Efficient Parameter Identification for Numerical Simulation Models

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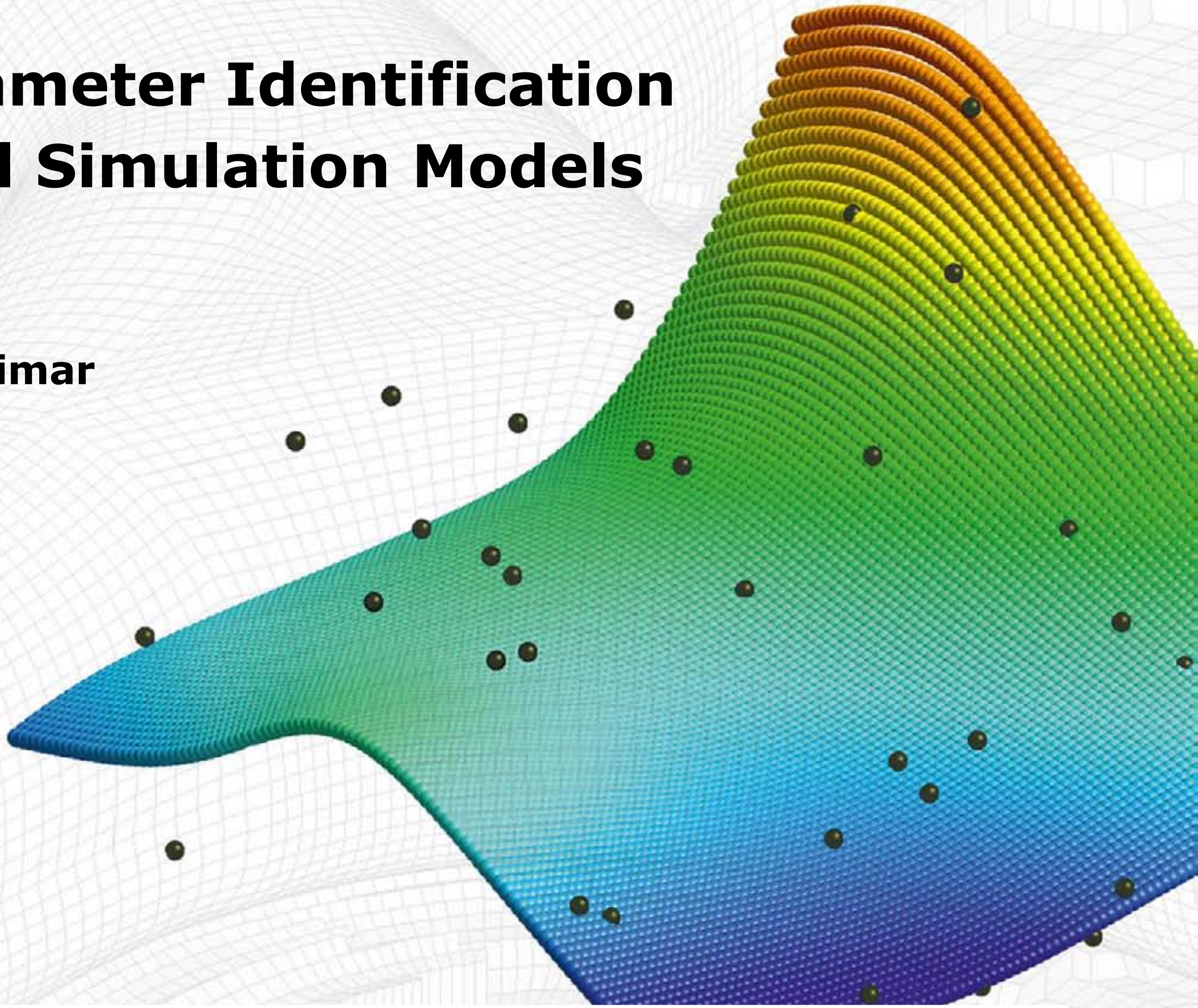
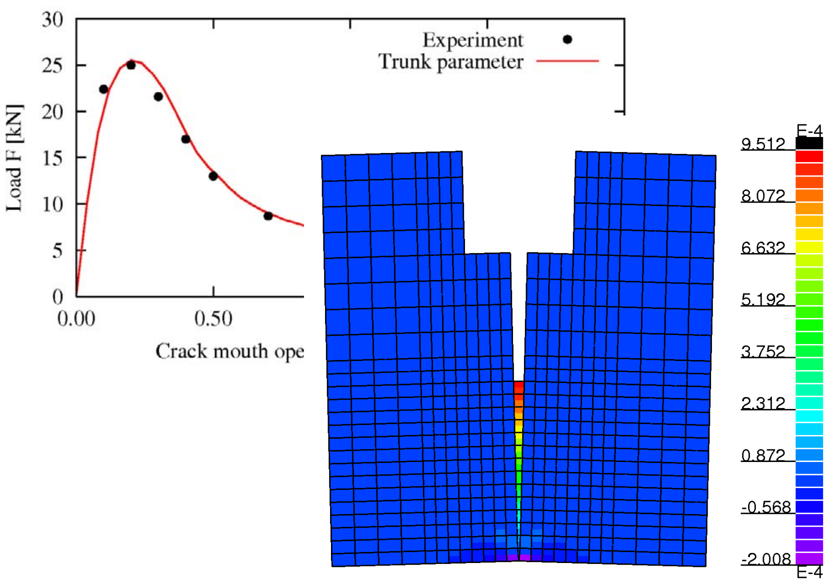
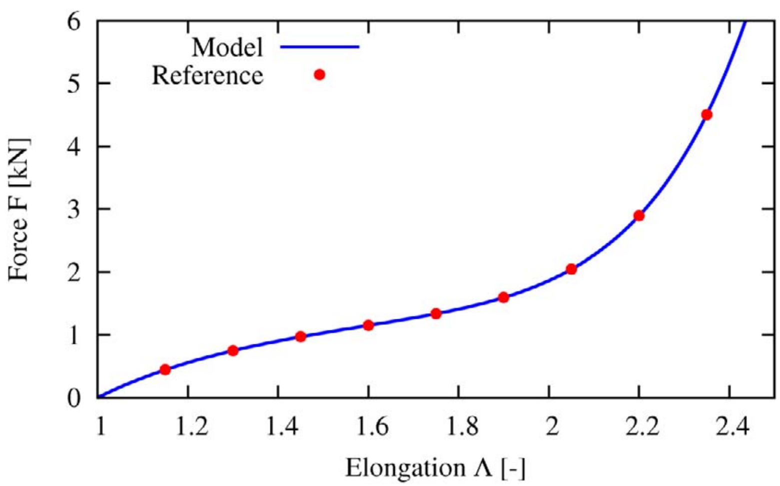


Outline

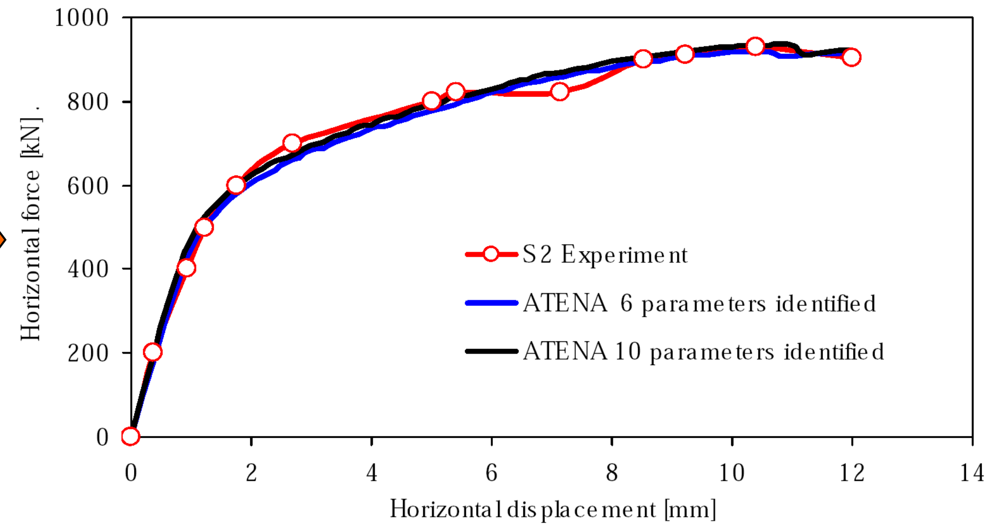
- Introduction
- Theoretical background
- Sensitivity analysis
- Least squares minimization
- Example: Identification of fracture parameters of concrete
- Example: Identification of hyperelasticity parameters of an OGDEN law





Introduction

Inverse Identification of Model Parameters



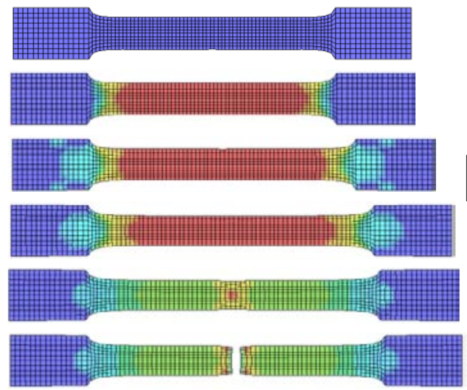
- Identification of unknown model parameters by the calibration of the model with respect to given measurements
- Direct relation between measurements and model parameters is known only inversely as forward simulation model

The Forward Simulation

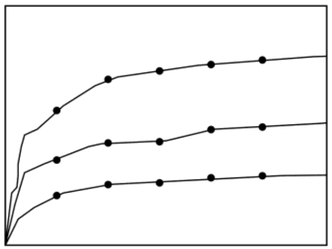
Model parameters

$$p_1, \; p_2, \; \vdots, \; p_m$$

Simulation model

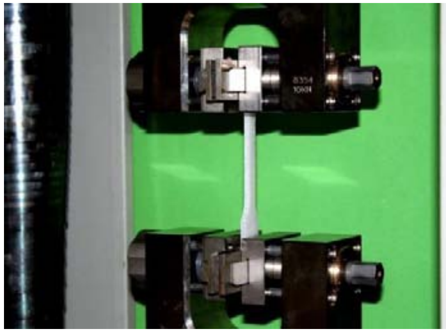


Model responses



$$y_1, \; y_2, \; \vdots, \; y_n$$

Measurements



$$y_1^*, \; y_2^*, \; \vdots, \; y_m^*$$

- For given set of model parameters **p** the model responses **y** can be calculated with a given simulation model
- Deviation of model responses and measurements **y*** can be evaluated
- For which parameter set $\mathbf{p}_{opt}$ model responses and measurement agree sufficiently well?

Theoretical Background

Least Squares Minimization

- The likelihood of the parameters is proportional to the conditional probability of measurements **y*** from a given parameter set **p**

$$L = k \cdot f(\mathbf{y}^*|\mathbf{p})$$

- For correct model (**y*** - **y**) is caused only by measurement errors

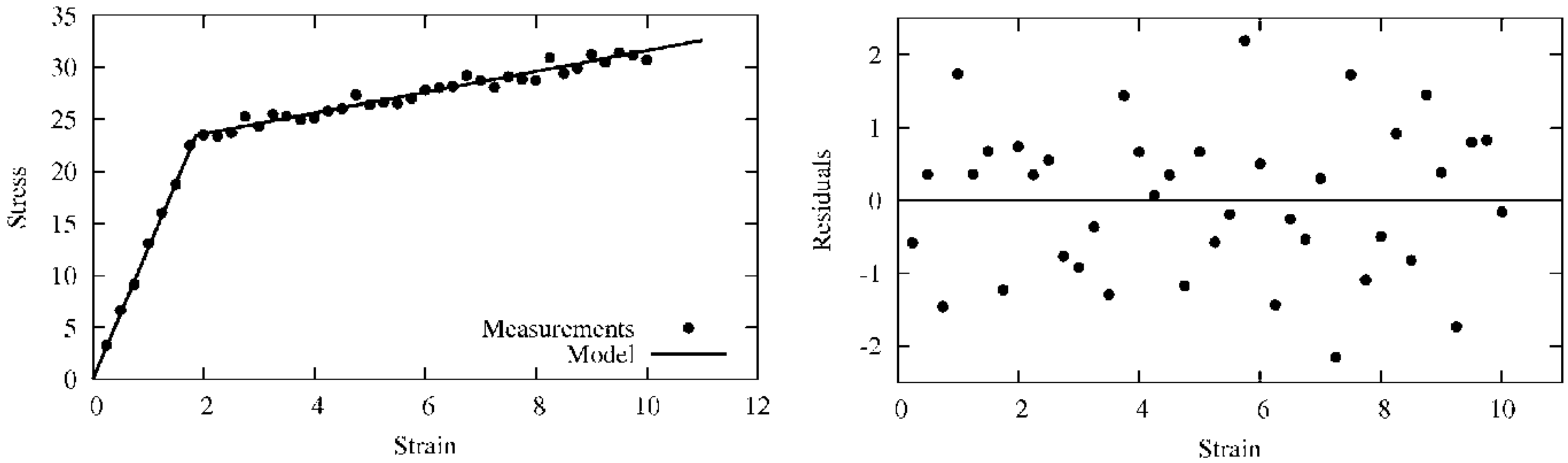
- Assuming **normally** distributed measurement errors:

$$P(\mathbf{y}^* - \mathbf{y}) = \frac{1}{\sqrt{(2\pi)^m |\mathbf{C_{yy}}|}} \exp\left[-\frac{1}{2}(\mathbf{y}^* - \mathbf{y})^T \mathbf{C}_{\mathbf{yy}}^{-1} (\mathbf{y}^* - \mathbf{y})\right]$$

- Maximizing the likelihood (minimizing the log-likelihood) leads to the least squares objective function

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

Least Squares Minimization



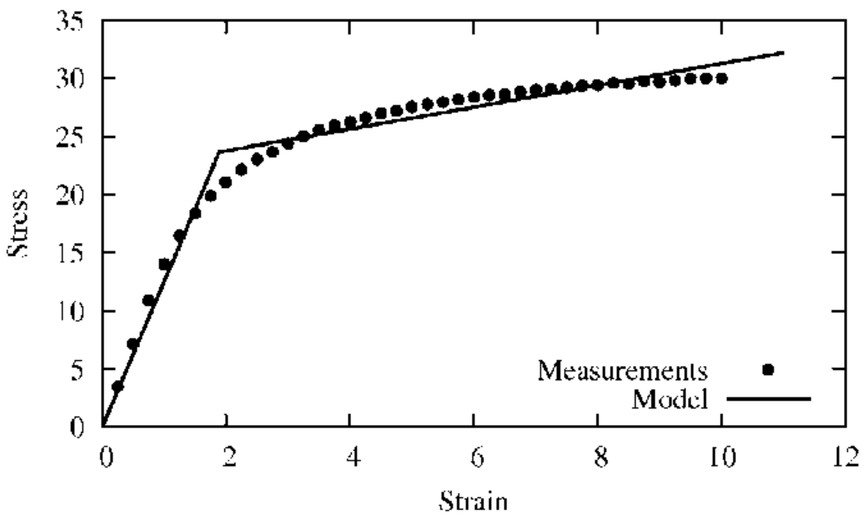
- If the errors are **independent** we obtain

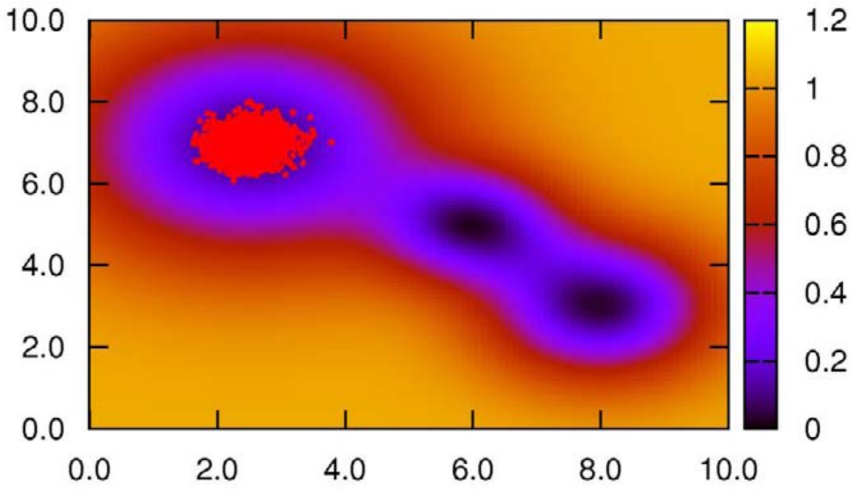
$$J(\mathbf{p}) = \sum_{i=1}^{n} w_i (y_i^* - y_i)^2, \quad w_i = \frac{1}{\sigma_{y,i}^2}$$

- With **constant** standard deviation the objective simplifies

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

Requirements to the Identification Procedure

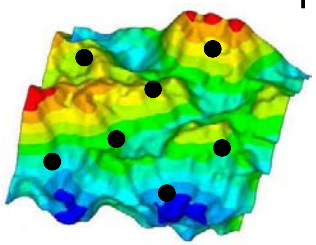




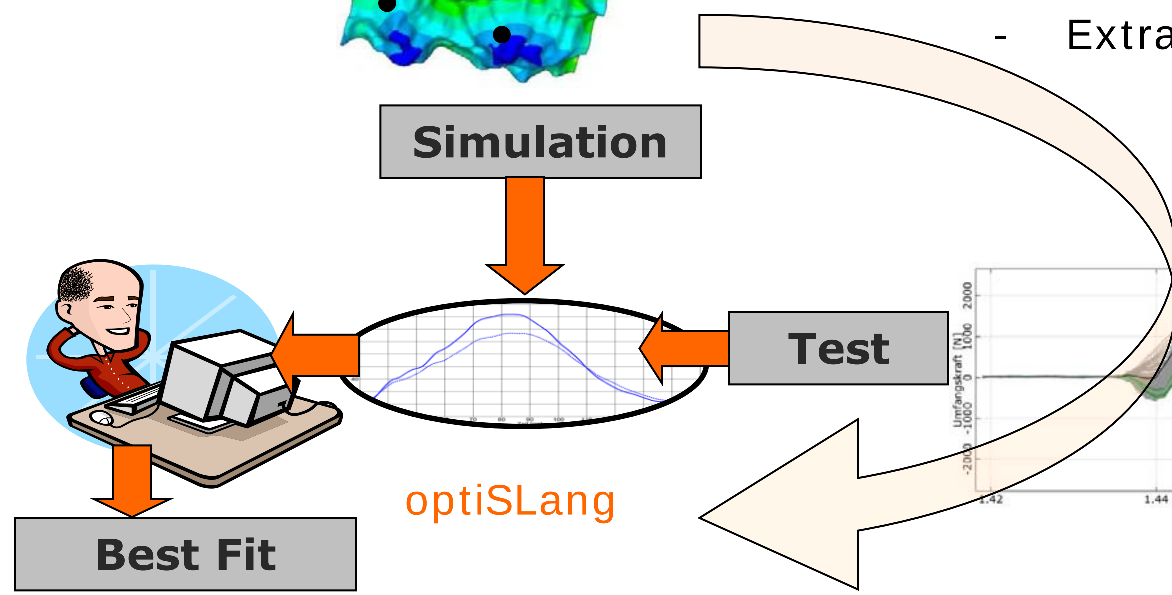
- The simulation model needs to represent the main physical behavior (systematic model errors are not considered)
- Since the least squares minimization may lead to a local optimum a global optimization strategy is necessary
- Only sensitive parameters can be identified
- Inverse problem needs to be well-posed
- Different parameter combinations may lead to a similar objective
- ➢ Uniqueness of identified parameters has to be assessed

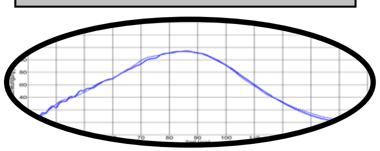
Calibration using optiSLang

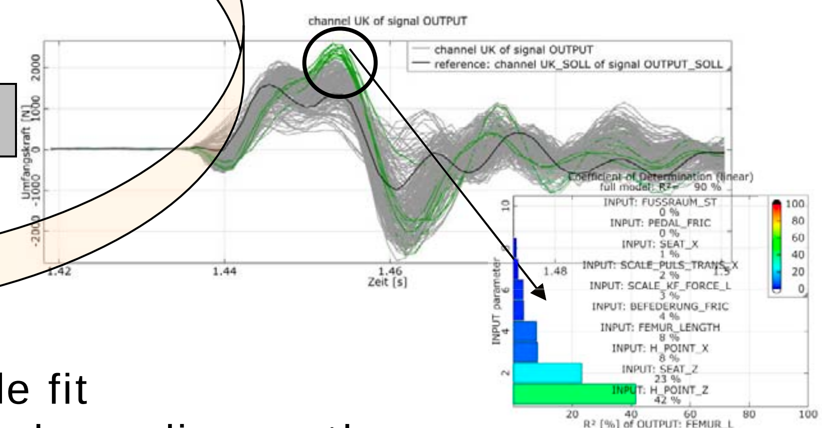
1) Define the Design space using continuous or discrete optimization variables



2) Scan the Design Space
- Check the variation
- Identify sensitive parameters and responses
- Check parameter bounds
- Extract start value



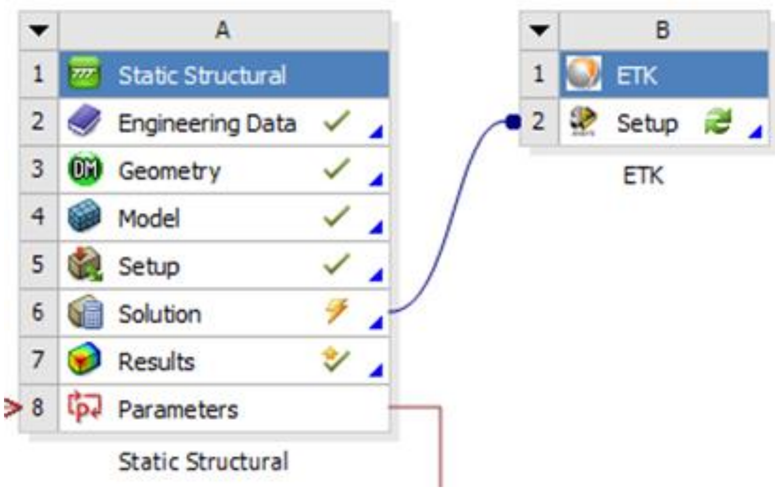


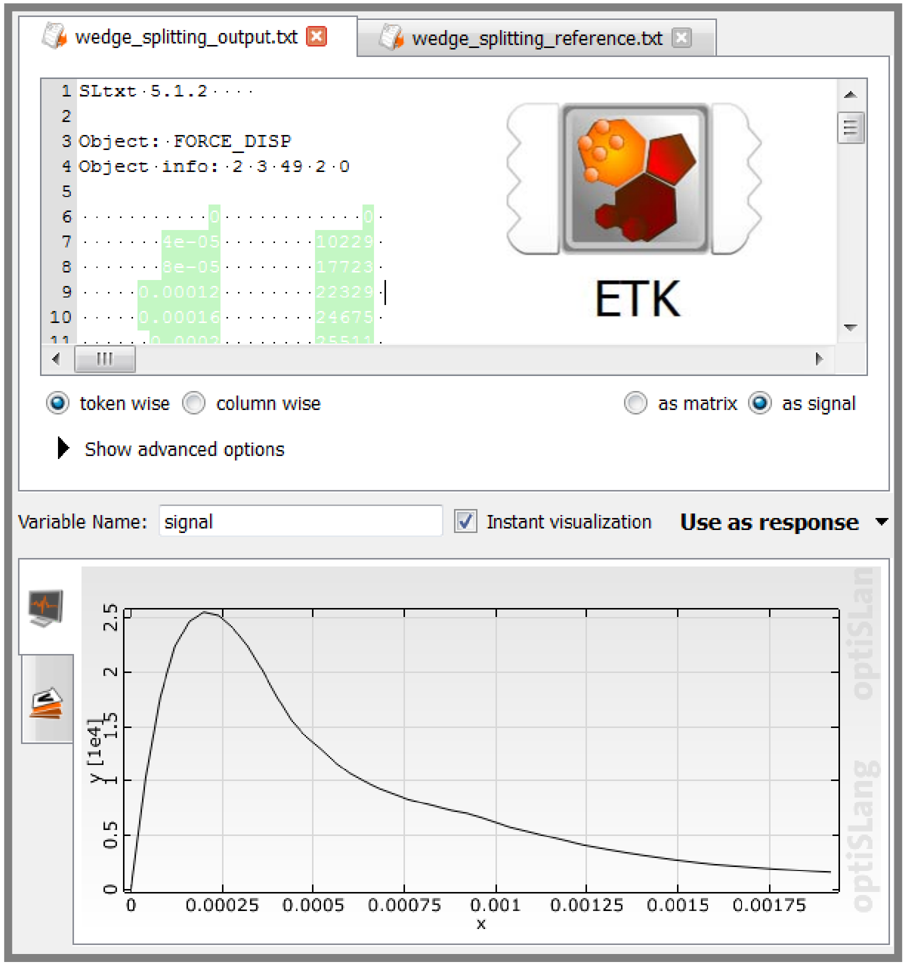


3) Find the best possible fit
- Choose an optimizer depending on the sensitive optimization parameter dimension/type

The Extraction Tool Kit (ETK)

- ETK is available in optiSLang and now in optiSLang inside ANSYS
- I can read signals, vectors and matrices from solver files in text and binary format
- It can perform arbitrary mathematical operations from extracted objects



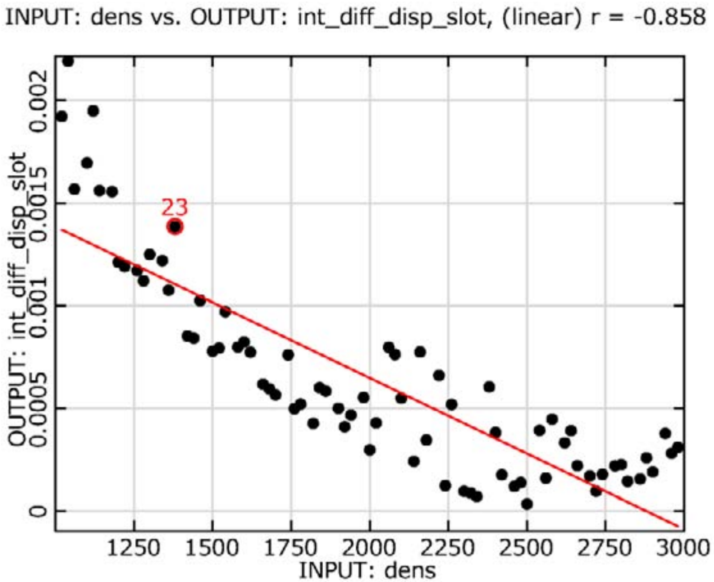


Sensitivity Analysis

Methods for Sensitivity Analysis

Local methods

- Local derivatives
- Standardized derivatives



Global methods

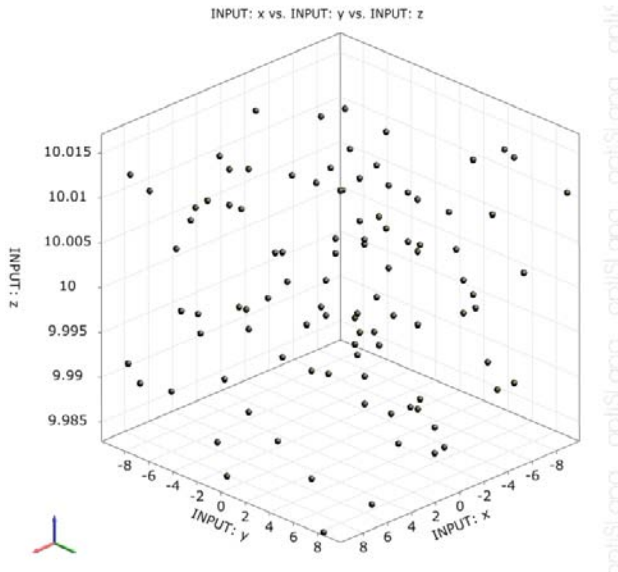
- Anthill plots
- Coefficients of correlation
- Rank order correlation
- Standardized regression coefficients
- Stepwise polynomial regression
- Varianced-based analysis: Sobol' indices

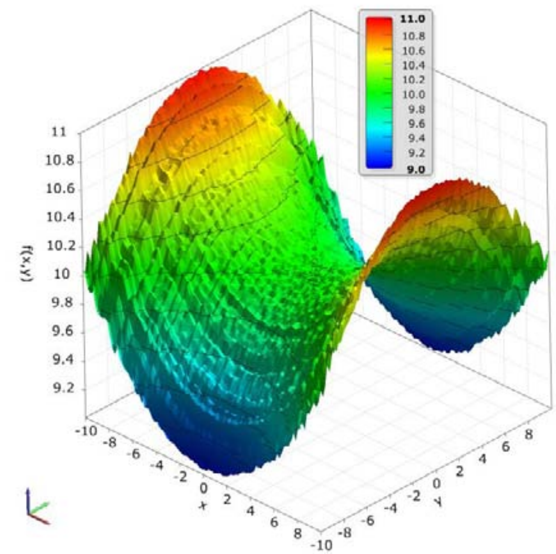
- **Advanced surrogate models including prediction analysis and optimal subspace detection: Metamodel of Optimal Prognosis**

Scanning the Design Space

Inputs | Design of Experiments | Solver evaluation | Outputs

$$\left.\begin{matrix} X_1 \\ X_2 \\ \vdots \\ X_k \end{matrix}\right\}$$



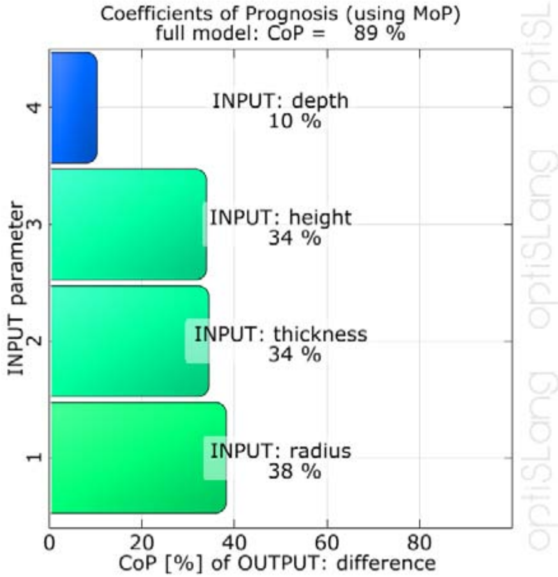


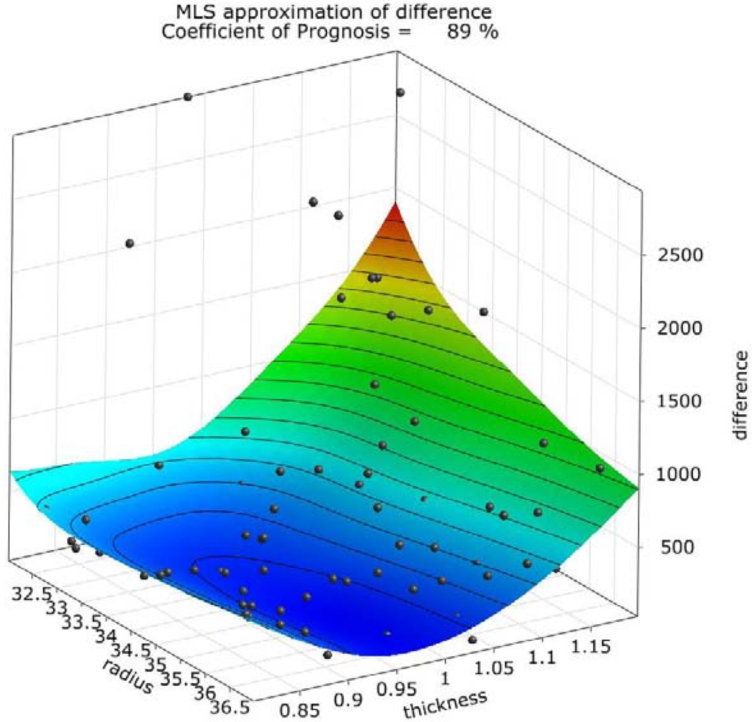
$$\left\{\begin{matrix} Y_1 \\ Y_2 \\ \vdots \\ Y_m \end{matrix}\right.$$

- Uniform distribution of inputs is represented by Latin Hypercube Sampling
- Minimum number of samples should represent statistical properties, cover the input space optimally and avoid clustering
- For each design all responses are calculated

Metamodel of Optimal Prognosis (MOP)

- Approximation of solver output by fast surrogate model
- Reduction of input space to get best compromise between available information (samples) and model representation (number of inputs)
- Determination of optimal approximation model
- Assessment of approximation quality
- Evaluation of variable sensitivities





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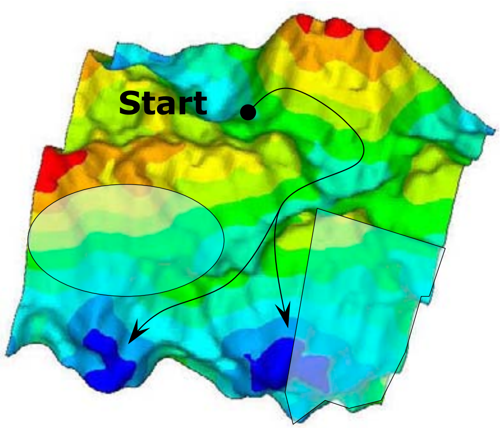
Least Squares Minimization

Optimization Algorithms

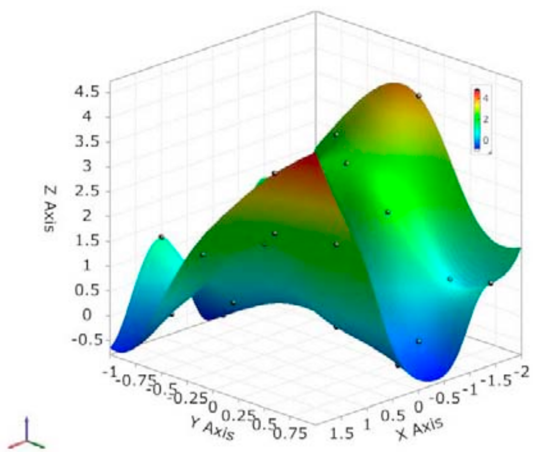
Gradient-based Methods

- Most efficient method if gradients are accurate enough
- Consider its restrictions like local optima, only continuous variables and noise



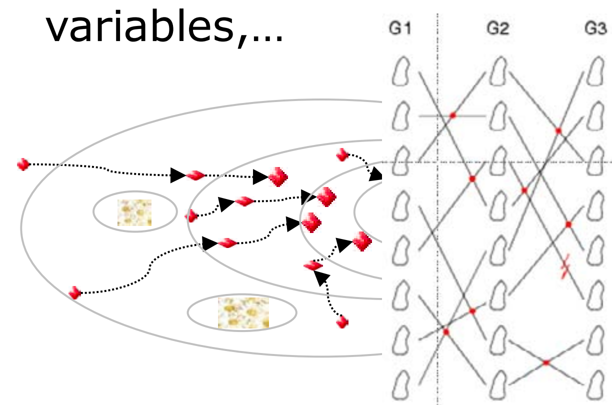
Adaptive Response Surface Method

- Attractive method for a small set of continuous variables (<20)
- Adaptive RSM with default settings is the method of choice



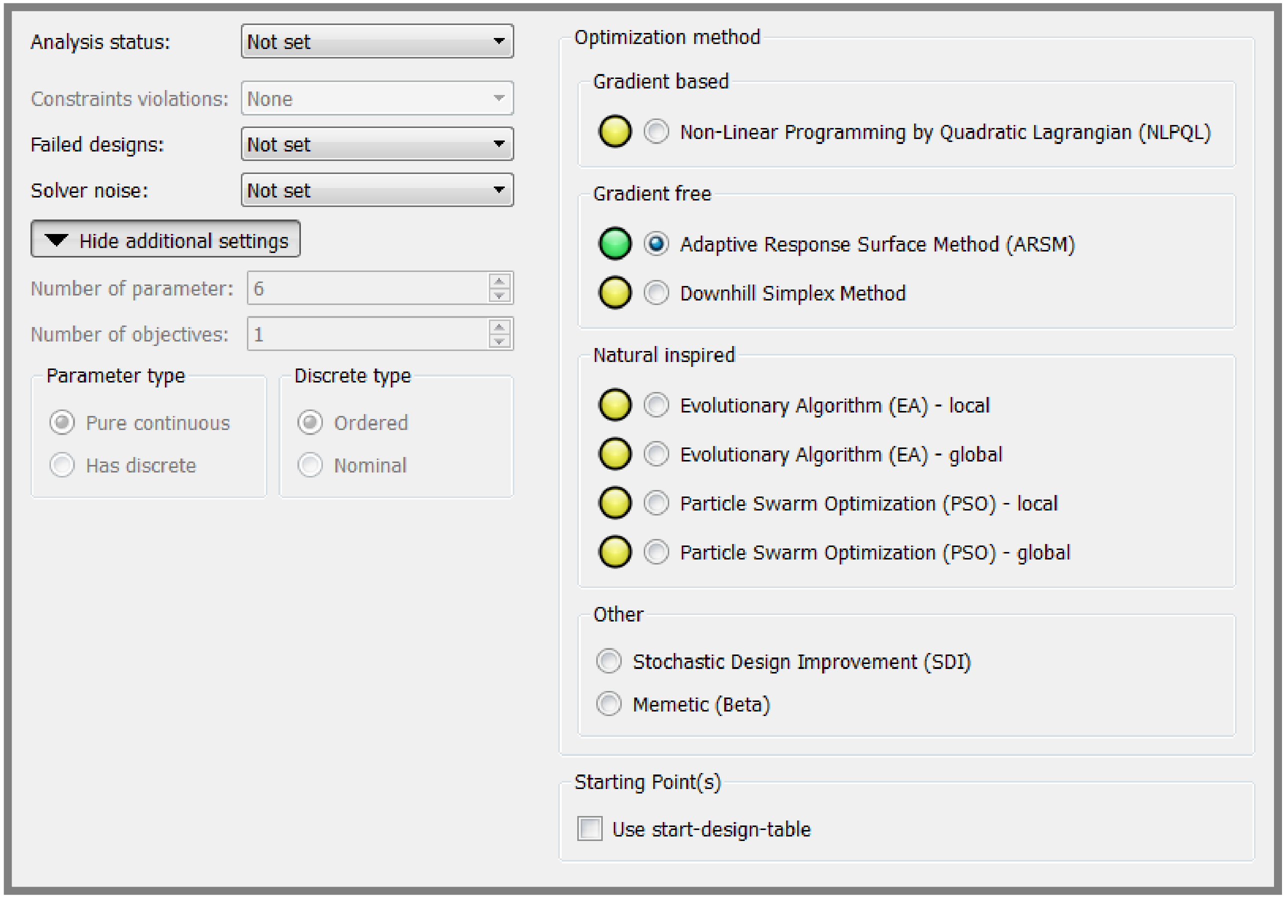
Nature inspired Optimization

- GA/EA/PSO imitate mechanisms of nature to improve individuals
- Method of choice if gradient or ARSM fails
- Very robust against numerical noise, non-linearity, number of variables,…



Decision Tree for Optimizer Selection

- optiSLang automatically suggests an optimizer depending on the parameter properties, the defined criteria and user specified settings

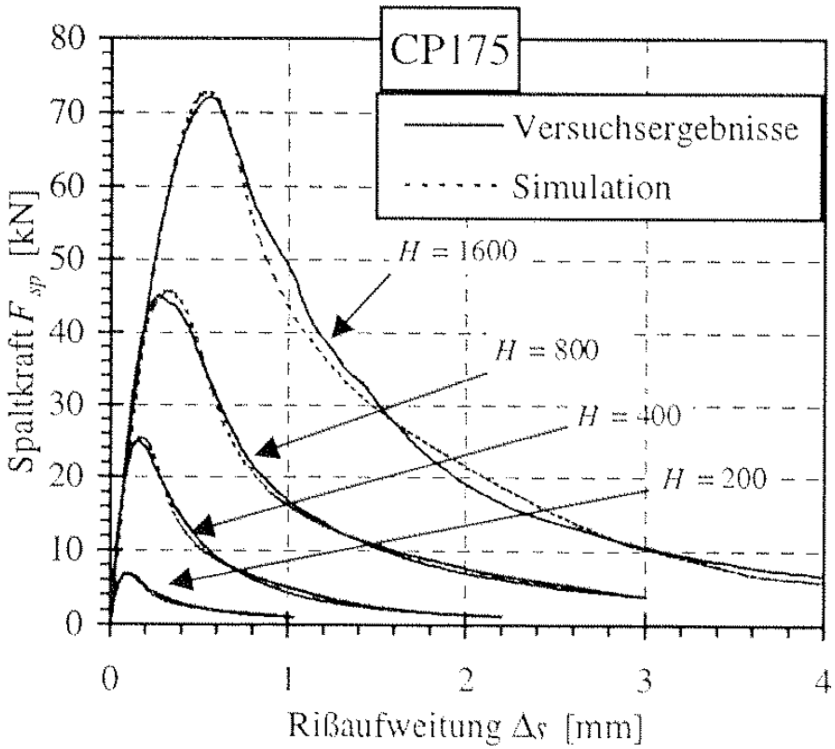


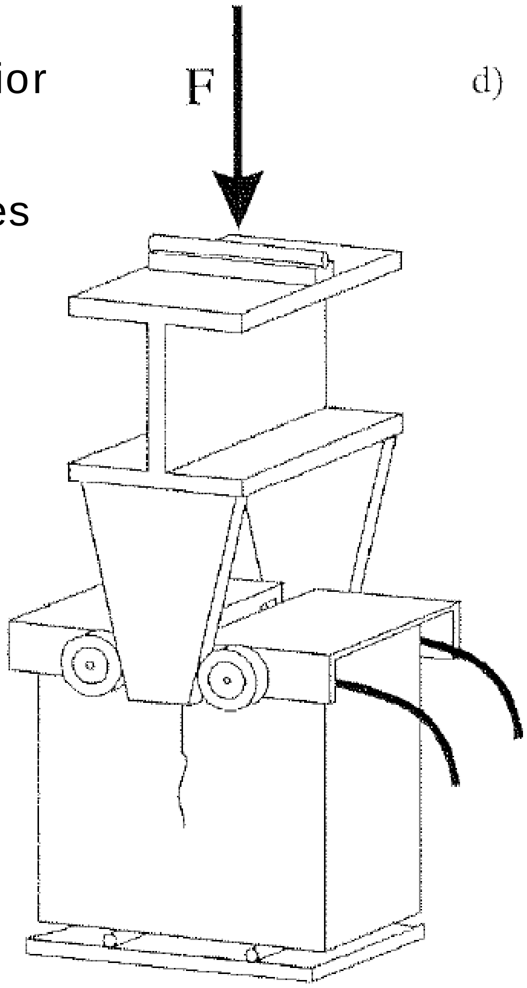
Examples

Wedge Splitting Test (Trunk 1999)

Experimental Set Up

- Measurements of cracking and softening behavior of dam concrete for different specimen sizes
- Identification of elasticity and fracture properties





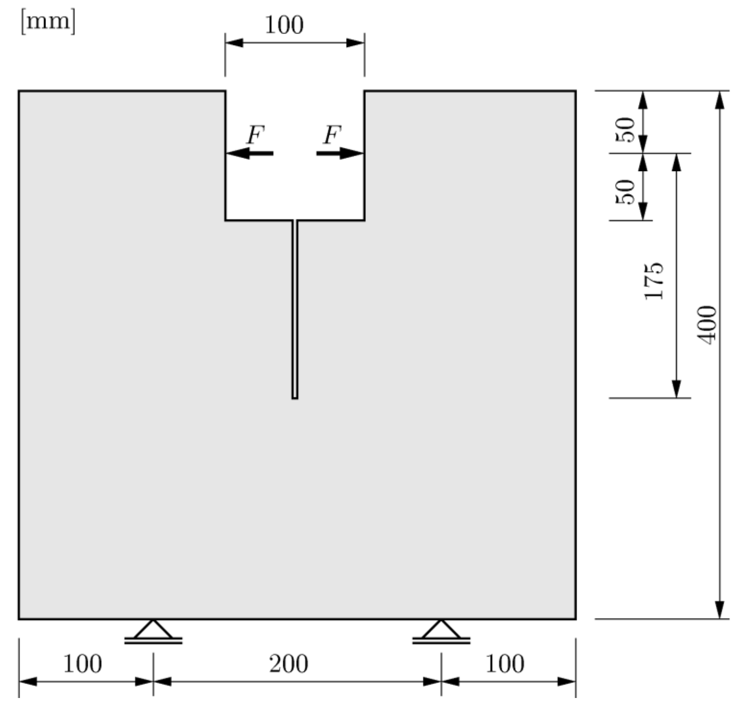
Wedge Splitting Test

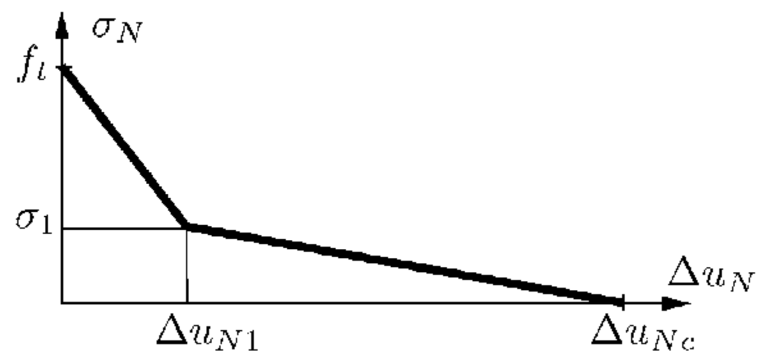
Simulation Model

- 2D linear elastic finite element model with predefined crack
- Bilinear softening for crack interface elements
- Unknown constitutive parameters:
  - Young's modulus *E*
  - Poisson's ratio υ
  - Tensile strength f_t
  - Fracture energy G_f
  - Shape parameters

$$\alpha_{f_t} = \sigma_1 / f_t$$

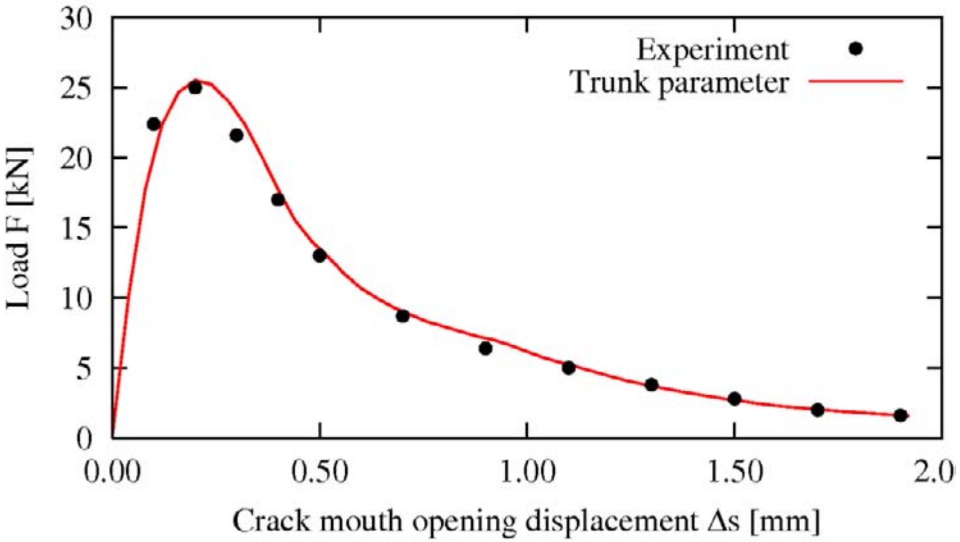
$$\alpha_{wc} = \Delta u_{N1} / \Delta u_{Nc}$$

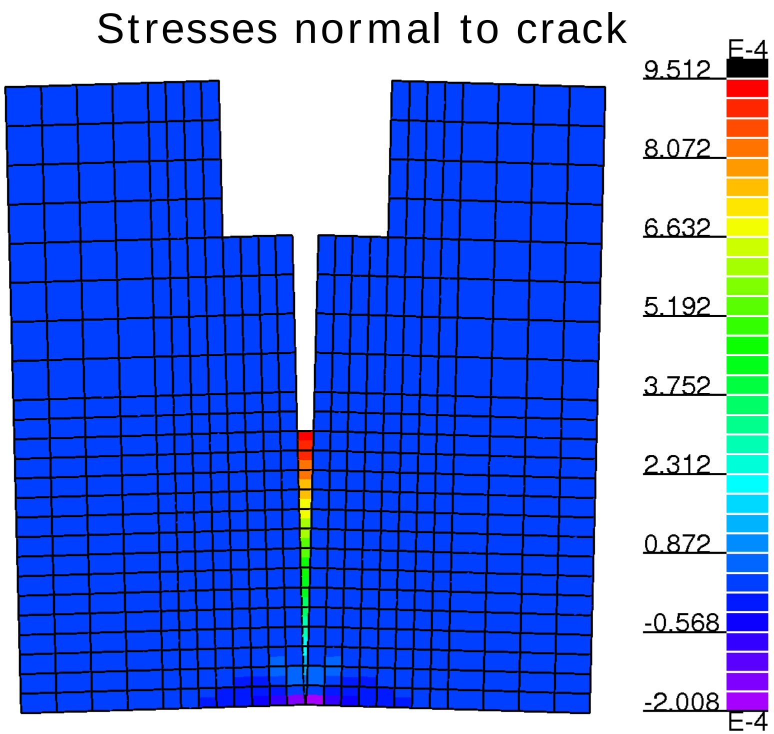




Wedge Splitting Test

Simulation with Reference Parameters

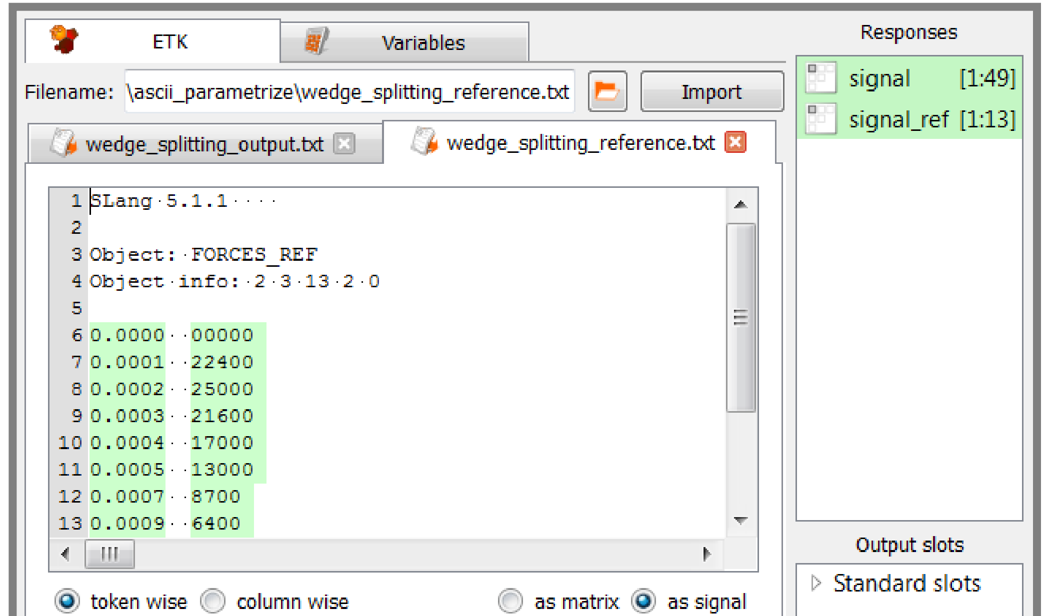


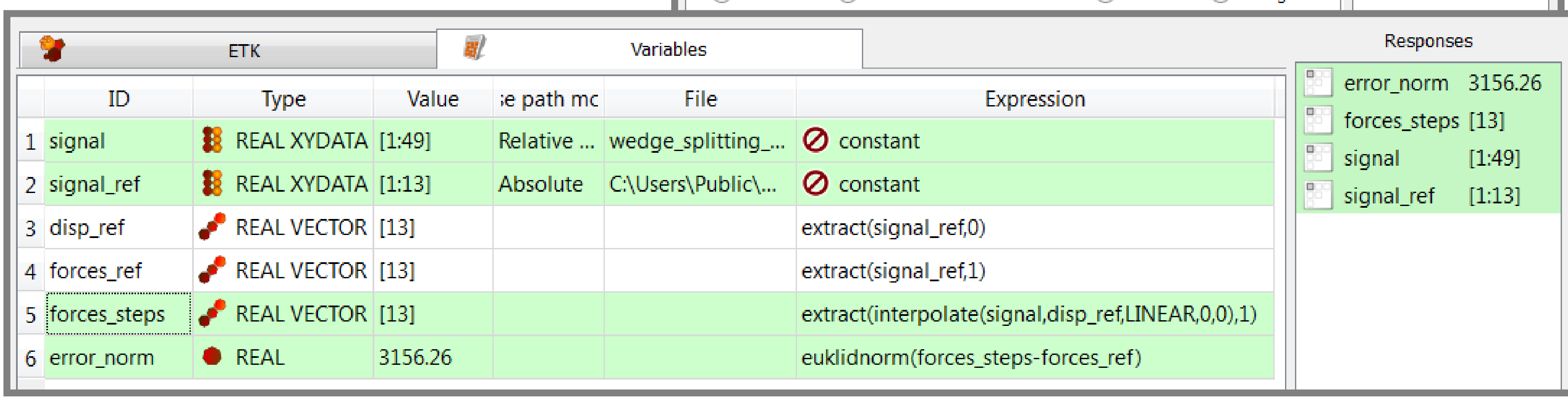


Wedge Splitting Test

Signal Functions

- Simulation and reference signals are included via text files
- Forces at reference displacement steps are interpolated from the signal
- Sum of squared errors is evaluated only at the reference points



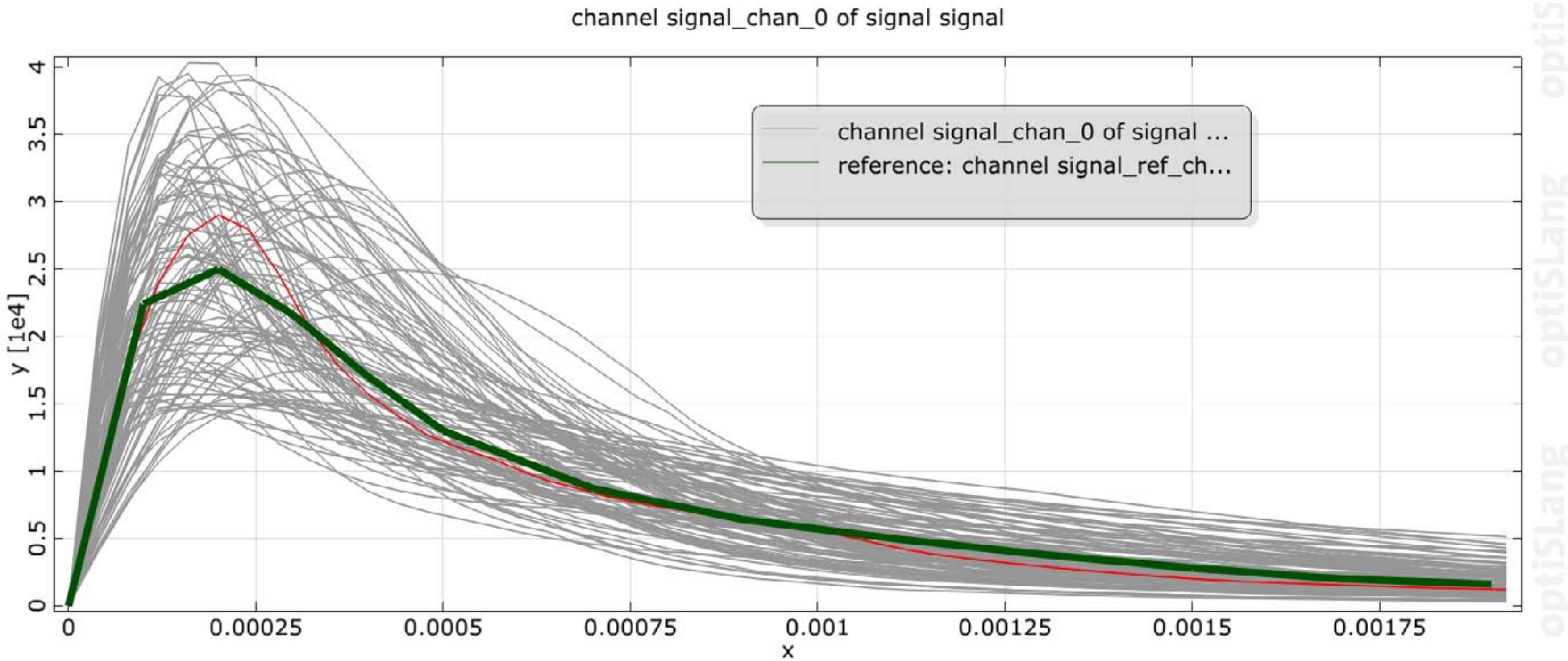


Wedge Splitting Test

Sensitivity Analysis

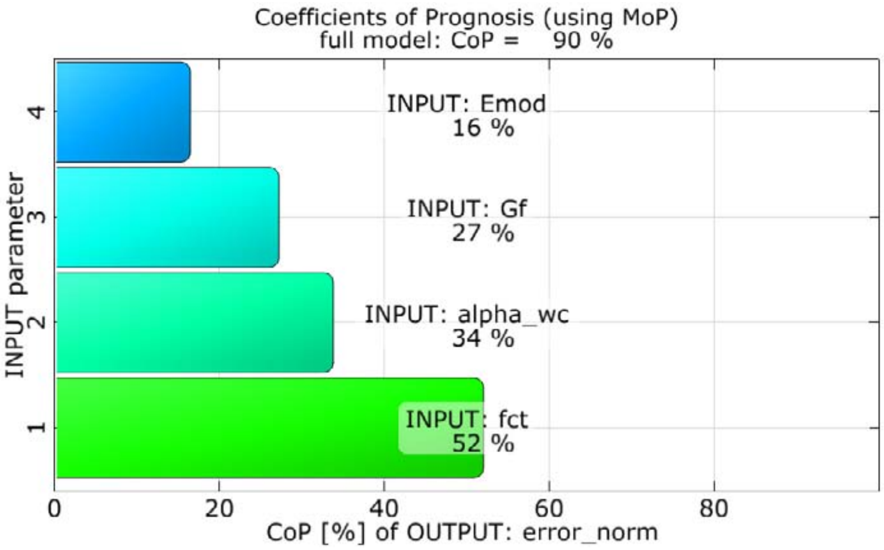
- The signals of each design are shown in the post-processing
- The range of the simulation signals covers the reference signal

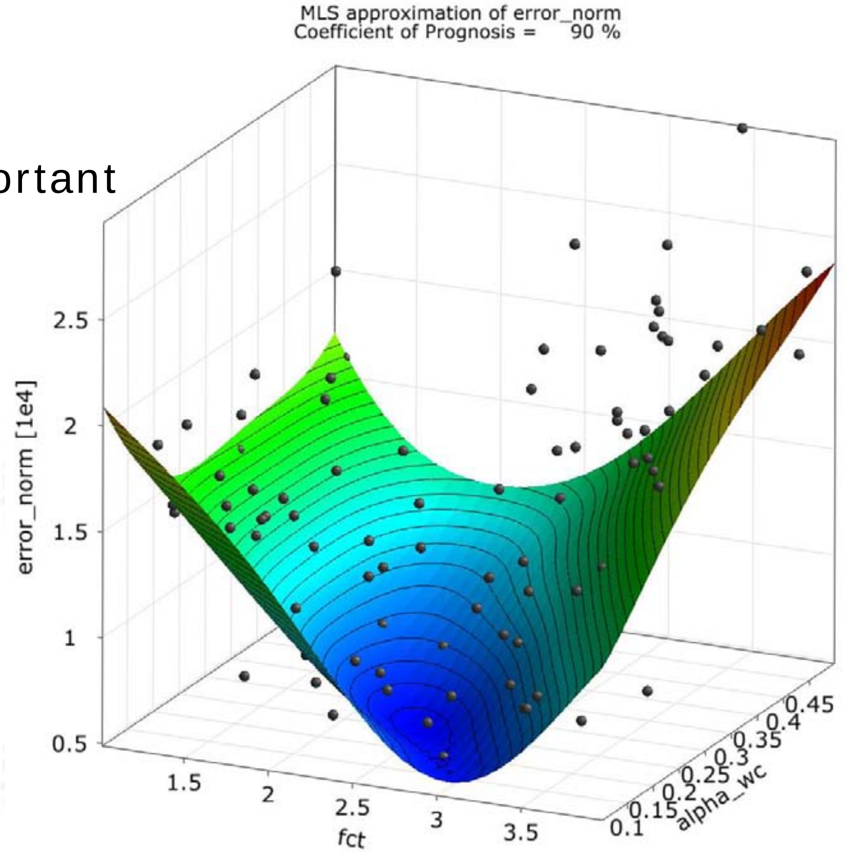
➢ Parameter bounds seem to be adequate



Wedge Splitting Test
Sensitivity Analysis

- Sum of squared errors can be explained with 90%
- Single global optimum is indicated
- Poisson's ratio and one of the shape parameters are not detected as important
- ➢ Check also single force values





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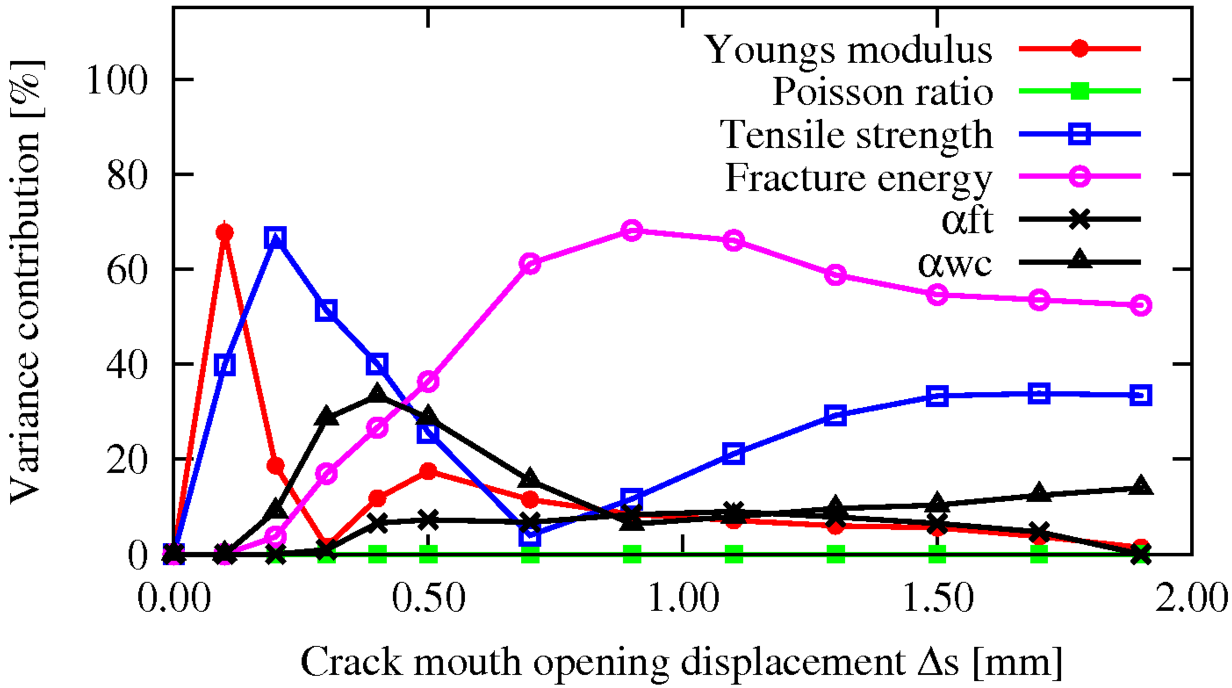
Wedge Splitting Test

Sensitivity Analysis

Wedge Splitting Test

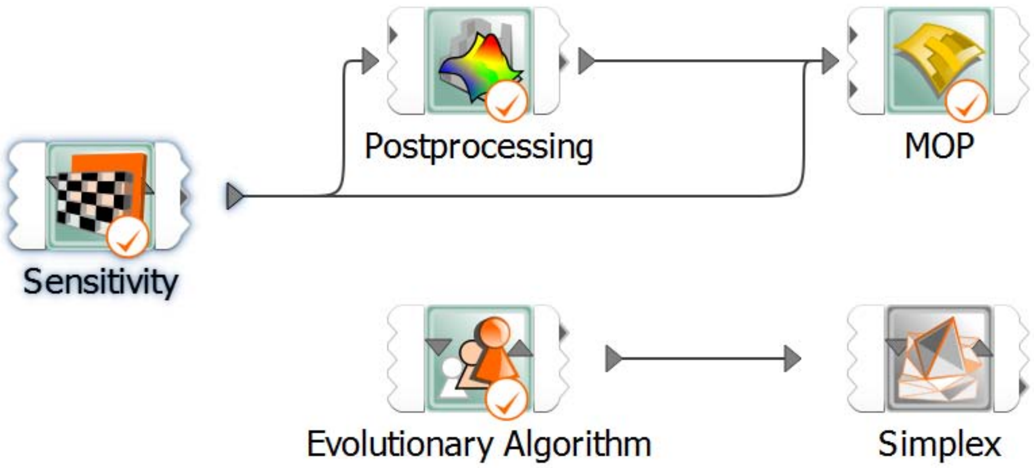
Sensitivity Analysis

- Young's modulus is most important at small displacements
- Poisson's ratio has no influence
- Tensile strength becomes important as the first cracks appear
- Fracture energy is most important during the softening process
- Shape parameters have minor influence



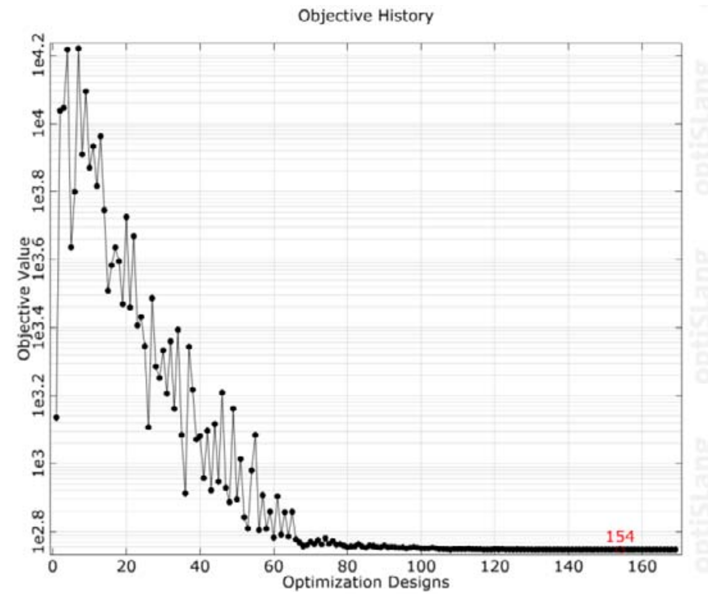
Wedge Splitting Test
Optimization

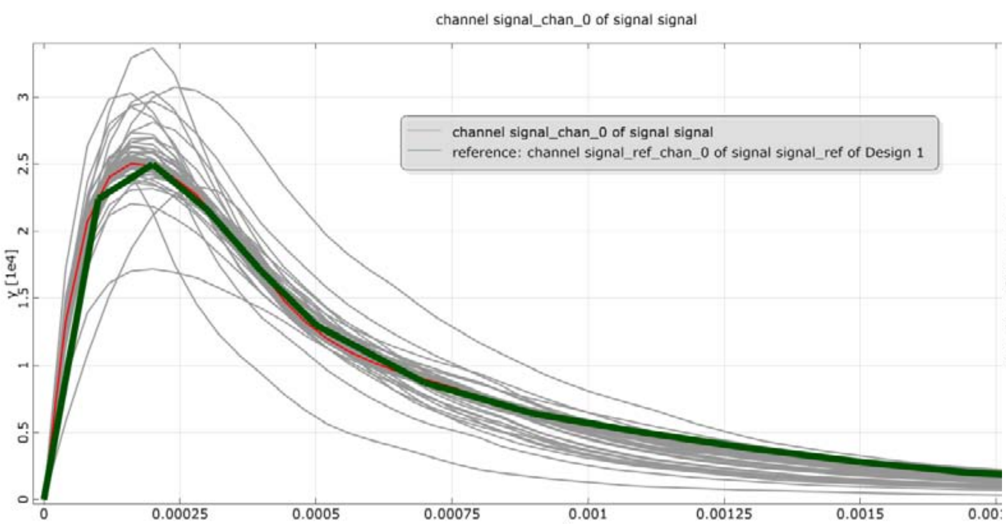
- Poisson’s ratio is not sensitive to any of the force values
- ➢ It can not be identified and is not considered in the optimization
- Other parameter bounds are kept
- Best designs of sensitivity are taken as start population
- Simplex optimizer eventually coupled with PSO or EA shows good convergence

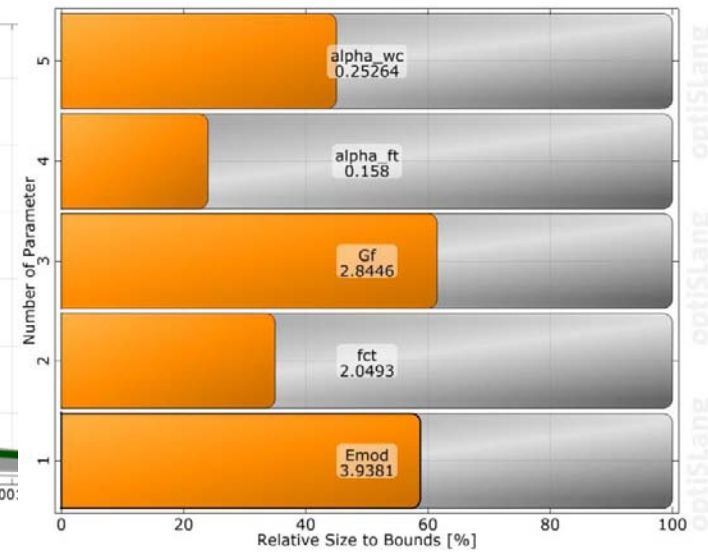


Wedge Splitting Test
Optimization

- The signal of the best design agrees very well with the reference
- The unknown parameters are identified by the optimizer



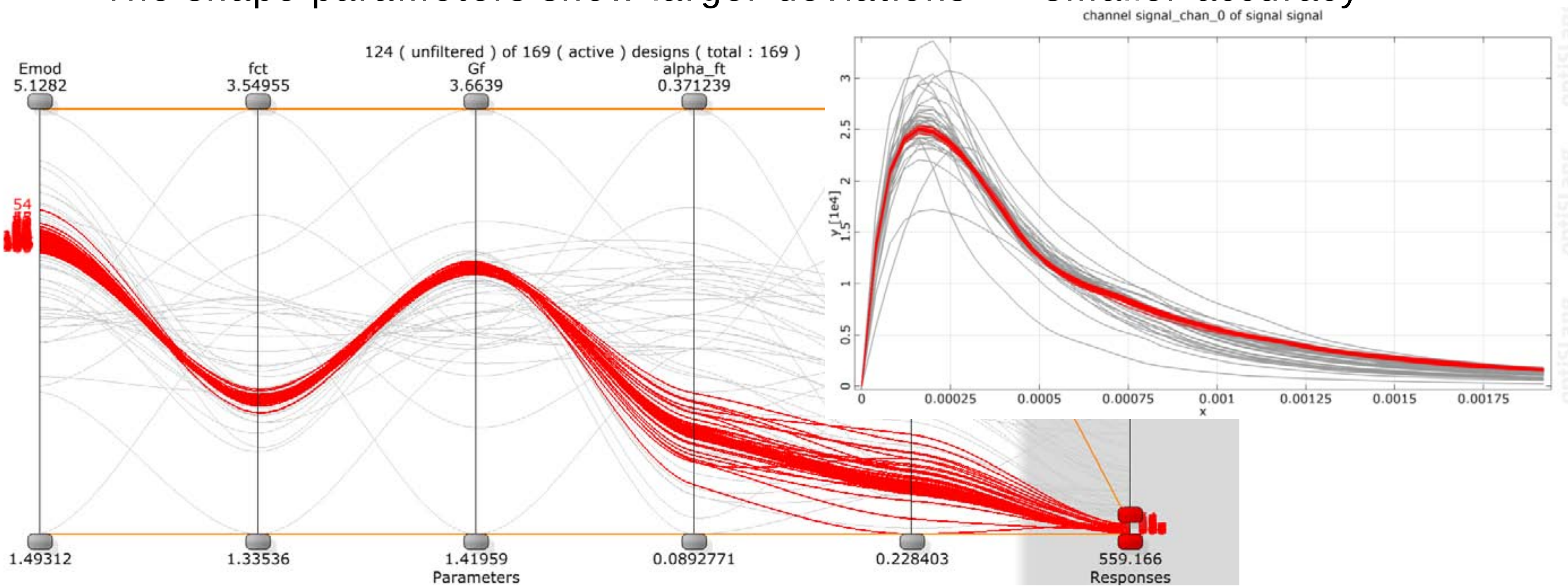




Wedge Splitting Test

Accuracy of the Identified Parameters

- Accuracy and uniqueness of identified parameters can be checked with a parallel coordinates plot by selecting the designs with small errors
- The corresponding signals agree very well with the reference
- The Young's modulus, the fracture energy and the tensile strength of these designs show small deviations, which indicates a good accuracy
- The shape parameters show larger deviations -> smaller accuracy

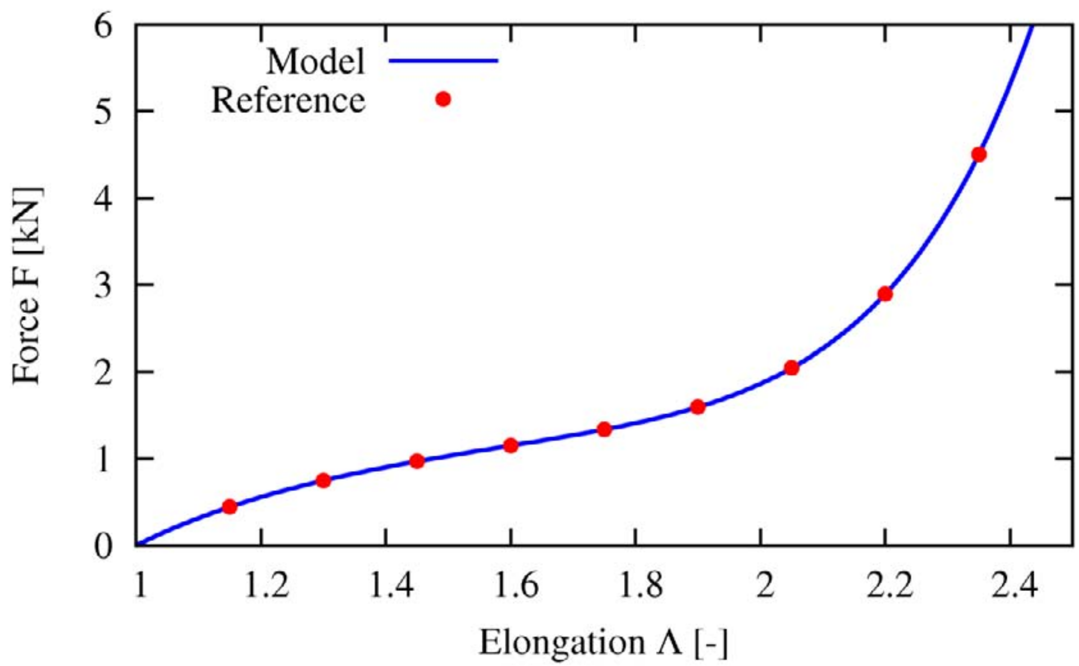


Ogden Hyperelasticity
Constitutive Model

- Hyperelastic model with exponential formulation of Cauchy stress depending on deformation
- One-dimensional case assuming incompressible behavior:

$$\sigma = \sum \mu_i (\Lambda^{\alpha_i} - \Lambda^{-\alpha_i/2})$$

- Often 2 or 3 pairs of μ and α are necessary
- μ and α are the unknown parameters in the identification
- How many terms of the OGDEN law are necessary for the given reference ?



Ogden Hyperelasticity

Sensitivity Analysis – Forces at Reference points

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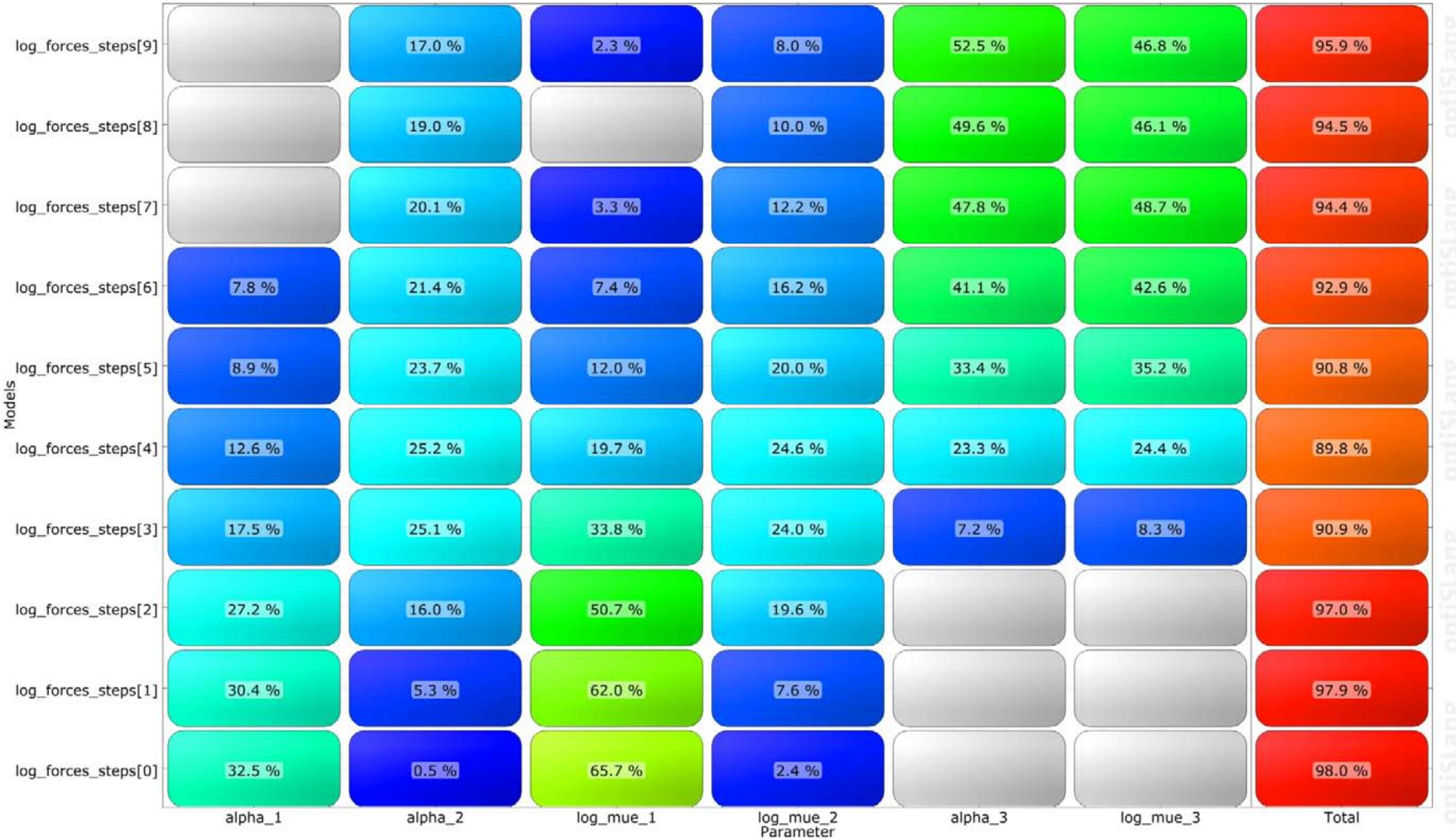
Ogden Hyperelasticity

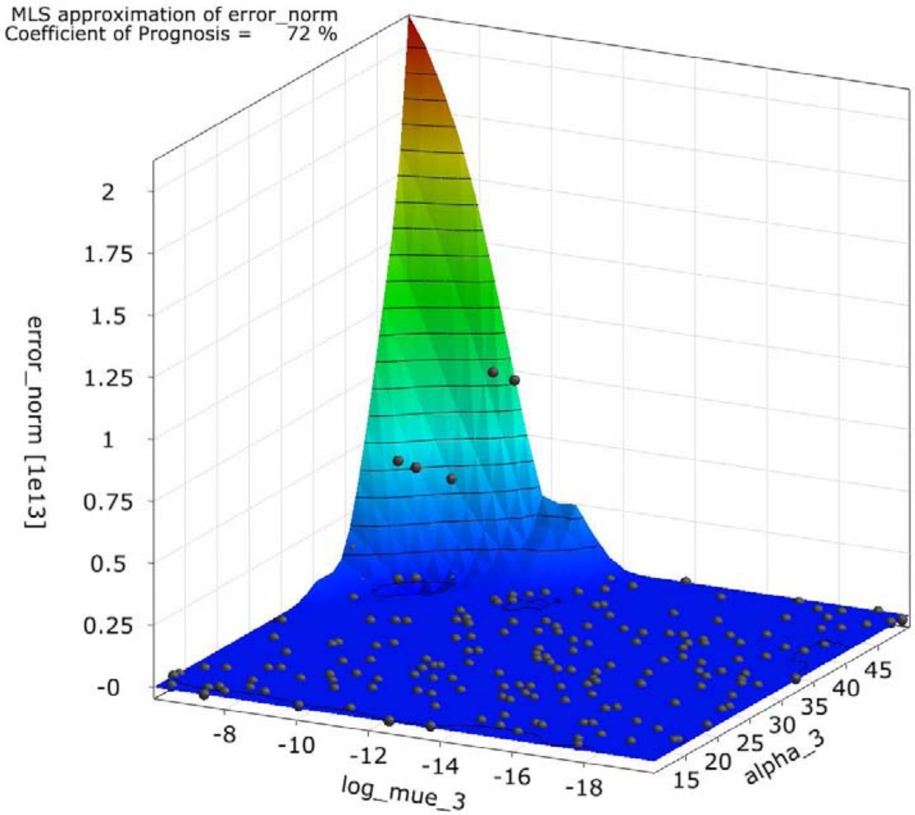
Sensitivity Analysis – Logarithmic Forces at Reference points

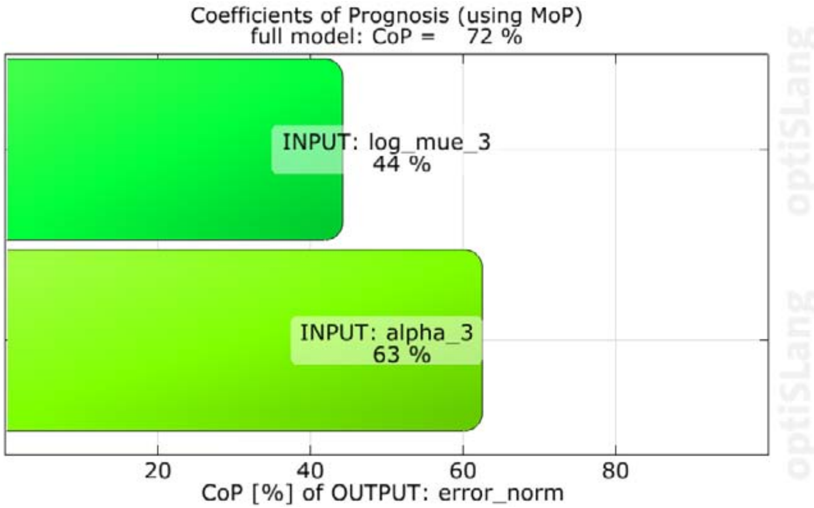


Ogden Hyperelasticity

Sensitivity Analysis – Sum of Squared Errors

- Logarithmic forces can be much better explained by input variables
- This is similar for the sum of squared errors
- With standard least squares, only 2 inputs seem to be important

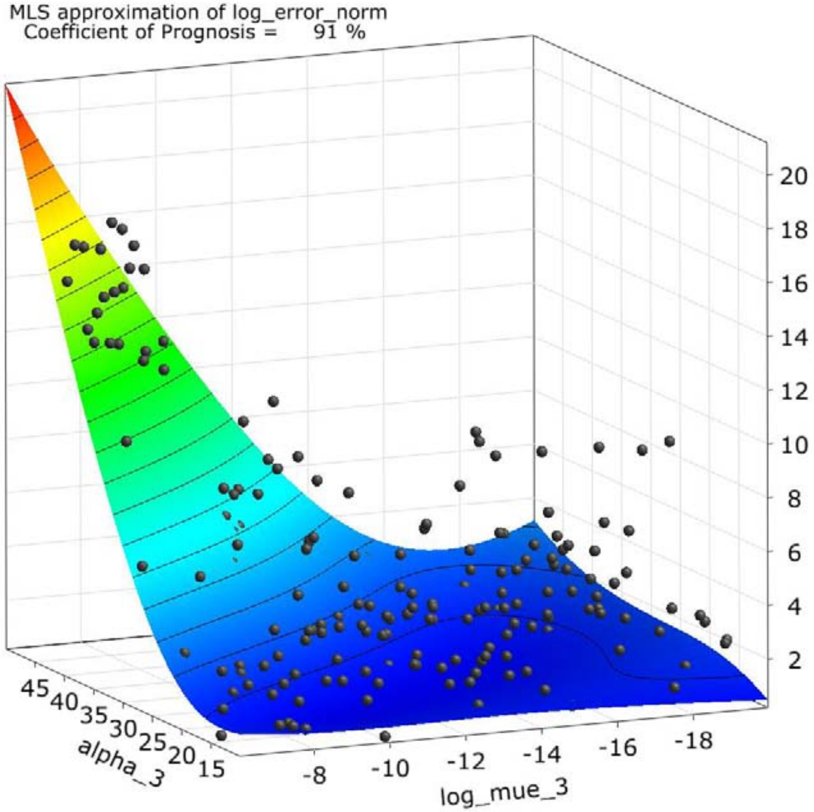


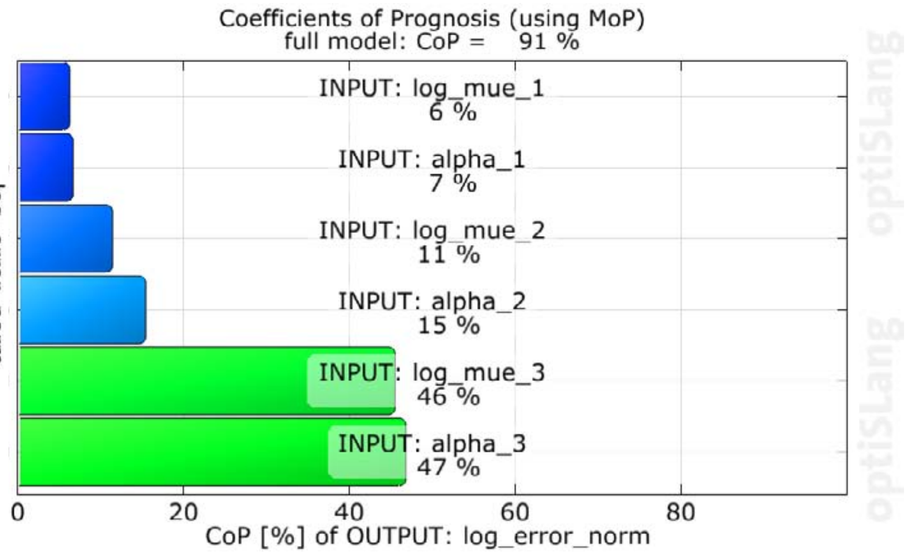


Ogden Hyperelasticity

Sensitivity Analysis – Sum of Squared Errors of Logarithmic Forces

- With logarithmic forces the sum of squared errors can be explained very well and is influenced by all input parameters

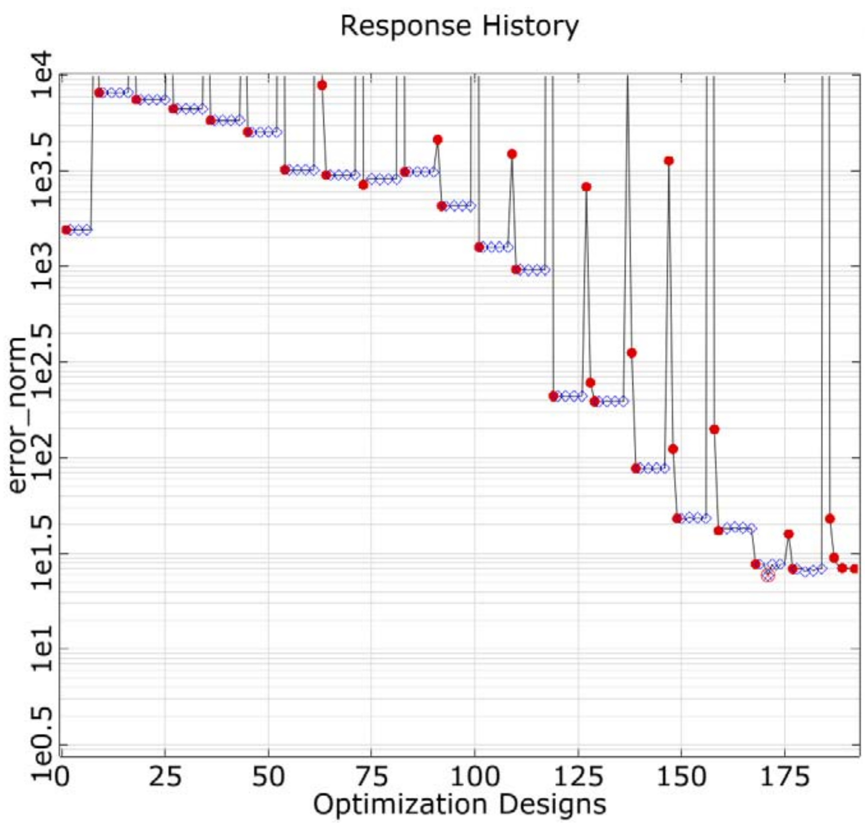


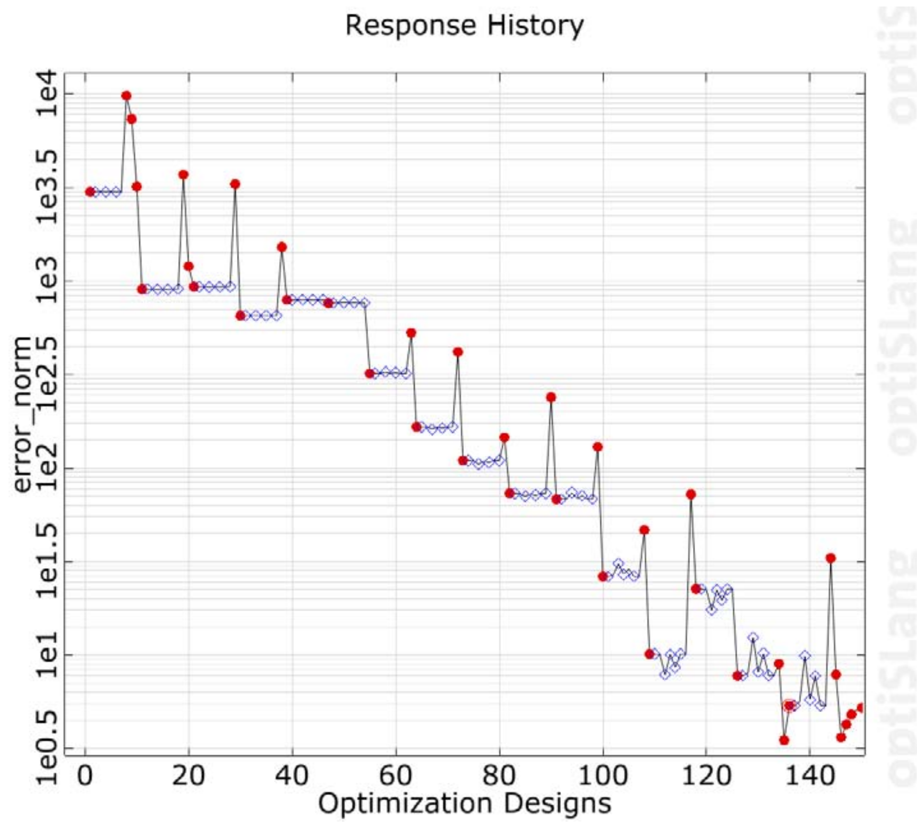


Ogden Hyperelasticity

Least Squares Minimization

- The optimizer converges faster to a better solution using the logarithmic forces

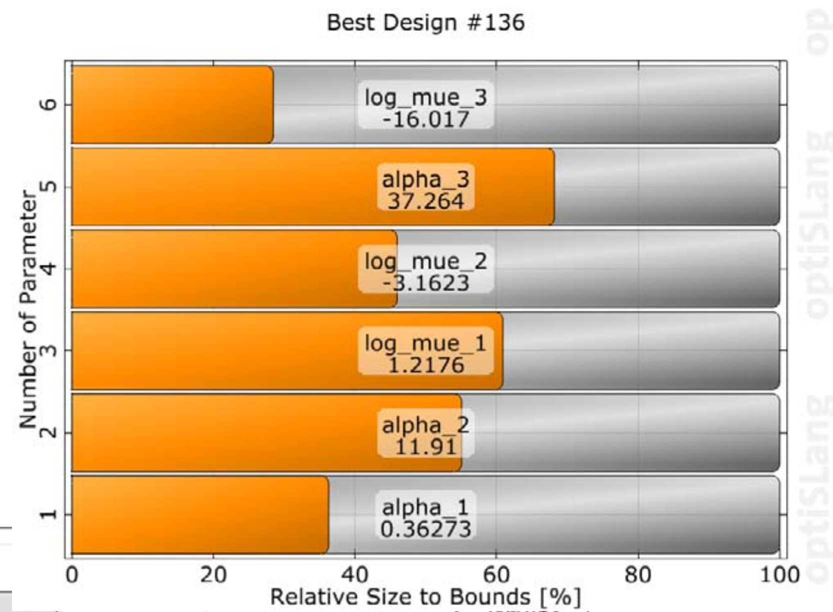


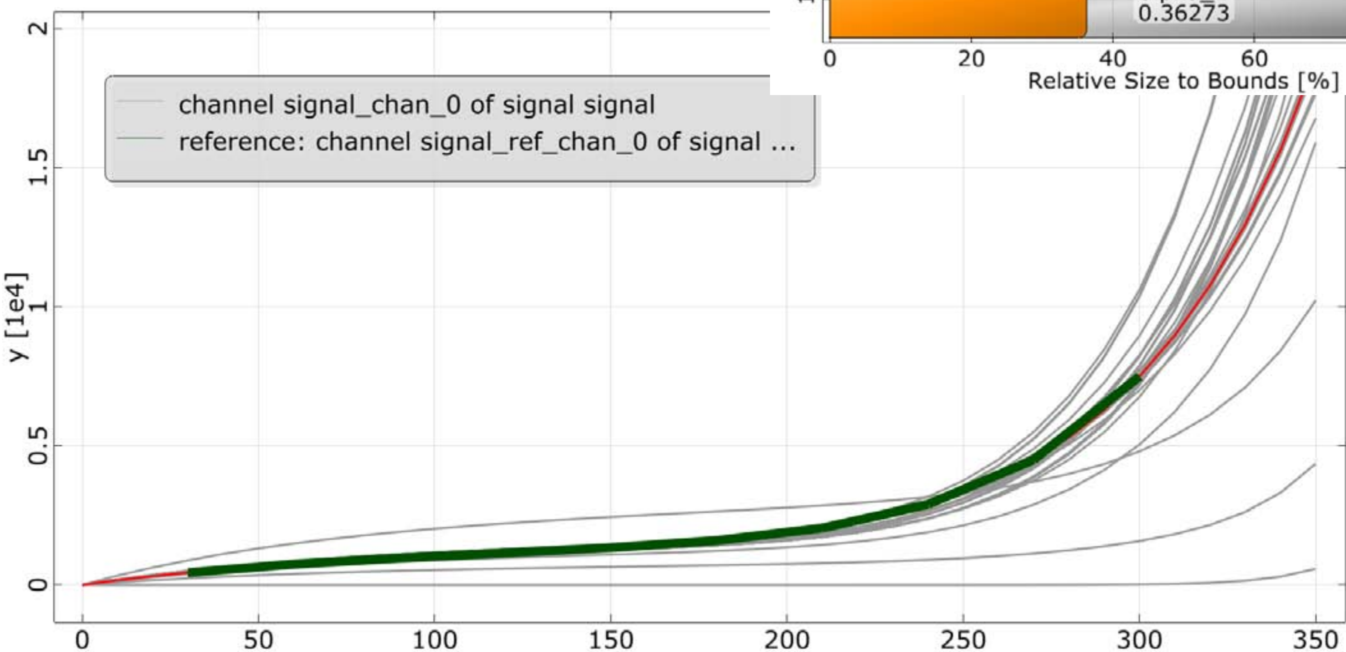


Ogden Hyperelasticity

Result

- The modulus μ of the third parameter pair is approximately zero
- ➢ Only two terms in the constitutive formulation are necessary
- Simulation and Reference agree perfectly:





Outlook

Parameter Accuracy

- Least squares objective function from maximum likelihood

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

- Linearization of objective function

$$\Delta\mathbf{p} = \left(\mathbf{A}^T \mathbf{C}_{\mathbf{yy}}^{-1} \mathbf{A}\right)^{-1} \mathbf{A}^T \mathbf{C}_{\mathbf{yy}}^{-1} \Delta\mathbf{y}, \quad \mathbf{A} = \frac{\partial \mathbf{y}}{\partial \mathbf{p}}$$

- Estimated covariance of optimal parameters (Markov estimator)

$$\mathbf{C}_{\mathbf{pp}} = \left(\mathbf{A}_{opt}^T \mathbf{C}_{\mathbf{yy}}^{-1} \mathbf{A}_{opt}\right)^{-1}$$

- For constant and independent measurement errors we obtain

$$\mathbf{C}_{\mathbf{pp}} = \sigma_y^2 \left(\mathbf{A}_{opt}^T \mathbf{A}_{opt}\right)^{-1}$$

Posteriori Error Estimation

- Estimated covariance for incorrect models

$$\hat{\mathbf{C}}_{\mathbf{pp}} = s_0^2 \mathbf{C}_{\mathbf{pp}} = s_0^2 \left(\mathbf{A}^T \mathbf{C}_{\mathbf{yy}}^{-1} \mathbf{A} \right)^{-1}$$

- Variance correction factor

$$s_0^2 = \frac{1}{N-P} \left(\mathbf{x}^* - \mathbf{x} \right)^T \mathbf{C}_{\mathbf{yy}}^{-1} \left(\mathbf{x}^* - \mathbf{x} \right)$$

- For constant and independent measurement errors we obtain

$$\hat{\mathbf{C}}_{\mathbf{pp}} = \frac{1}{N-P} \sum_{i=1}^{n} (y_i^* - y_i)^2 \left(\mathbf{A}_{opt}^T \mathbf{A}_{opt} \right)^{-1}$$

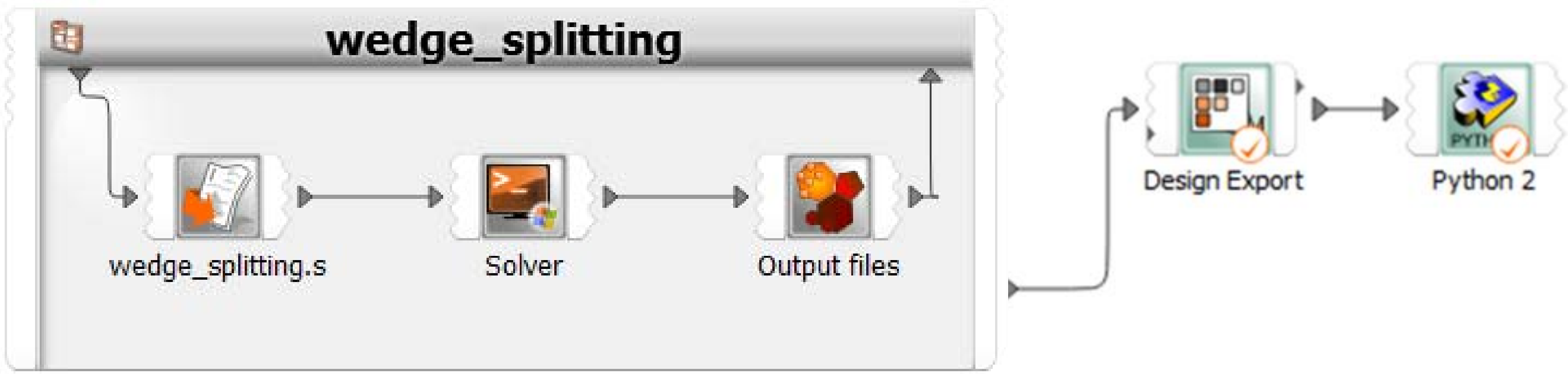
Wedge Splitting Test
Estimation of Parameter Accuracy

- Define a local sensitivity at the best design
- Add small interval of 0.01 for all identified parameters in the start design table

Status	Emod	Gf	alpha_ft	alpha_wc	fct	nue
Succeeded	4.17742	2.8497	1.49243	2.57183	2.0017	1.8
Needs reevalua...	4.18742	2.8497	1.49243	2.57183	2.0017	1.8
Needs reevalua...	4.17742	2.8597	1.49243	2.57183	2.0017	1.8
Needs reevalua...	4.17742	2.8497	1.50243	2.57183	2.0017	1.8
Needs reevalua...	4.17742	2.8497	1.49243	2.58183	2.0017	1.8
Needs reevalua...	4.17742	2.8497	1.49243	2.57183	2.0117	1.8

Wedge Splitting Test
Estimation of Parameter Accuracy

- Export the designs to a CSV-file
- Connect a python node and load the python-script *covariance_parameter.py*



Wedge Splitting Test

Estimation of Parameter Accuracy

- The python script writes a result file *parameter_accuracy.txt*
- The result file indicates, that the fracture energy and the tensile strength can be identified with the highest accuracy
- The shape parameters and the Young’s modulus can be identified with worse accuracy
- The estimated model error is about 200 N

Estimated standard deviation of identified parameters

Emod	0.0772	0.1595
Gf	0.0164	0.0339
alpha_ft	0.0504	0.1042
alpha_wc	0.0610	0.1261
fct	0.0148	0.0307
s0	206.5816	

Summary

- Sensitivity analysis is an important method within the calibration framework
- It can be used to check, if the parameters can be identified
- Different formulations of the error function can be investigated
- Choosing a better explainable error measure may significantly improve the optimization procedure
- The Metamodel of Optimal Prognosis with the included prediction assessment and the variance based sensitivity measures is a reliable and suitable tool for calibration task in real world applications