

## Lectures

# Effective Parameter Identification to Validate Numerical Simulation Models

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# EFFECTIVE PARAMETER IDENTIFICATION TO VALIDATE NUMERICAL SIMULATION MODELS

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## 1. Introduction

In the field of numerical simulation a variety of abstract physical models is used to describe observable phenomena. An important class of these models are material or constitutive models that represent the phenomenological behavior of different materials and material combinations. To apply these models within a complex 3D FEM model, one of the main questions is often how the model parameters have to be chosen. Simple models like isotropic elasticity allow to directly determine model parameters like Young's modulus and Poisson ratio from measurements. For more complex models, like deterioration or crack models of brittle materials, model approximations are often chosen that can only be described with a greater amount of model parameters. For these models it is often not possible to decouple the influence of each single parameter from each other and to determine these by direct measurements. For those problems an inverse approach is suitable in which a simulation model is used that represents the real geometry, boundary conditions and the sequence of the measurement setup. The unknown parameters are then determined by an iterative approach by comparison between measurement and simulation data. This process is called model calibration.

In this paper the basics of this approach and their practical realization will be discussed. An important aspect additional to the standard method is the analysis of the identifiability of the parameters. Due to very efficient sensitivity analysis methods, it is first detected which parameters actually have an influence on the simulation results and the calibration procedure. Furthermore, the analysis helps to define suitable measures to quantify the difference between measurement and simulation. If such a measure can be described by the unknown model parameters with high certainty, the successful calibration with global and local optimization methods can be performed in a next step. Finally, it has to be analyzed whether the inverse problem can be solved nonambiguously, that means there is a unique parameter combination that allows optimal matching between measurement and simulation. In

this paper approaches for this kind of calibration tasks and the software based realization by means of several examples will be presented.

## 2. Basic concept

### *Minimization of Least Squares*

In the field of parameter identification several methods have been established. Very well-known is the minimization of the sum of squared errors. This approach assumes that the simulation model can accurately represent the physical properties. In this case, the only deviation between simulation and measurement were caused by measurement errors. If these measurement errors are considered as multidimensional normal distribution the following objection function can be formulated using the maximum likelihood estimation [Beck 1977]:

$$J = (\mathbf{y}^* - \mathbf{y})^T \mathbf{C}_{yy}^{-1} (\mathbf{y}^* - \mathbf{y}) \rightarrow \min$$

where  $\mathbf{C}_{yy}$  is the covariance matrix of the measurement points. As this measure is often unknown, the measurement errors are considered as independent. This leads to weighted squared errors. Assuming a constant measurement error for all measurement points the well-known sum of squared errors is obtained:

$$J(\mathbf{p}) = \sum_{i=1}^n (y_i^* - y_i)^2$$

For the identification task this sum of squared errors is to be minimized. In the case of many experiments the corresponding measurement curves can be merged additively in one objective function.

For complex models the objective function is often a highly non-linear function with multiple local minimums. For this reason for the search of the optimal parameter set it is recommended to couple a global optimization algorithm, like evolutionary algorithms, with a local algorithm like Simplex- or gradient based methods.

Alternative approaches for the minimization of the sum of squared errors like Kalman filter or Bayesian Updating consider the parameters as statistical measures but more information about the covariance of the measurement points are necessary. Often, these methods are extensive why they are not considered in this study. A methodical comparison can be found in [Most 2010].

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## *Identifiability of parameters*

The minimization of squared errors is an inverse approach where the model parameters are matched indirectly to the measurement results. If the model parameters have no influence on the model responses it is not possible to identify them. This can be evaluated with an initial sensitivity analysis. In this case it is important to examine not only one-dimensional dependencies like local derivatives or correlation coefficients, but also parameter interactions.

In this study a multivariate sensitivity analysis was applied that has been based on response surfaces and variance based sensitivity indices to evaluate the influence of each parameter [Most 2011]. The response surface based so called Metamodel of Optimal Prognosis (MOP) acts as surrogate model to approximate the solver response. Its algorithm automatically determines the most appropriate approximation model and reduces the number of input parameters to the important ones. As quality measure serves the Coefficient of Prognosis (CoP) which allows to validate the model concerning its ability to predict upcoming design points. This approach is very efficient and can evaluate the sensitivities with only 50-100 simulation runs.

Furthermore, the unambiguity of the parameters to be identified will be investigated. In complex models different parameter combinations can lead to similar simulation results. This ambiguity can be analyzed after a global optimization run. Alternatively, several optimization runs can be performed to compare the identified parameters afterwards.

### **3. Example: Identification of concrete fracture parameters from a wedge splitting test**

The following example will explain the basic procedure using a wedge splitting test regarding Trunk [Trunk1999]. During this experiment, a pre-slotted specimen was loaded vertically along a predefined crack edge (Figure 1). With this setup, the experimental measurement of the post-cracking behavior was possible.

The simulation model represents the specimen as a linear elastic continuum containing 2D plane-stress elements (Figure 2). The theoretical crack evolution was represented by 2D interface elements, whereby the softening behavior was modeled using a common bilinear softening law. The tensile strength  $f_t$  and the specific fracture energy  $G_f$ , as well as the two shape parameters  $\alpha_{ft}$  and  $\alpha_{wc}$  describing the kink of

the bilinear curve, serve as fracture parameters. The simulation was conducted path-controlled causing a steadily increased crack opening width.

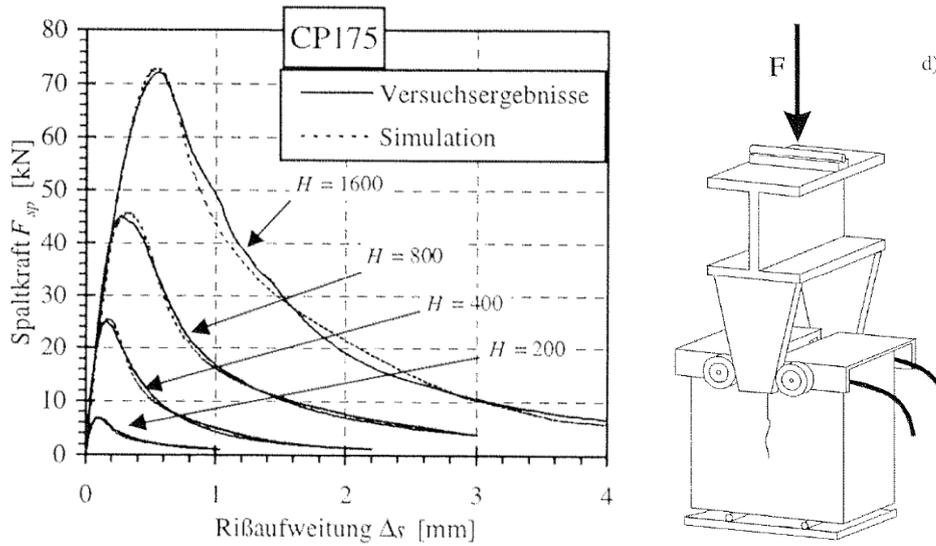
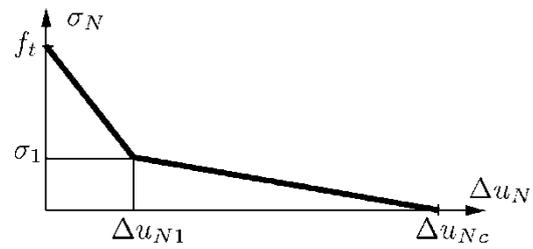
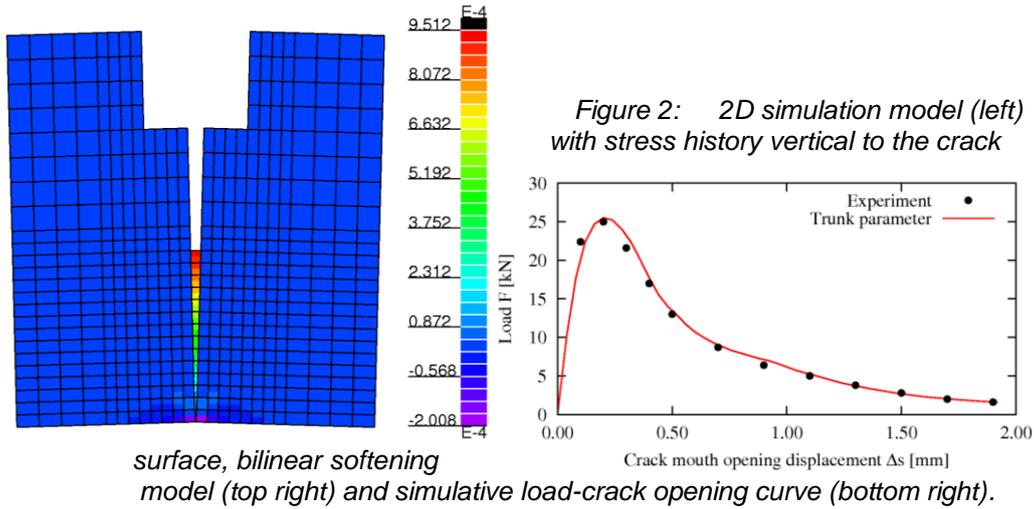


Figure 1: Wedge splitting test regarding Trunk, experimental setup and measured load displacement curves for different specimen.



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In the first step, a sensitivity analysis was performed. Here, the Young's modulus  $E$ , the Poisson's ratio  $\nu$  and the four fracture parameters were varied. As design-of-experiments scheme, a correlation-optimized Latin Hypercube Sampling was used [optiSLang 2014]. The simulation curves were calculated and imported in optiSLang via a signal module for each of the 100 samples. The reference signal is covered by the curves which indicates that the chosen range of parameters is well adjusted (Figure 3). An identification with the estimated parameter ranges seems possible.

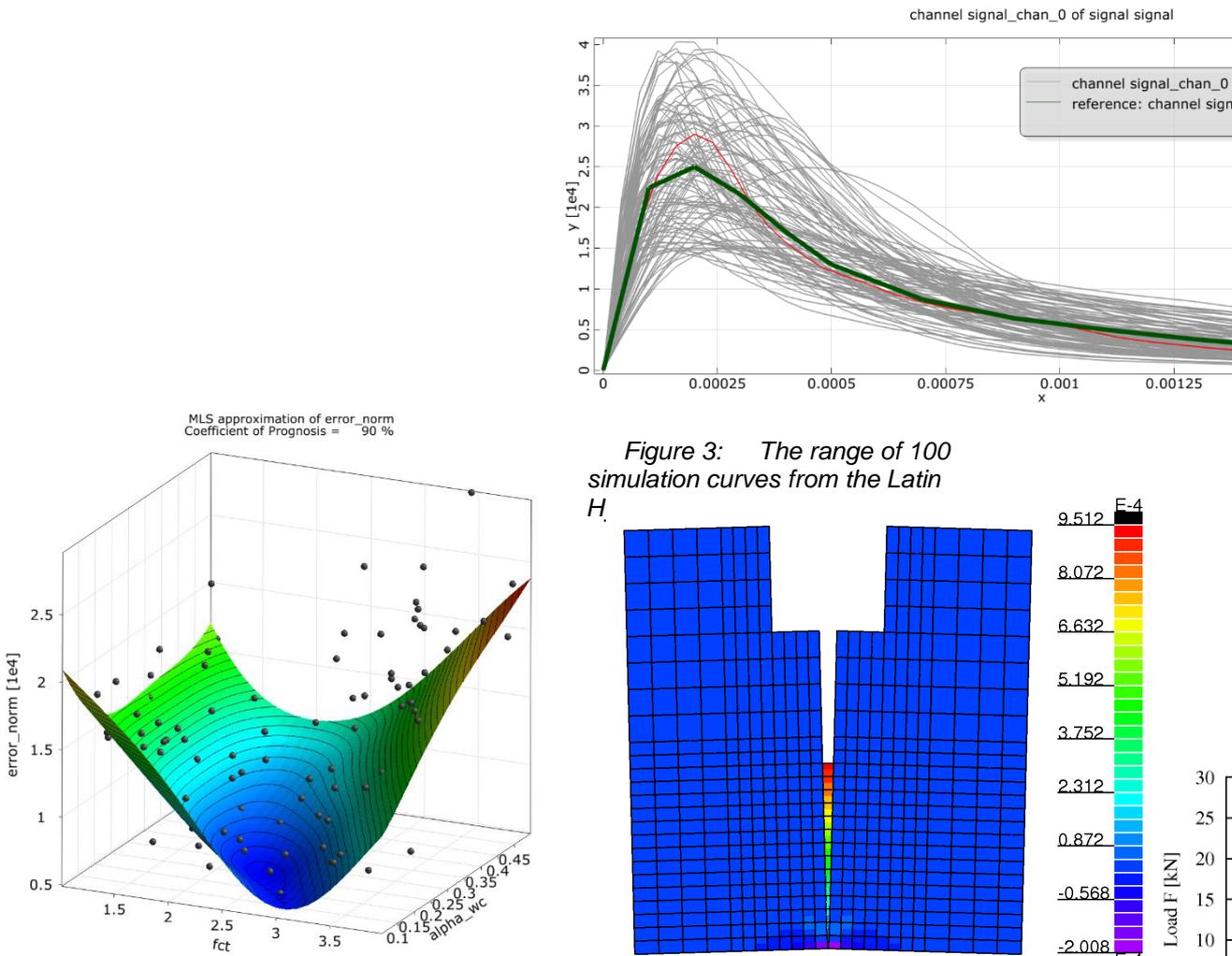
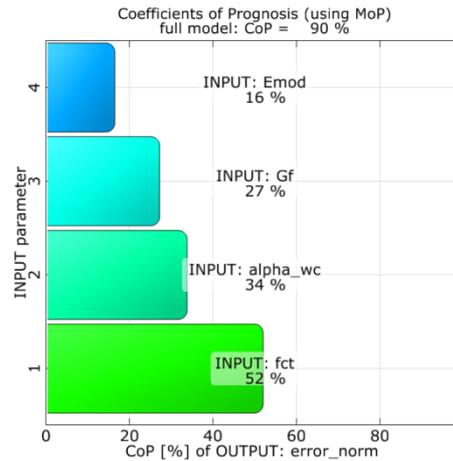


Figure 4: Approximation of the sum of squared errors using Moving Least Squares (left) and variance-based sensitivity indices of the parameters to be identified (right).



Furthermore, the influence of the model parameters on the response variables was analyzed using the Metamodel of Optimal Prognosis (MOP) [Most 2011]. Figure 4 shows the meta-model and the parameter influence concerning the sum squared errors. It can be seen that the Poisson's ratio and one of the form parameters most likely cause no effect. However, the approximation quality was not ideal and less important factors were not identified due to insufficient sampling points.

To ensure that only parameters without influence were excluded from the identification, effects occurring during the softening process were analyzed more detailed. The loads at the reference points (Figure 2) were extracted from the signals of the simulation model and, for each value, a sensitivity analysis was conducted. This could be done without any further simulation runs because the additional scalar values were just extracted from the calculated response signals. The displacement dependent sensitivity indices are shown in Figure 5.

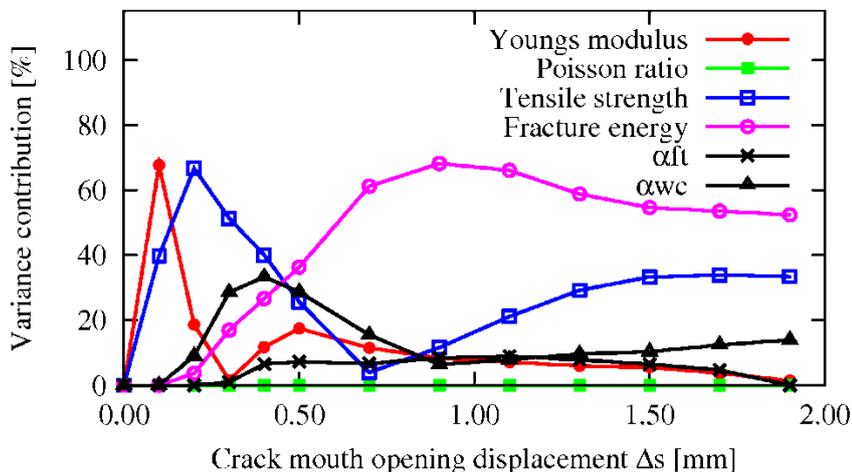


Figure 5: Sensitivity indices for all input parameters depending on the crack opening width.

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Figure 5 illustrates that the Poisson's ratio had no influence. Apart from that, all parameters caused at least a partial effect during the displacement process. Thus, the conclusion can be drawn that all parameters except the Poisson's ratio were identifiable from the measurement data.

The next step was the conduction of a global optimization using an Evolutionary Algorithm with the 10 best designs of the sensitivity study as a start population. This improves the convergence of the optimization process significantly. The best design was then used as a start design for a local optimization. For the local search, the Simplex-Nelder-Mead method was used.

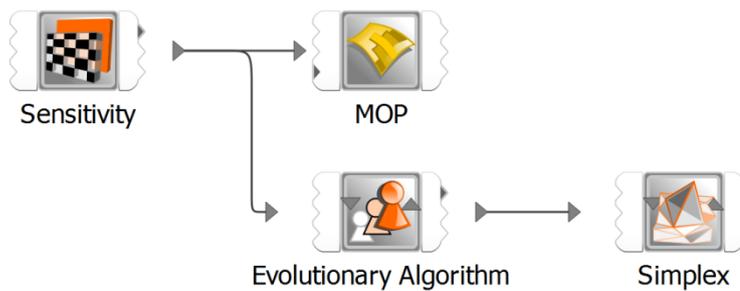


Figure 6: Flow chart of identification: the sensitivity analysis generated the DoE designs as well as a response surface model using the Metamodel of Optimal Prognosis. For global search, the best designs served as a start population for the Evolutionary Algorithm. The resulting best design was then used as the starting point of the local search using Simplex Nelder-Mead.

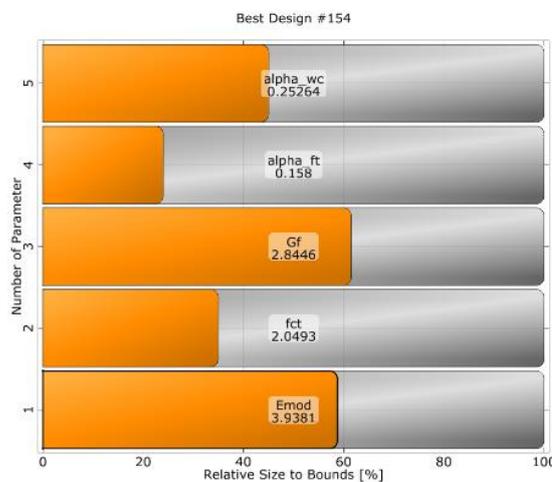
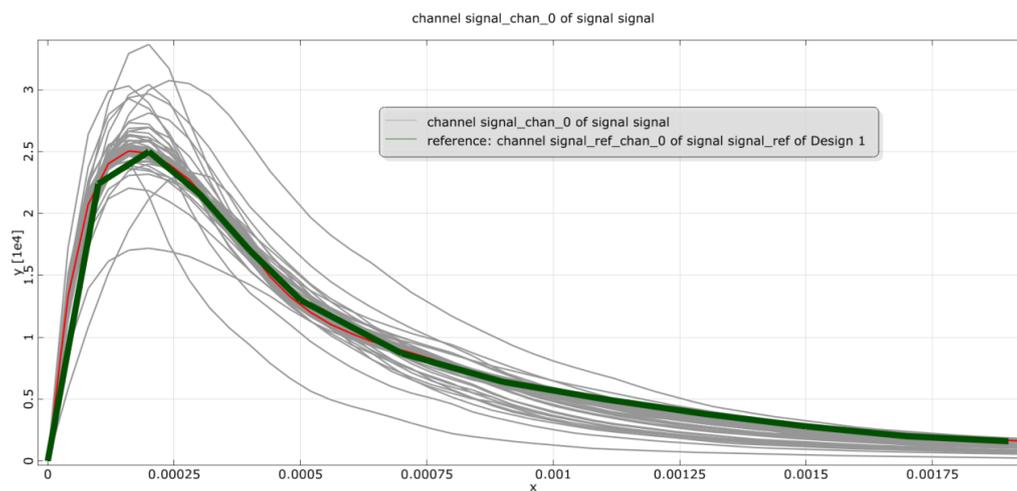


Figure 7: Locally optimized simulation curves (upper panel) and optimal parameters (lower panel) showing a very good agreement between measurement and simulation.

In Figure 7 the optimized simulation curves and the optimized parameters are illustrated. The figure shows a good matching between measurement and simulation.

Finally, the issue of ambiguity was verified in detail. For this purpose, the designs of the local optimization were depicted as a parallel coordinates plot. The range of the sum of squared errors was tightly restricted. Thus, only simulation curves with a very similar course were shown. In reference to the accompanying parameter ranges, it was illustrated that the modulus of elasticity, the tensile strength as well as the fracture energy show very small intervals. Consequently, they were sufficiently identifiable. The two shape parameters showed very similar results but with a larger deviation. Therefore, they were identifiable with less accuracy using the available measurement points. Here, the consideration of further experimental data would certainly improve the validity.

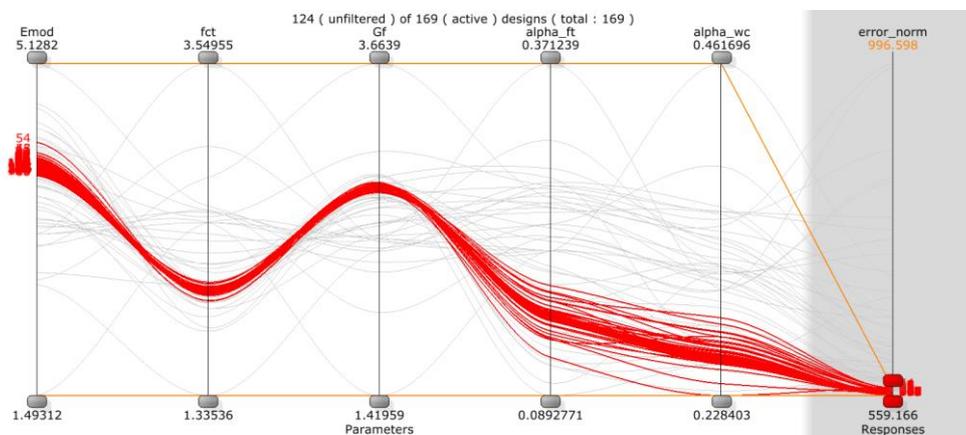


Figure 8: Parallel coordinates plot of the best optimization designs for all considered material parameters and the sum of the least squares.

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### 4. Example: Target optimization of the frequencies of a tuning fork

Target optimization is a special identification task. With the simple example of a tuning fork the whole parameter identification workflow is presented comprising sensitivity analysis and optimization in optiSLang. A modal analysis with a fixed support of the tuning fork and an undamped oscillation is performed.

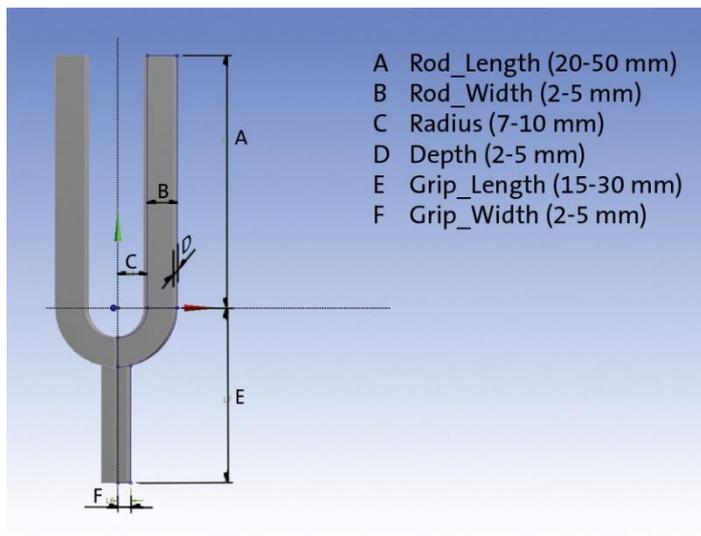


Figure 9: Geometry input parameters of the tuning fork design.

For the sensitivity analysis and optimization 6 input parameters were considered. Namely, these are the geometry parameters rod length, rod width, grip length, grip width, radius and depth (Figure 9). At the same time four output parameters are evaluated: the three lowest eigenfrequencies obtained by the modal analysis and the mass.

The aim of the optimization was to equalize the first eigenfrequency to 440 Hz and the higher frequencies to the duplicate and triplicate respectively. Thus, we performed a single objective target optimization by taking the sum of the quadratic deviation to the target value and the mass. The objective function which should be minimized is  $(\text{frequency}_1 - 440)^2 + (\text{frequency}_2 - 880)^2 + (\text{frequency}_3 - 1320)^2 + \text{mass}$ .

As a pre-optimization step and for the identification of the most important inputs a sensitivity analysis was performed by means of the MOP. Figure 10 (A) shows the matrix of the estimated sensitivity indices and the total CoP values of the corresponding approximation models. It can be seen that the rod length and the grip width of the tuning fork have a main influence on the eigenfrequencies. On the other hand, the

rod width and depth have a major impact on the mass. The radius has a low influence on all outputs. Therefore, its identifiability is expected to be low. As an example, the metamodel for the first eigen-frequency is illustrated in Figure 10 (B) showing the dependency on the two inputs that influence this eigenfrequency most.

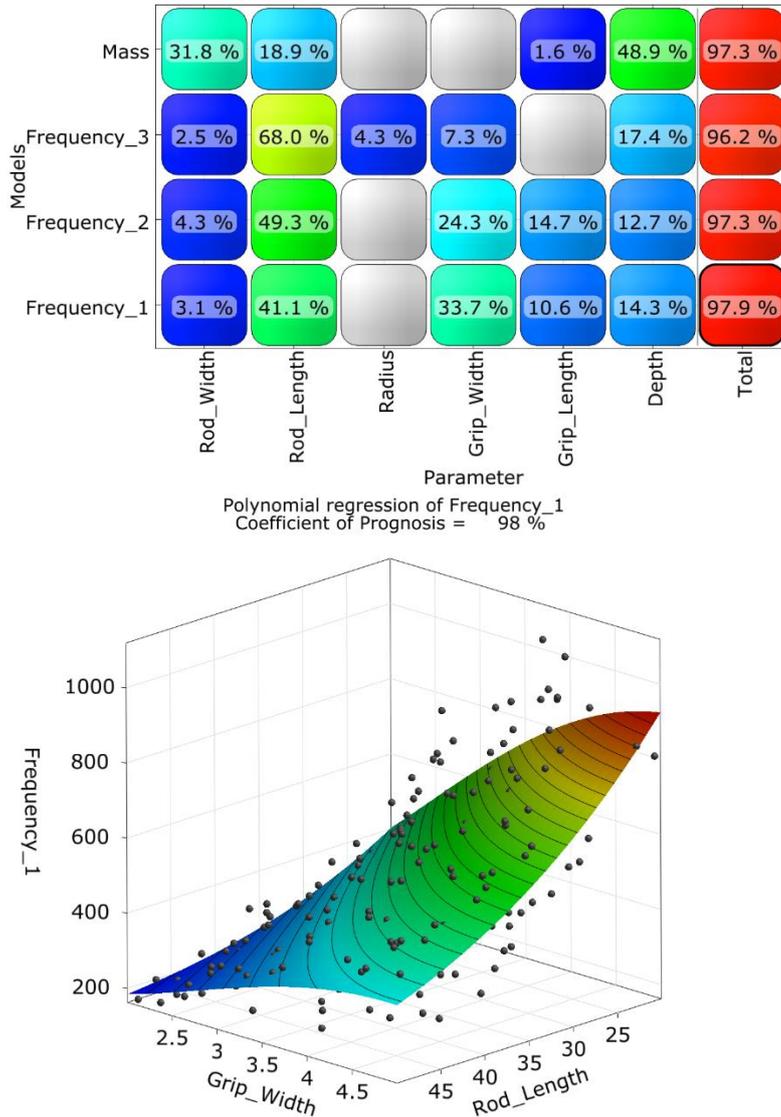


Figure 10: Results of the sensitivity analysis: Matrix of the variance based sensitivity indices (upper panel) and Metamodel of Optimal Prognosis for the first eigenfrequency as a function of the two most important inputs (lower panel). All design points are projected to this subspace, the other input parameters are set to their mean value.

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First, a gradient-based optimization on the MOP was performed to determine a good start design for the subsequent optimization with direct solver calls. As optimizer the Adaptive Response Surface Method (ARSM) was applied due to its robustness to failed solver calls and noise. The optimizer converged in eight iterations with 112 solver calls. A comparison between initial and optimized design is illustrated in Figure 11.



Figure 11: Comparison of the initial versus optimal design of the tuning fork.

### 5. Example: Effective signal extraction to analyze a complex material model for copper thin films

Metallic thin films often show a different physical behavior than bulk solids made of the same material. This requires the determination of new parameters of corresponding material models. One example is thin film copper produced by electro-chemical deposition (ECD). It is widely used in semiconductor industry because of its excellent electrical and thermal conductivity. The functionality of semiconductor products depends strongly on mechanical performance of ECD-Cu under broad temperature range. Therefore, the stress-strain response of this special copper is measured at different temperatures. To this end, the wafer curvature approach serves as standard method [Wimmer 2014]. It measures the change of curvature radius due to mismatch in thermal extension coefficients between the film and substrate for a temperature profile. Silicon is often used as substrate since its mechanical properties are well defined and well-known.

In the following example an inelastic material model consisting of seven parameters was validated for ECD copper of 10 μm thickness subjected to cyclic thermal loading (Figure 12).

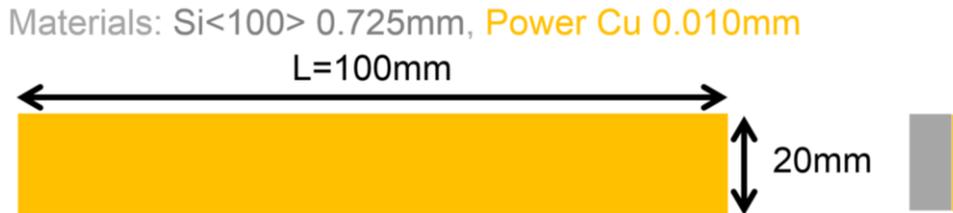


Figure 12: Bimetallic strip in top view and cross section, silicon in grey, copper in yellow.

The raw measured quantity is the curvature radius. It is usually used for the calculation of the bow (maximal deflection of sample) and stress in the film using Stoney's formula which is valid for the elastic and non-elastic range:

$$\sigma_{Cu} = \frac{E_{Si} h_{Si}^2}{6h_{Cu}} \frac{1}{R}$$

where  $\sigma_{Cu}$  describes the average film stress in the direction of the length side of the strip,  $h_{Si}$  is the substrate thickness,  $R$  is the radius of the curvature and  $E_{Si}$  is the Young's modulus of the substrate.



Figure 13: Curvature radius a Cu-Si bimetallic strip is the raw measured quantity. The bow is calculated afterwards and compared with simulation results.

The measurement of the mechanical properties of the Cu-Si bimetallic strip was performed by a cyclical thermal exposure that is illustrated in Figure 14. The corresponding measurement data deduced from the curvature of the substrate is shown in Figure 15.

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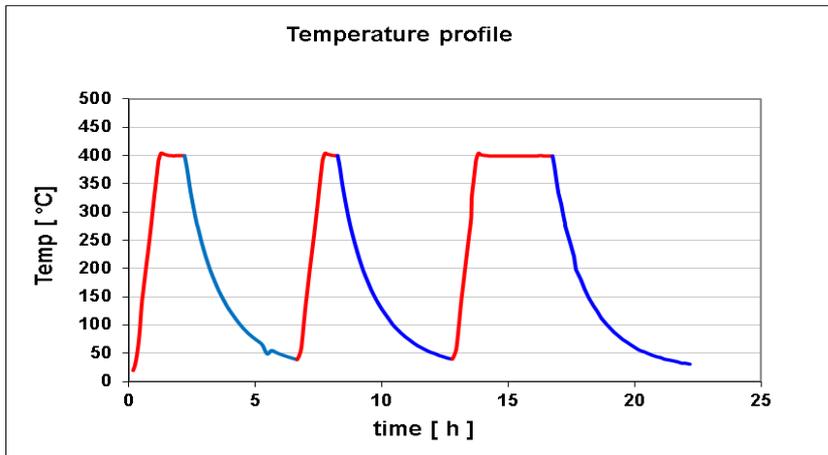


Figure 14: A typical cyclical heating and cooling process during a measurement of a Cu-Si bimetallic strip.

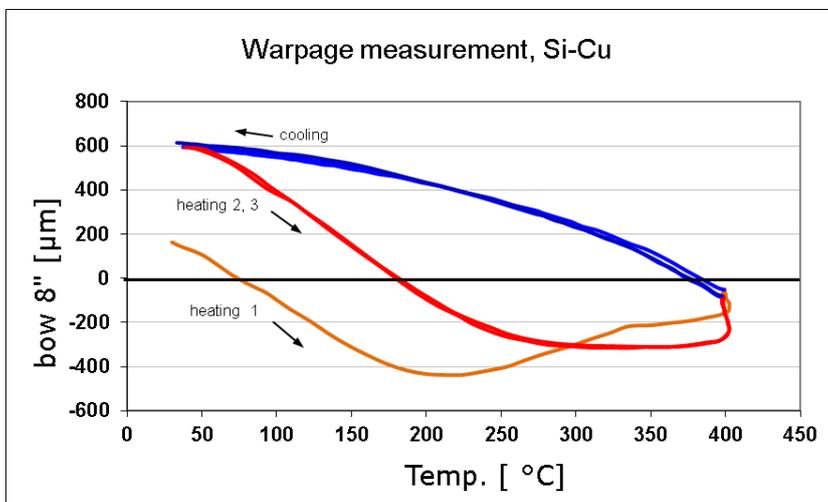


Figure 15: Bow evolution displayed as a function of temperature clearly demonstrates complex the inelastic behavior of ECD copper.

The aim of optimization was to match the reference signal (bow vs. time) from the experiment with the simulated signal from the FEM calculations. A "manual" validation was extremely time-consuming: it took about 3 weeks for 70 simulations. Problem was not a time for one run (it was less than 10 min), but the analysis of results and decision how to change the parameters values in order get closer to experimental results. Before every run it had to be decided in which extent each parameter should be changed. For this purpose, gradients of the objective function were built manually as sensitivity measures using Excel. And even after achieving a satisfactory result it was not clear, if the parameter set can be improved further or not.

In comparison to that, the optimization has been performed with optiSLang applying the least squares approach. Within one day, the automated optimization was finished after 284 simulation runs. It can be seen that the agreement of the curves of the automated optimization is significantly better than the agreement of the manual optimization (Figure 16, right panel). Additional advantage is the possibility to repeat parameter fitting, if, for example, some model parameters will become known from independent experiments. For manual validation such situation would be a real nightmare, because simulation engineer would have to start from the beginning.

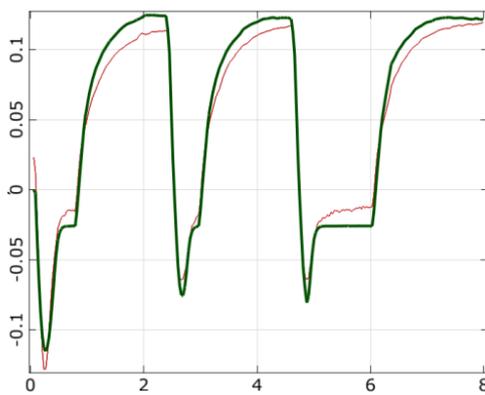
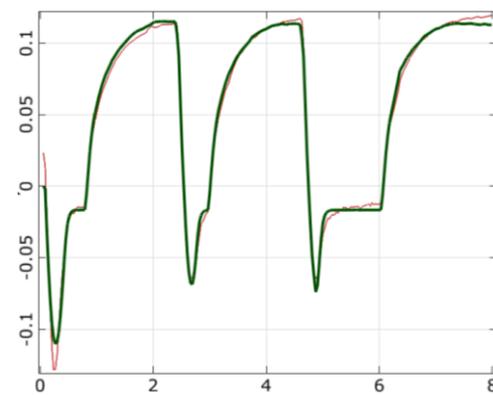


Figure 16: Bow vs. time. Left panel: The outcome of the manual optimization was a good agreement between reference and simulation signal but with much effort.



Right panel: The automated optimization resulted in an almost perfect match within a shorter time (green - simulation, red - experiment).

## 6. References

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