) - \sum_{i=1}^{n_c} \beta_i r_i(\mathbf{p_m}) - \mathbf{Z}(\mathbf{p_m}) \tag{8}$$

the constant error value is calculated, where $\mathbf{F}_{\text{Measure}}(\mathbf{p_m})$ is the measurement result for parameter combination $\mathbf{p_m}$. It is already sufficient to carry out a single measurement on any parameter constellation. The evaluation in Tab. 1 for different constellations shows that the parameter combinations hardly plays a role. However, a parameter constellation that is as central as possible in the parameter space should be preferred, since possible effects at the edges are avoided.

-	const.1	const. 2	const. 3	const.4	const. 5
RMSE	0.0078	0.0079	0.0076	0.0076	0.0078
Distance to space center (in % of the parameter space)	52	36	29	23	2

Table 1: RMSE for different constellations including Δ_{Measure}

A disadvantage of the method is a risk to integrate the error of a single measurement into the whole model. For this reason, this risk can be greatly minimized by forming an average value.

4.2 Concept of superposed surrogate models

If measurements are available or possible, the question arises whether a surrogate model based exclusively on the measurement data makes more sense. However, it has to be considered that measurements are very expensive and they should be avoided as far as possible. Therefore, in the following, a hybrid method is presented, which uses the simulation based surrogate model from section 2 and generates another surrogate model on the measurement data. For the measurement based surrogate model we assume, that the number of sampling points is significantly smaller than the number of sampling points of simulation based model, $|\mathbf{P}_{\text{Measure}}| << |\mathbf{P}_{\text{Sim}}|$. Since the simulation based model for the cold forging example has only nine sampling points, the measurement based model is here limited to only three sampling points. For both surrogate models Eq. 5 is used.

The linear combination of the models

$$\hat{\mathbf{F}}_{\text{hybrid}}(\mathbf{p}) = b_1 \hat{\mathbf{F}}_{\text{sim}}(\mathbf{p}) + b_2 \hat{\mathbf{F}}_{\text{Measure}}(\mathbf{p}), \tag{9}$$

defines a hybrid method. By the factors b_1 and b_2 with $b_1 + b_2 = 1$ the influence of the respective surrogate model can be adjusted depending on the quality of the simulation and the measurements. In case of a lack of knowledge there should be a 50/50 ratio.

With the first column in Tab. 2 it becomes clear that the measurement based model using only three sampling points already has a better significance than the simulation based model using nine sampling points. Nevertheless, the hybrid model shows an optimum between $\frac{1}{10} < b_1 < \frac{1}{3}$, where the influence of the simulation based surrogate model is nearly 25%. A disadvantage of this method comes up with consideration of the measurement uncertainty in section 4.4.

b_1	0	$\frac{1}{10}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{9}{10}$
b_2	1	$\frac{9}{10}$	$\frac{3}{4}$	$\frac{2}{3}$	$\frac{1}{2}$	$\frac{1}{10}$
RMSE	0.0064	0.0058	0.0057	0.0060	0.0073	0.0122

Table 2: RMSE for different constellations including hybrid model

4.3 Comparison of the different methods

Since it was shown in the last section that the accuracy of the measurement based surrogate model is higher than the accuracy of a simulation based model, a surrogate model based only on the measurements is to be generated as a reference, which has as many sampling points as the simulation based model. It must be taken into account that the measurement data cover only a part of the parameter space and therefore no full factorial design is possible. Nine constellations are selected so that the distance between the evaluation points is as large as possible. The RMSE for this surrogate model is 0.0078 and thus also in the order of magnitude of the concept with constant error Δ_{Measure}. Fig. 5 shows the involutes of the five different variants for one parameter constellation.

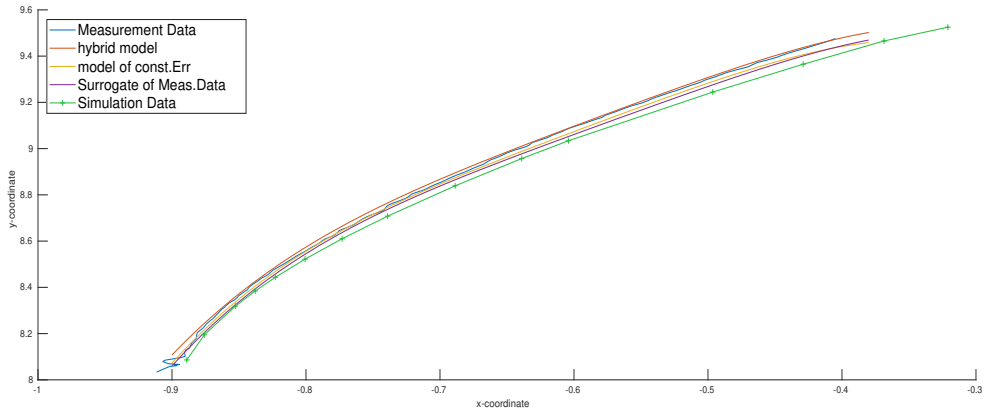


Figure 5: Comparison of all variants

This corresponds approximately to the results of the RMSE evaluation. It is quite surprising that the measurement based surrogate model is not able to convert the much larger information content into accuracy. This circumstance is due to the measurement uncertainty and perhaps the location of the sampling points, which were fixed due to experimental restrictions.

4.4 Integration of measurement uncertainty

As already mentioned in section 3, the locally resolved estimation of the measurement precision results in a distribution (random measurement error), whose standard deviation must be taken into account. This leads to a range of measurement results. Thus, if a measurement is performed only once, the result is subject to uncertainties. A consideration of the measurement uncertainty can therefore be generated by using fuzzy numbers. The fuzzy numbers form intervals, but their values are not necessarily a complete part of the interval. For each value,

a membership function is assumed whose values are between zero and one. A membership function of one means that the value is in the interval, while a membership function of zero means that the value is definitely not in the interval. In contrast to classical set theory, where the values only have a membership function of zero or one, values in the fuzzy interval can also have a value in between. Thus, all kinds of uncertainties can be described with fuzzy quantities. Fuzzy arithmetic contains many characteristic features, which are shown e.g. in [18, 19]. Fuzzy numbers can be discretized with α-cuts, where classical intervals are formed with a fixed membership function value.

If the measurement uncertainty is applied to the surrogate model by means of such α-cuts, bands, whose boundaries according to the tolerance for risk, are formed. For the width of the bands in Fig. 6 applies $w(\mu = 0) = 3\sigma$. The other bands for $\mu > 0$ are automatically generated based on the selected fuzzy number. In Fig. 6 a truncated gauss fuzzy number is used. The crisp value $(\mu = 1)$ is the involute of the surrogate model with the concept of constant error.

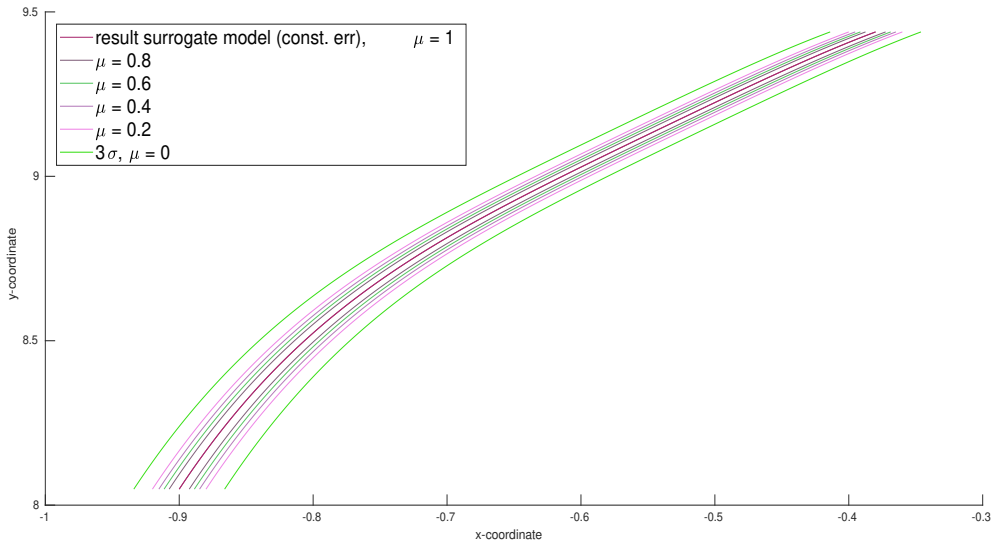


Figure 6: Measurement uncertainty implemented with fuzzy numbers

For the concept of constant error, the result is finally

$$\tilde{\hat{\mathbf{F}}}_{\Delta\,\mathrm{err}}(\mathbf{p}) = \hat{\mathbf{F}}_{\mathrm{Sim}}(\mathbf{p}) + \tilde{\Delta}_{Measure}. \tag{10}$$

The uncertainty in the result is only due to the measurement uncertainty and can therefore be handled very easily. This is different with a uncertainty analysis of the hybrid model. Here

$$\tilde{\hat{\mathbf{F}}}_{\mathrm{hybrid}}(\mathbf{p}) = b_1\hat{\mathbf{F}}_{\mathrm{Sim}}(\mathbf{p}) + b_2\tilde{\hat{\mathbf{F}}}_{\mathrm{Measure}}(\mathbf{p}) \tag{11}$$

shows, that the uncertainty is integrated in the surrogate model itself. A crisp value at $\mu = 1$ does not exist, instead it must already be assumed, that the involute for $\mu = 1$ is uncertain. This cannot be verified exactly.

5 Conclusions

The deviations between simulation and surrogate model, which is based exclusively on these simulations, are significantly smaller than the deviations between simulation and real measurements. An optimization of the simulation based surrogate model has no significant influence and therefore remains unconsidered.

Forming a new surrogate model based exclusively on the measurement data improves the accuracy, but the effort is significantly higher than one of the presented methods in section 4. However, if the simulation is good enough, only a few measurements can be sufficient, since the simulation can correctly map the trend. It is shown that the accuracy does not increase with the number of measurements, since the measurement error only consists of a random contribution, because the systematic contribution is regarded as zero. This uncertainty is reflected in the result functions and is taken into account by means of a band around the surrogate model results. For that case the concept of constant error is easier to handle in contrast to the hybrid concept.

A classification of such surrogate models in tolerance management is a special challenge. In addition to the measurement uncertainty, the tolerance has to be considered. This makes it even more difficult to distinguish between good and bad parts. An estimation under almost 100% coverage of the measurement uncertainty and the tolerance results in a narrow band and can lead to many rejects or tight tolerances. It is at the discretion of the designer to choose suitable tolerances .

The methods presented here make it possible to approximate a process by means of simulation and measurements and to take the measurement uncertainty into account. It was shown, that it is possible to generate a ”good” surrogate model with simulation based models and few measurement data.

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