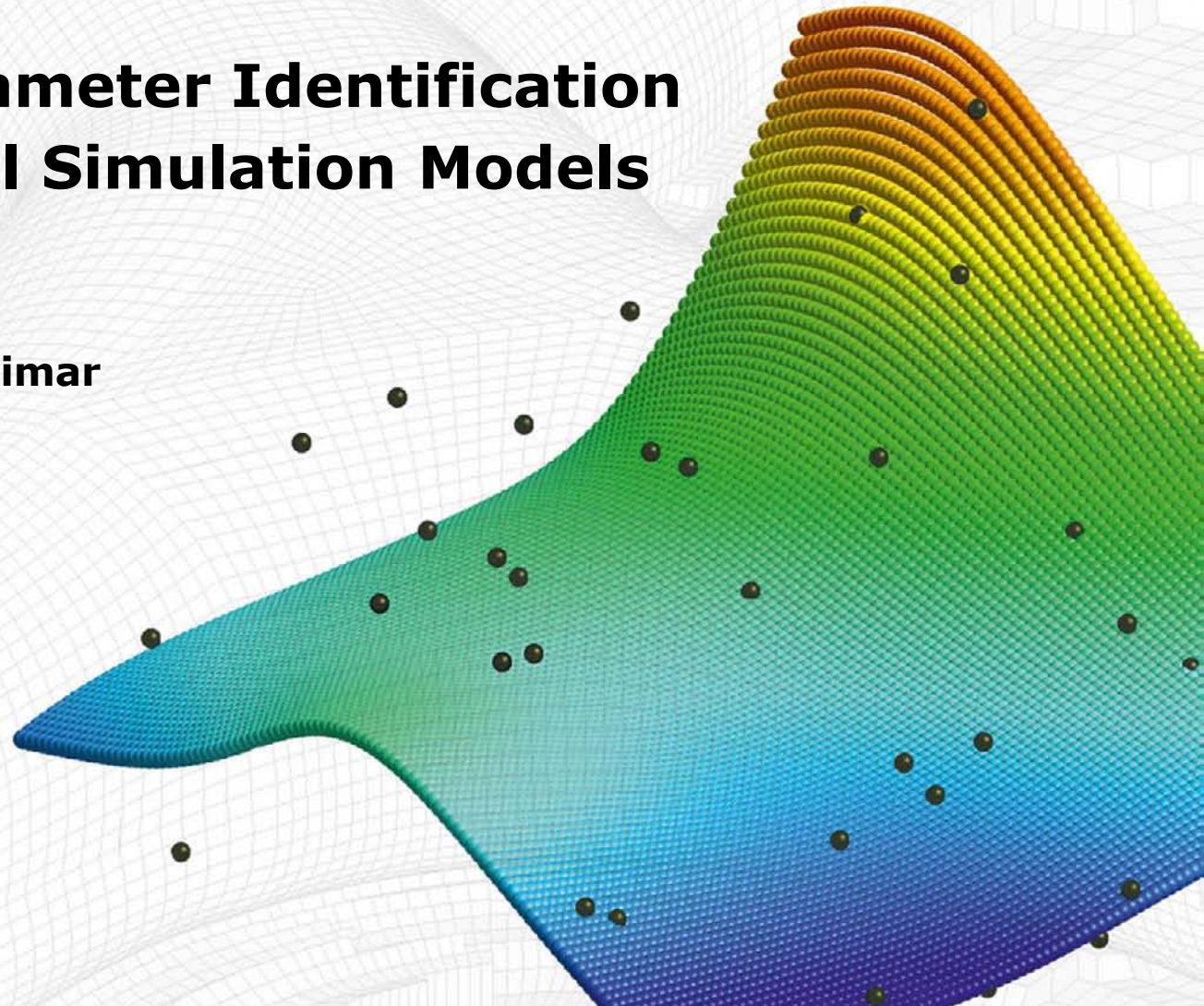


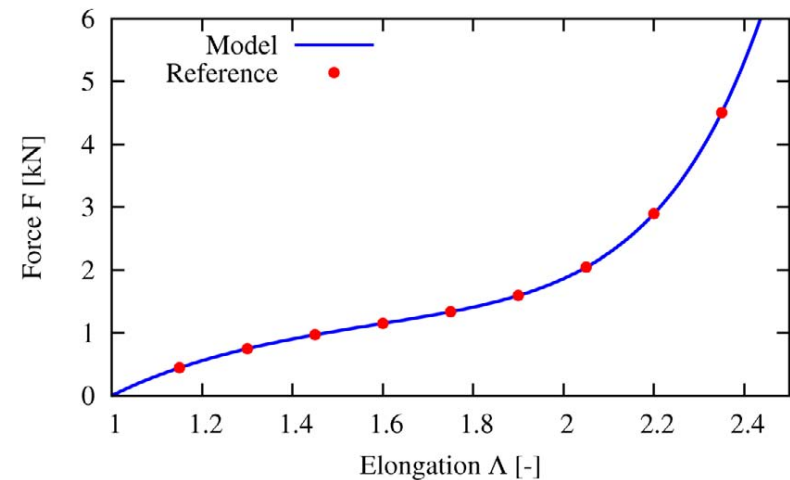
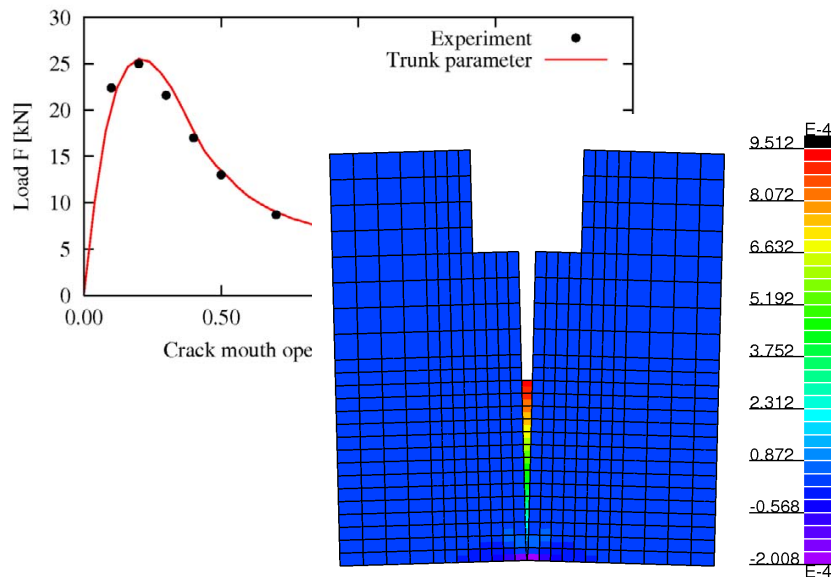
# Efficient Parameter Identification for Numerical Simulation Models

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Dynardo GmbH, Weimar



# Outline

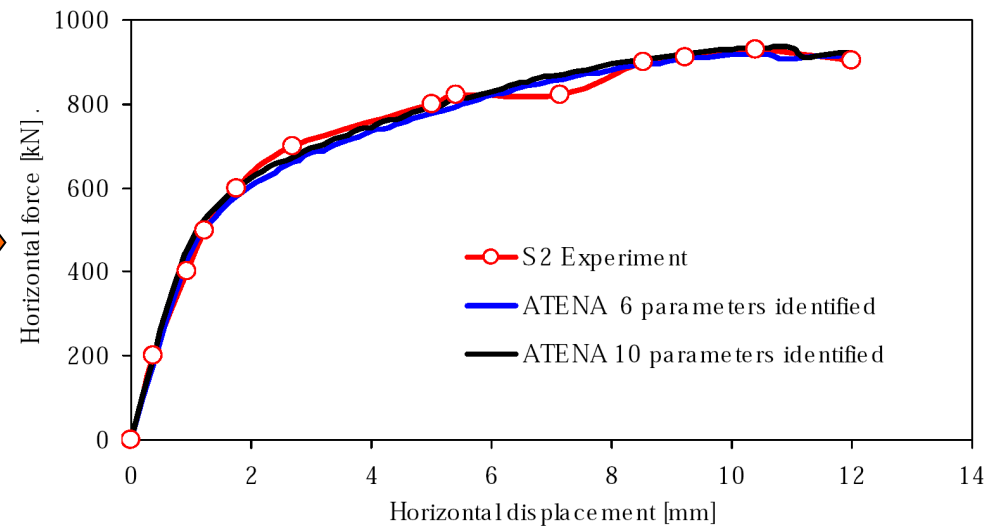
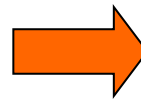
- Introduction
- Theoretical background
- Sensitivity analysis
- Least squares minimization
- Example: Identification of fracture parameters of concrete
- Example: Identification of hyperelasticity parameters of an OGDEN law



# Introduction

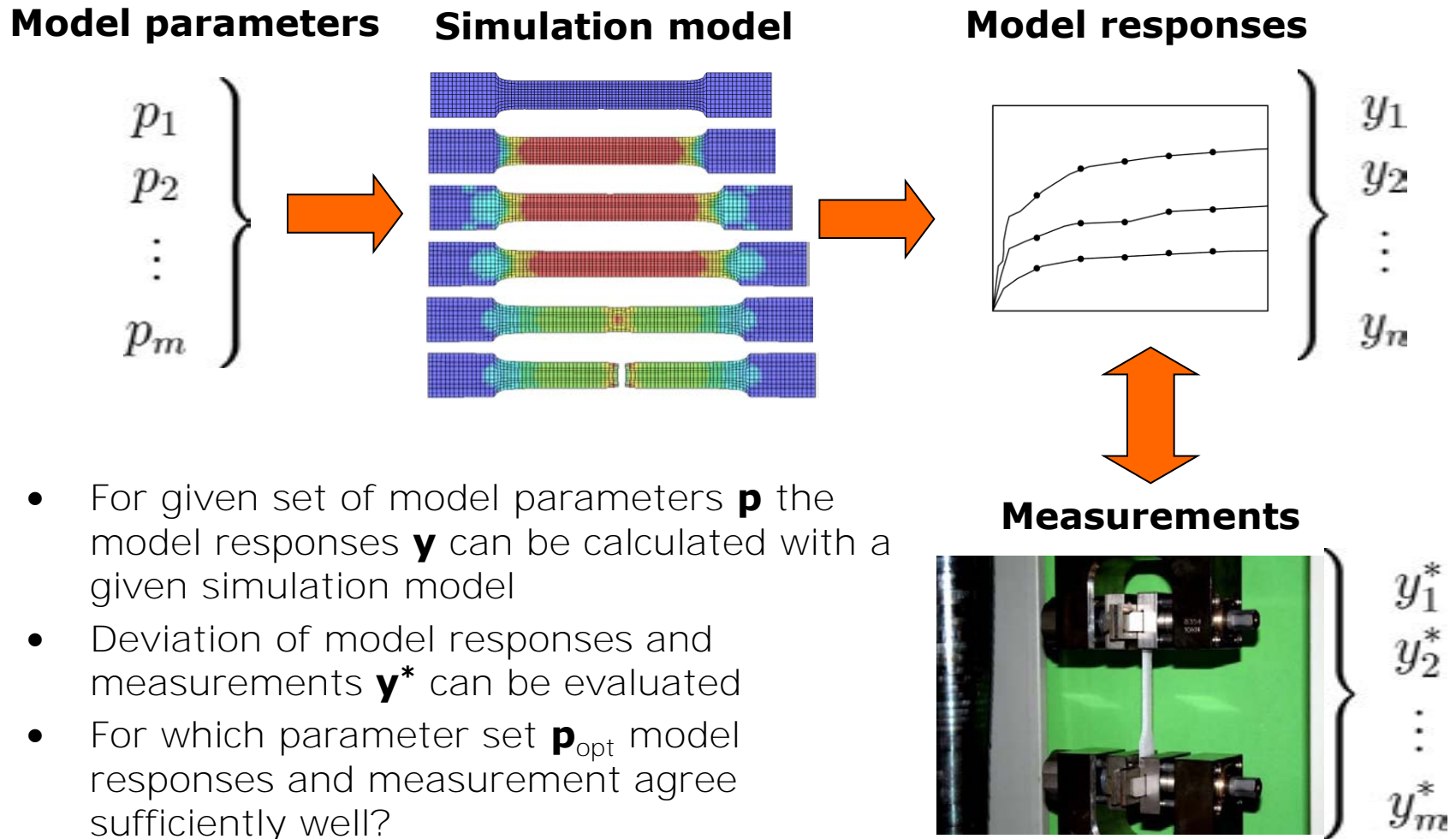


# Inverse Identification of Model Parameters



- 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



# Theoretical Background



## Least Squares Minimization

- The likelihood of the parameters is proportional to the conditional probability of measurements  $\mathbf{y}^*$  from a given parameter set  $\mathbf{p}$

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

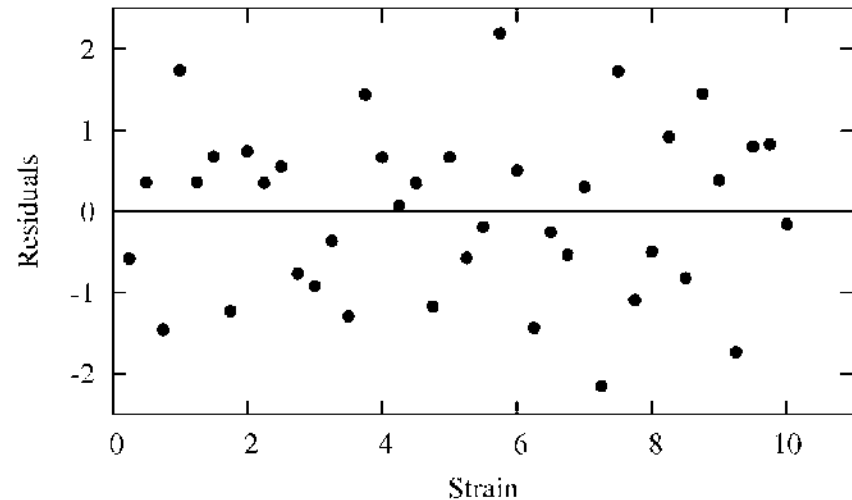
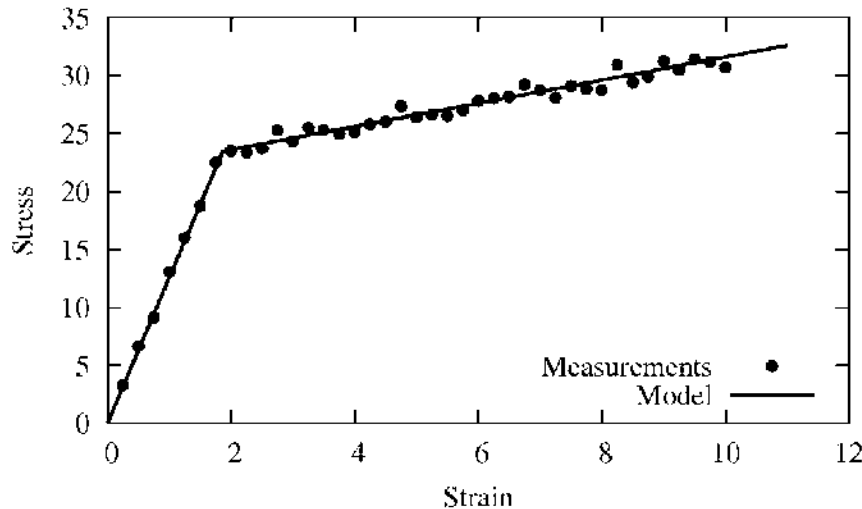
- For correct model  $(\mathbf{y}^* - \mathbf{y})$  is caused only by measurement errors
- Assuming **normally** distributed measurement errors:

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

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

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

# Least Squares Minimization



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

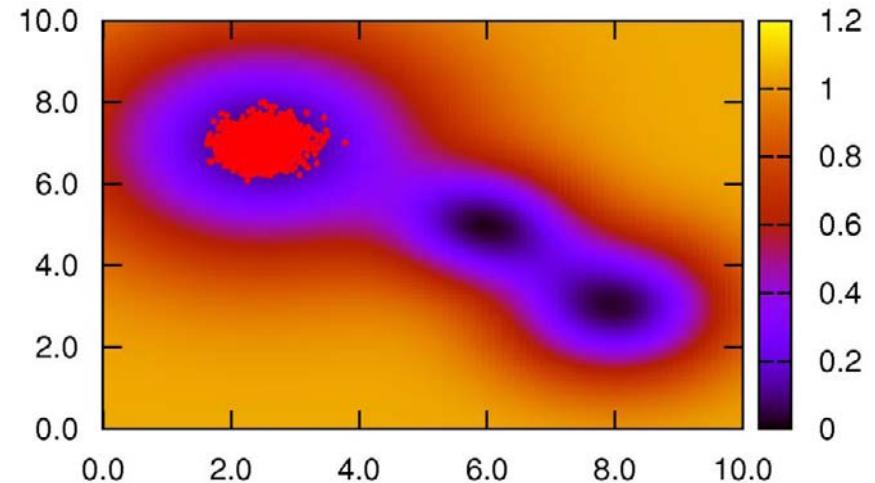
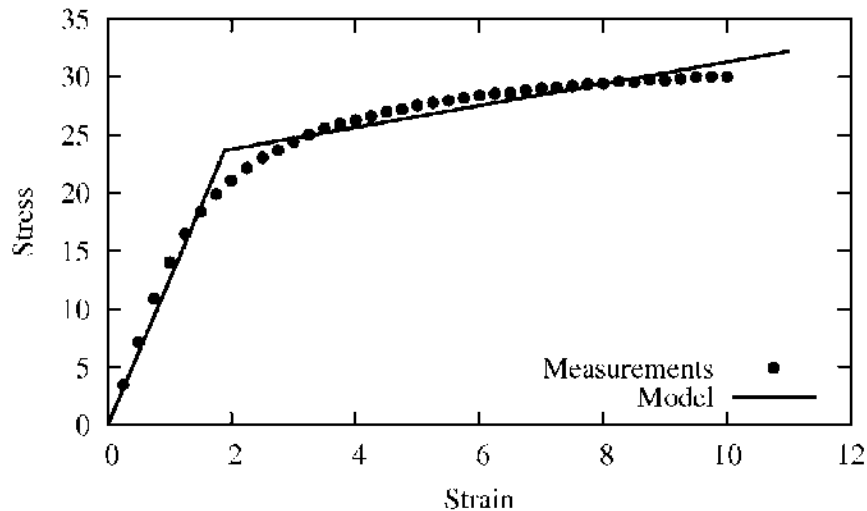
$$J(\mathbf{p}) = \sum_{i=1}^n w_i (y_i^* - y_i)^2, \quad w_i = \frac{1}{\sigma_{y,i}^2}$$

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

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



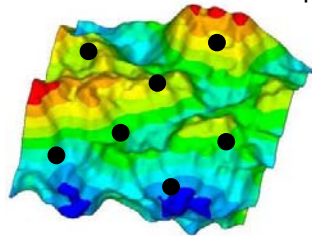
## Requirements to the Identification Procedure



- 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

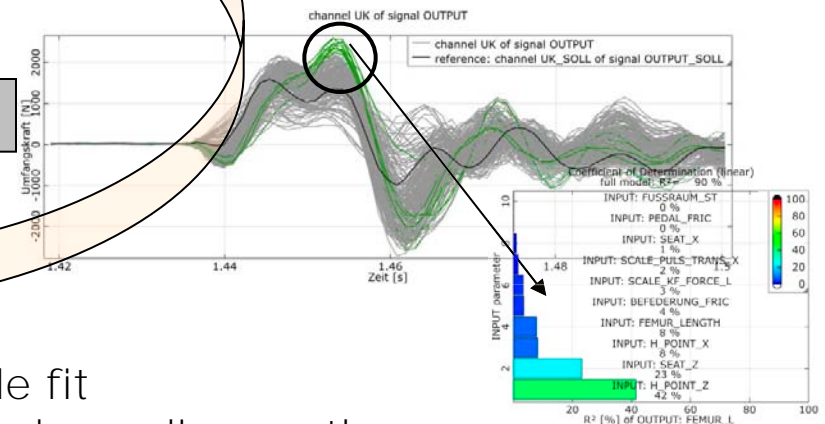
- Check the variation
- Identify sensitive parameters and responses
- Check parameter bounds
- Extract start value

**Simulation**

**Test**

optiSLang

**Best Fit**

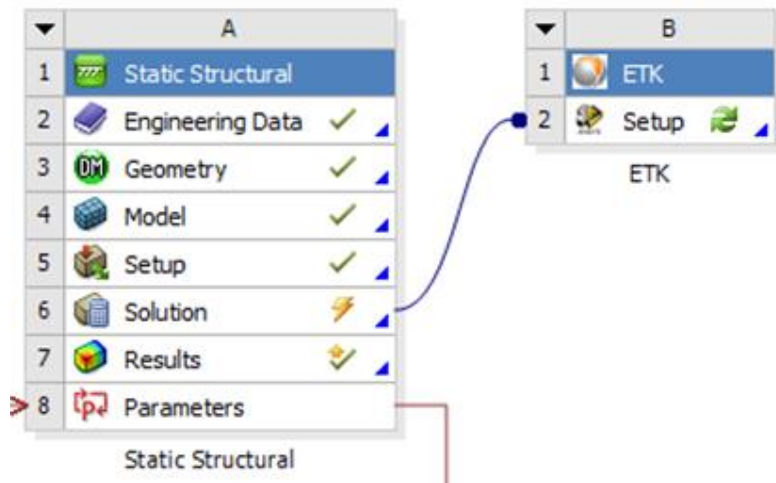


3) Find the best possible fit

- 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



The screenshot displays the ETK software interface. At the top, two tabs are visible: 'wedge\_splitting\_output.txt' and 'wedge\_splitting\_reference.txt'. The main window shows a text editor with the following content:

```

1 SLtxt:5.1.1.2 .....
2
3 Object: FORCE_DISP
4 Object info: 2·3·49·2·0
5
6 .....0.....0..
7 .....3e-05.....10229
8 .....3e-05.....17729
9 .....0.00012.....22329
10 .....0.00016.....24675
11 .....0.0003.....25511
  
```

To the right of the text editor is a 3D model of a wedge-shaped object with orange and red surfaces, labeled 'ETK'. Below the text editor, there are radio buttons for 'token wise' (selected), 'column wise', 'as matrix', and 'as signal'. A 'Show advanced options' button is also present. Below these controls, the 'Variable Name' is set to 'signal', and 'Instant visualization' and 'Use as response' are checked. At the bottom, a graph shows the signal over time. The y-axis is labeled 'Y [1e4]' and ranges from 0 to 2.5. The x-axis is labeled 'x' and ranges from 0 to 0.00175. The graph shows a curve that rises to a peak of approximately 2.4 at x ≈ 0.00025 and then decays towards zero.

# Sensitivity Analysis



# Methods for Sensitivity Analysis

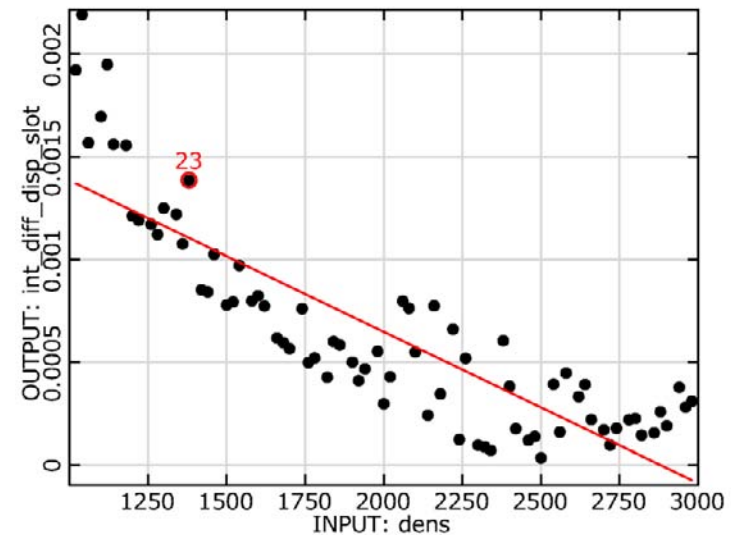
## Local methods

- Local derivatives
- Standardized derivatives

## Global methods

- Anthill plots
- Coefficients of correlation
- Rank order correlation
- Standardized regression coefficients
- Stepwise polynomial regression
- Variance-based analysis: Sobol' indices
- **Advanced surrogate models including prediction analysis and optimal subspace detection: Metamodel of Optimal Prognosis**

INPUT: dens vs. OUTPUT: int\_diff\_disp\_slot, (linear)  $r = -0.858$

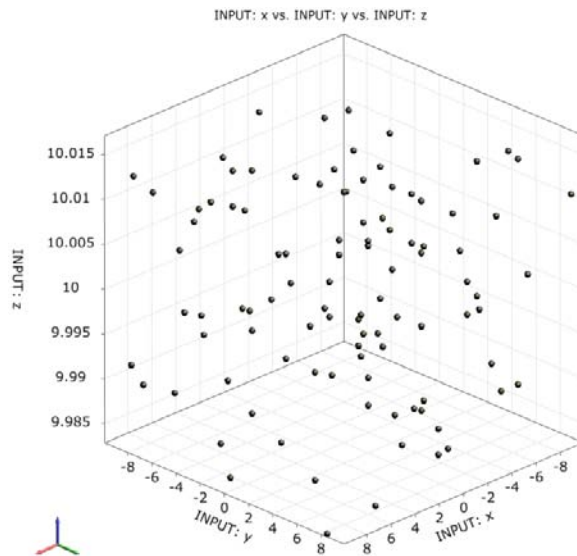


# Scanning the Design Space

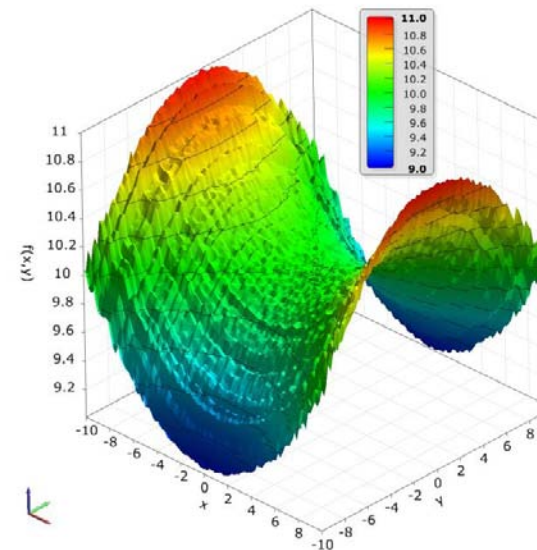
Inputs

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

Design of Experiments



Solver evaluation



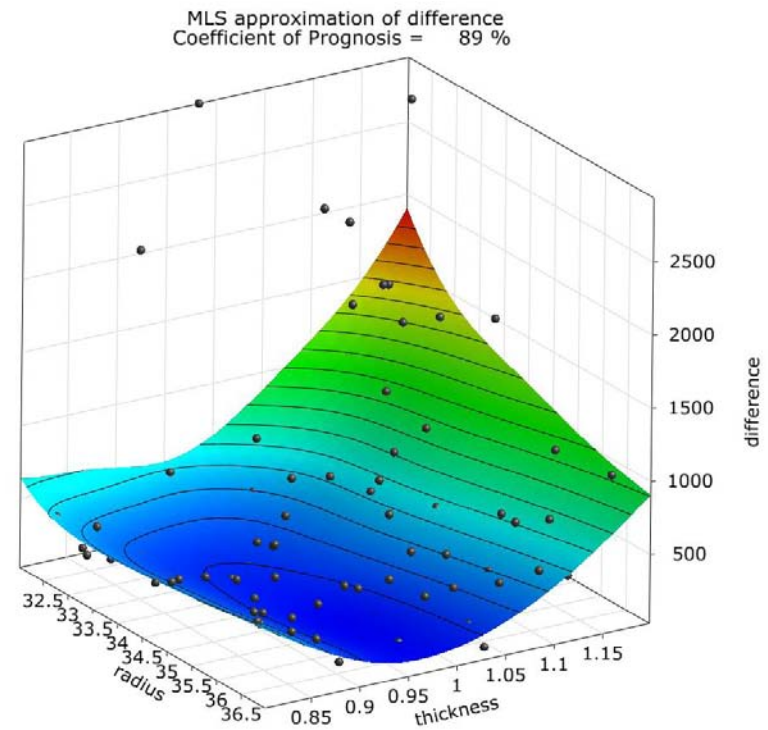
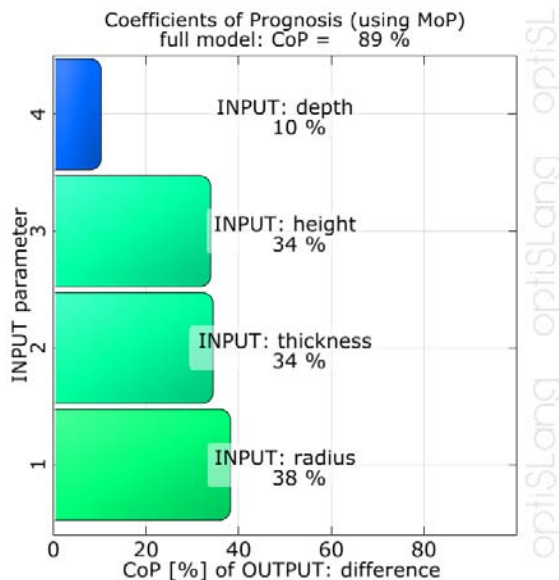
Outputs

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

- 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



# Least Squares Minimization

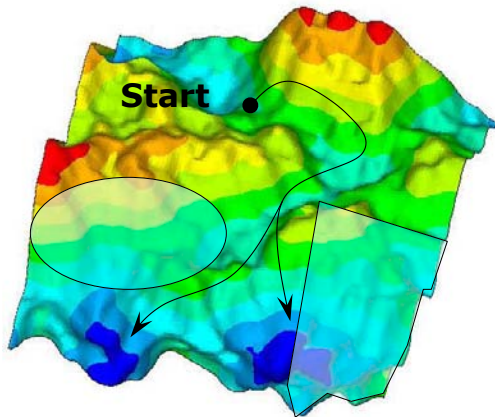




# Optimization Algorithms

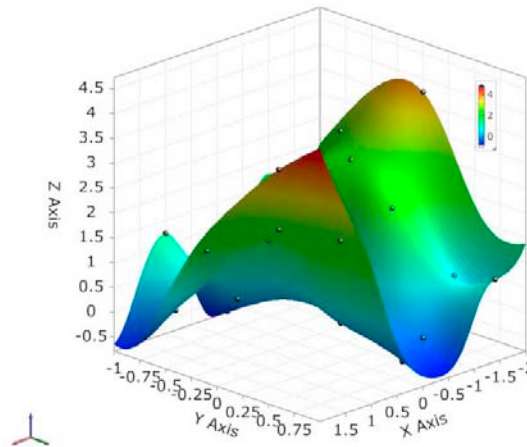
## Gradient-based Methods

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



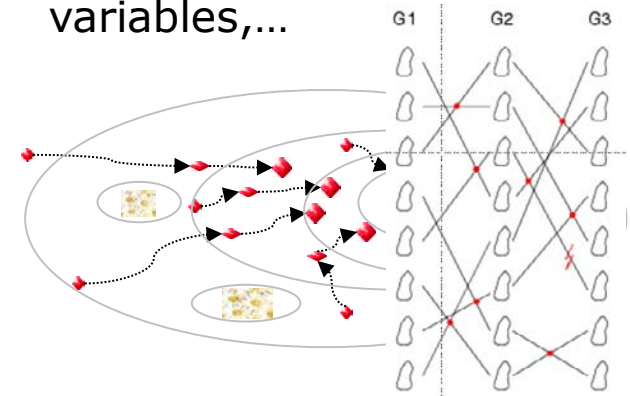
## Adaptive Response Surface Method

- 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

Analysis status:

Constraints violations:

Failed designs:

Solver noise:

Number of parameter:

Number of objectives:

Parameter type

Pure continuous

Has discrete

Discrete type

Ordered

Nominal

Optimization method

Gradient based

Non-Linear Programming by Quadratic Lagrangian (NLPQL)

Gradient free

Adaptive Response Surface Method (ARSM)

Downhill Simplex Method

Natural inspired

Evolutionary Algorithm (EA) - local

Evolutionary Algorithm (EA) - global

Particle Swarm Optimization (PSO) - local

Particle Swarm Optimization (PSO) - global

Other

Stochastic Design Improvement (SDI)

Memetic (Beta)

Starting Point(s)

Use start-design-table

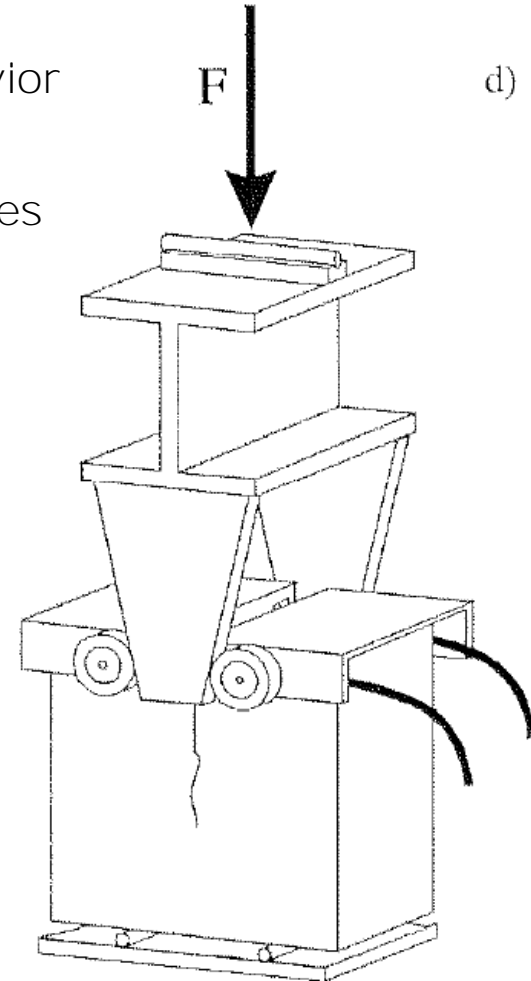
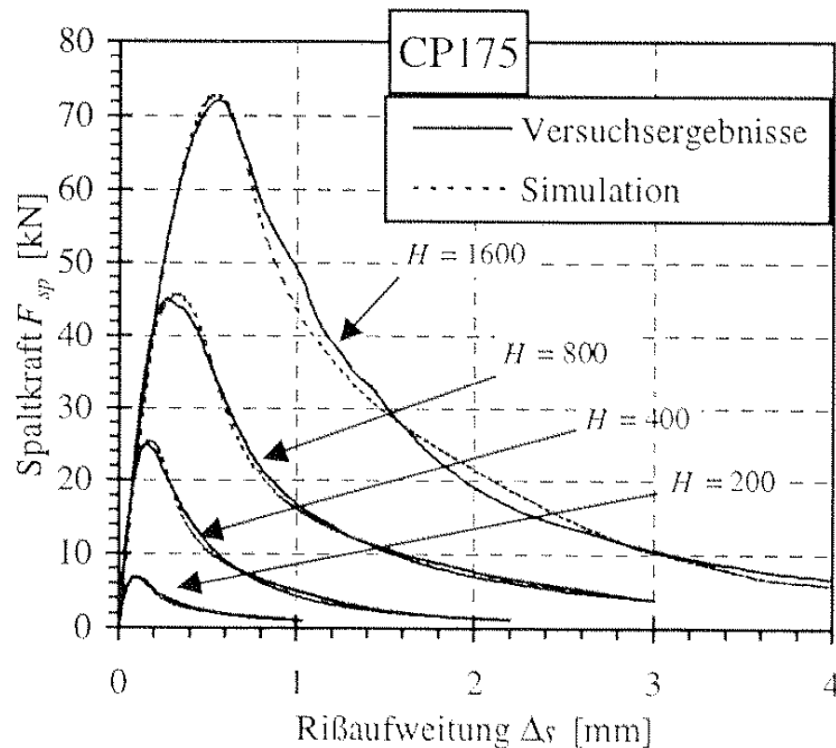
# Examples



# 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



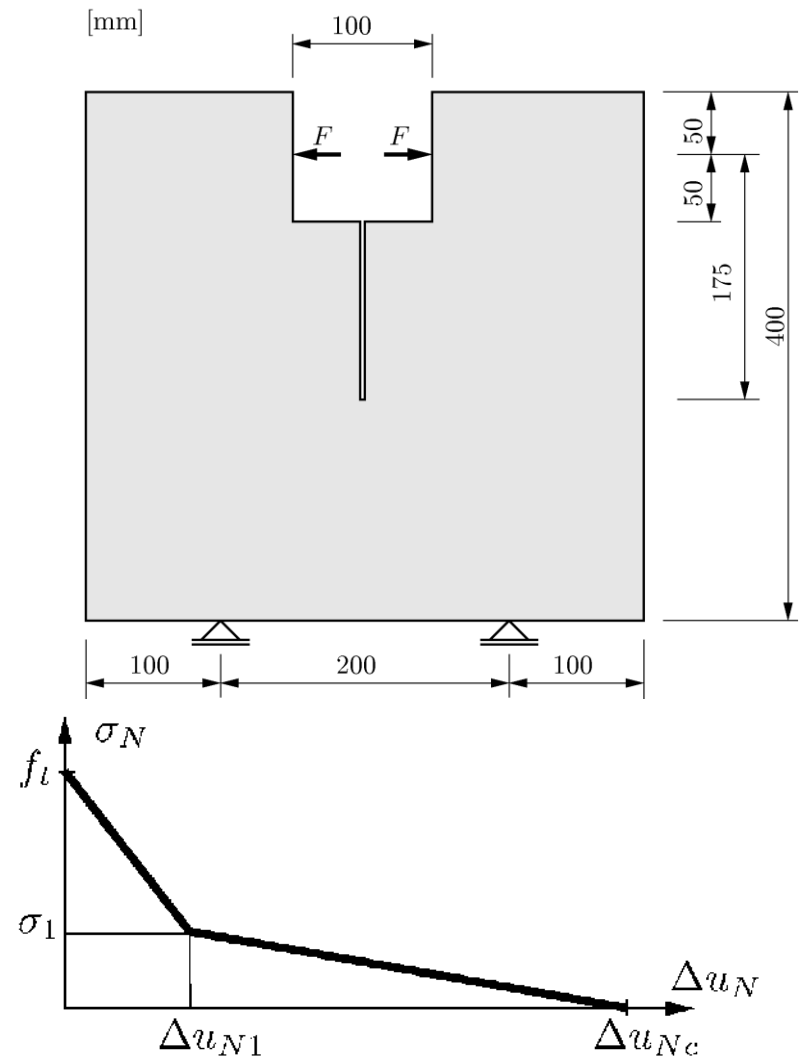
# Wedge Splitting Test

## 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  $\nu$
  - Tensile strength  $f_t$
  - Fracture energy  $G_f$
  - Shape parameters

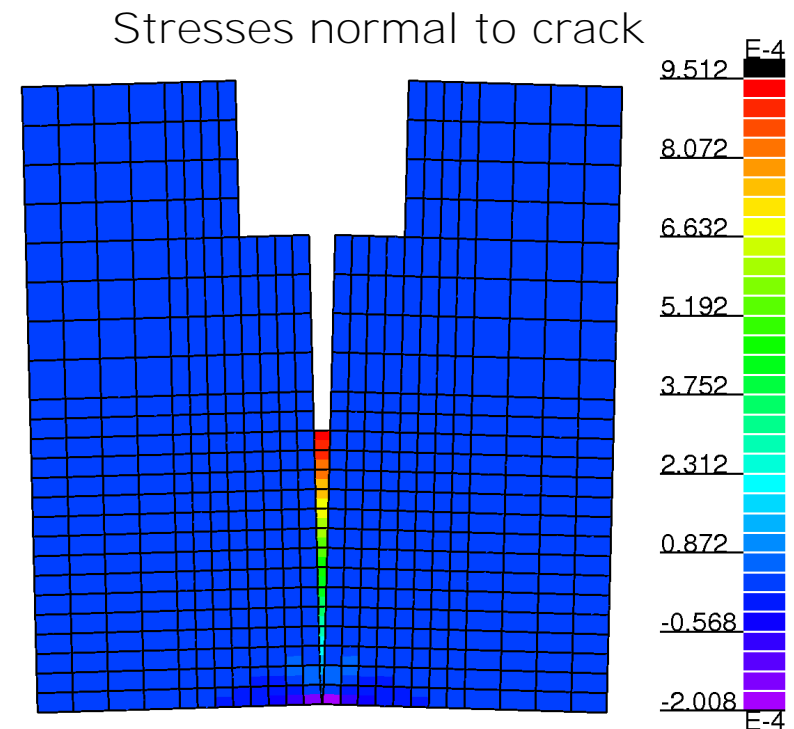
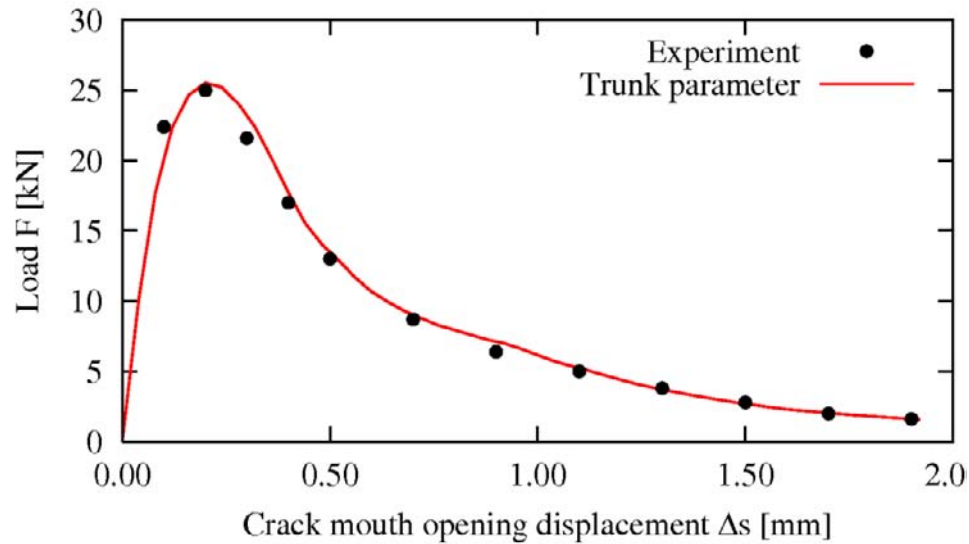
$$\alpha_{ft} = \sigma_1 / f_t$$

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



# 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

The screenshot shows the Dynardo software interface. The main window displays a text file named 'wedge\_splitting\_output.txt' with the following content:

```

1 SLang 5.1.1...
2
3 Object: FORCES_REF
4 Object info: 2 3 13 2 0
5
6 0.0000 00000
7 0.0001 22400
8 0.0002 25000
9 0.0003 21600
10 0.0004 17000
11 0.0005 13000
12 0.0007 8700
13 0.0009 6400
  
```

The interface also shows a 'Responses' panel on the right with two entries: 'signal [1:49]' and 'signal\_ref [1:13]'. At the bottom, there are radio buttons for 'token wise', 'column wise', 'as matrix', and 'as signal', with 'as signal' selected.

The screenshot shows the Dynardo software interface with a table of variables and a responses panel. The table has the following columns: ID, signal, Type, Value, ie path mc, File, and Expression.

ID	signal	Type	Value	ie path mc	File	Expression
1	signal	REAL XYDATA	[1:49]	Relative ...	wedge_splitting_...	constant
2	signal_ref	REAL XYDATA	[1:13]	Absolute	C:\Users\Public\...	constant
3	disp_ref	REAL VECTOR	[13]			extract(signal_ref,0)
4	forces_ref	REAL VECTOR	[13]			extract(signal_ref,1)
5	forces_steps	REAL VECTOR	[13]			extract(interpolate(signal,disp_ref,LINEAR,0,0),1)
6	error_norm	REAL	3156.26			euklidnorm(forces_steps-forces_ref)

The 'Responses' panel on the right shows the following entries:

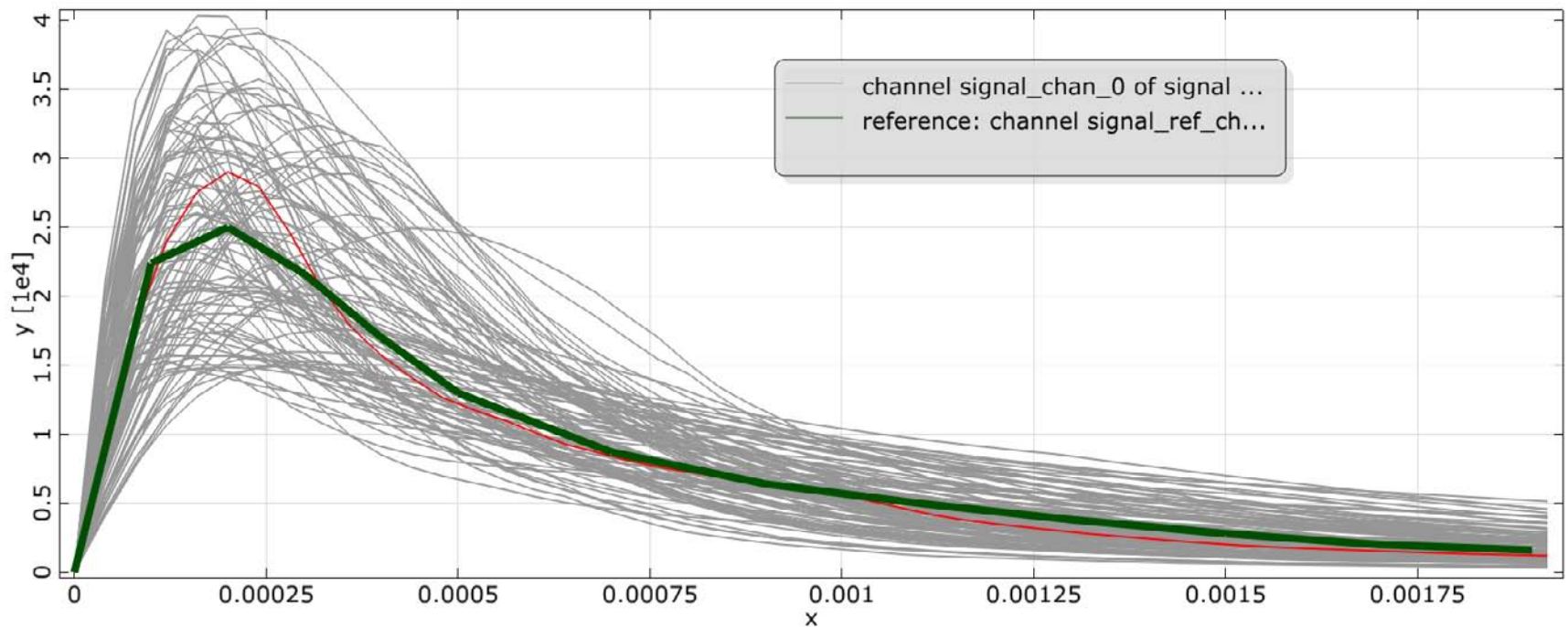
- error\_norm 3156.26
- forces\_steps [13]
- signal [1:49]
- signal\_ref [1:13]

# 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

channel signal\_chan\_0 of signal signal

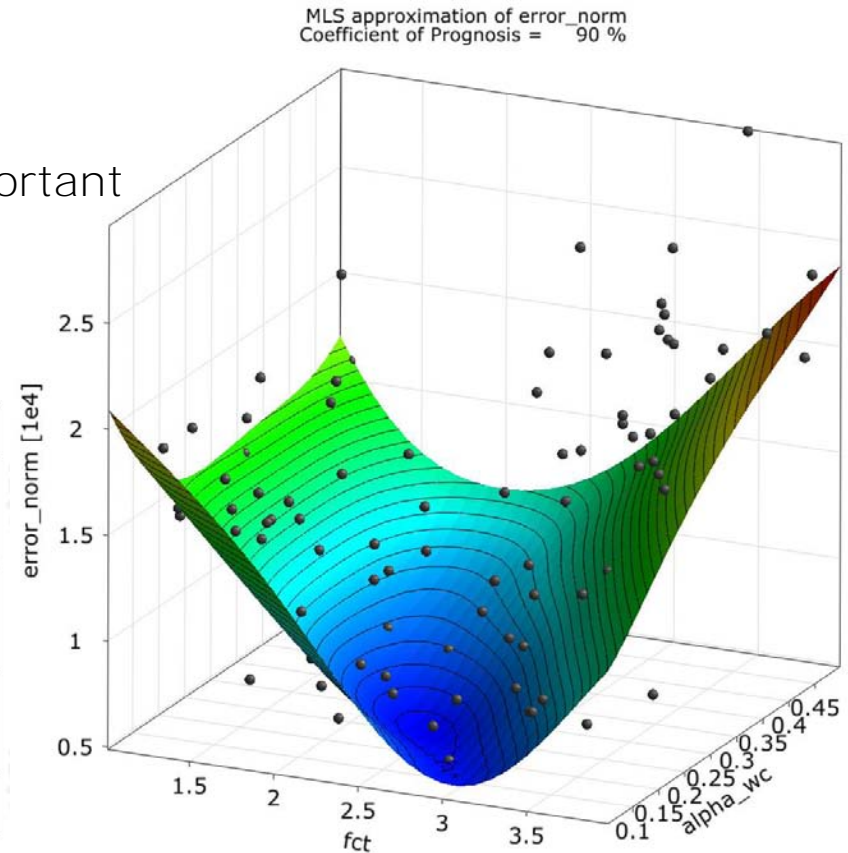
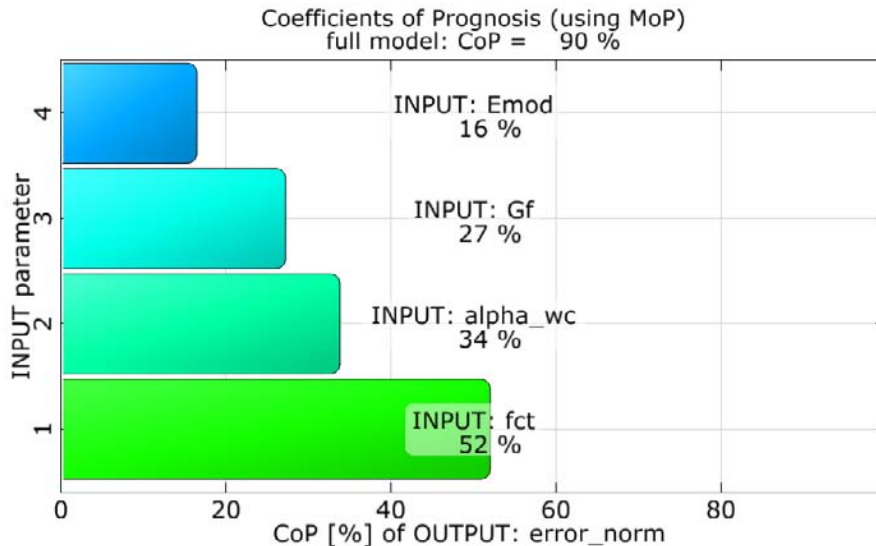




# Wedge Splitting Test

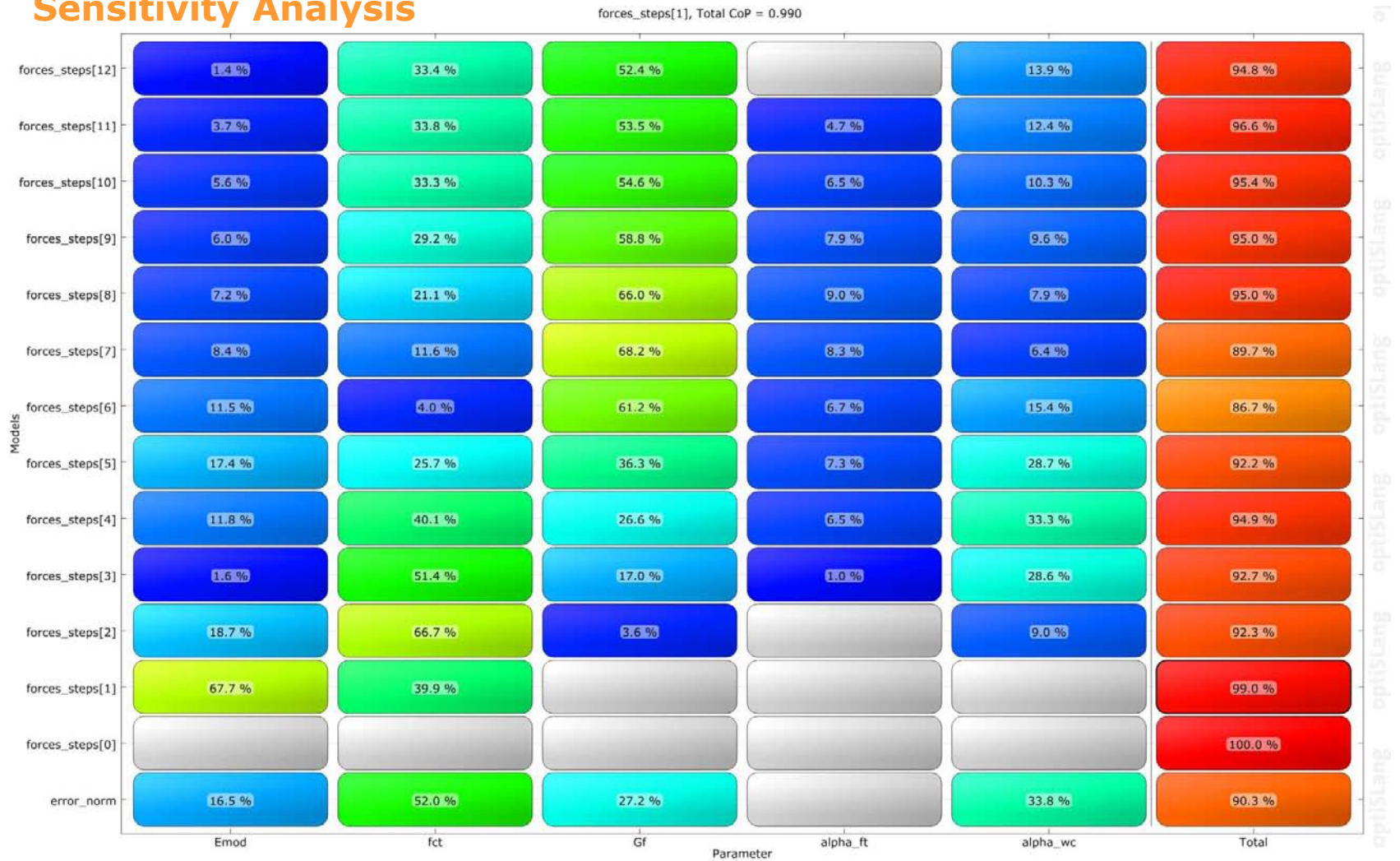
## Sensitivity Analysis

- 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



# Wedge Splitting Test

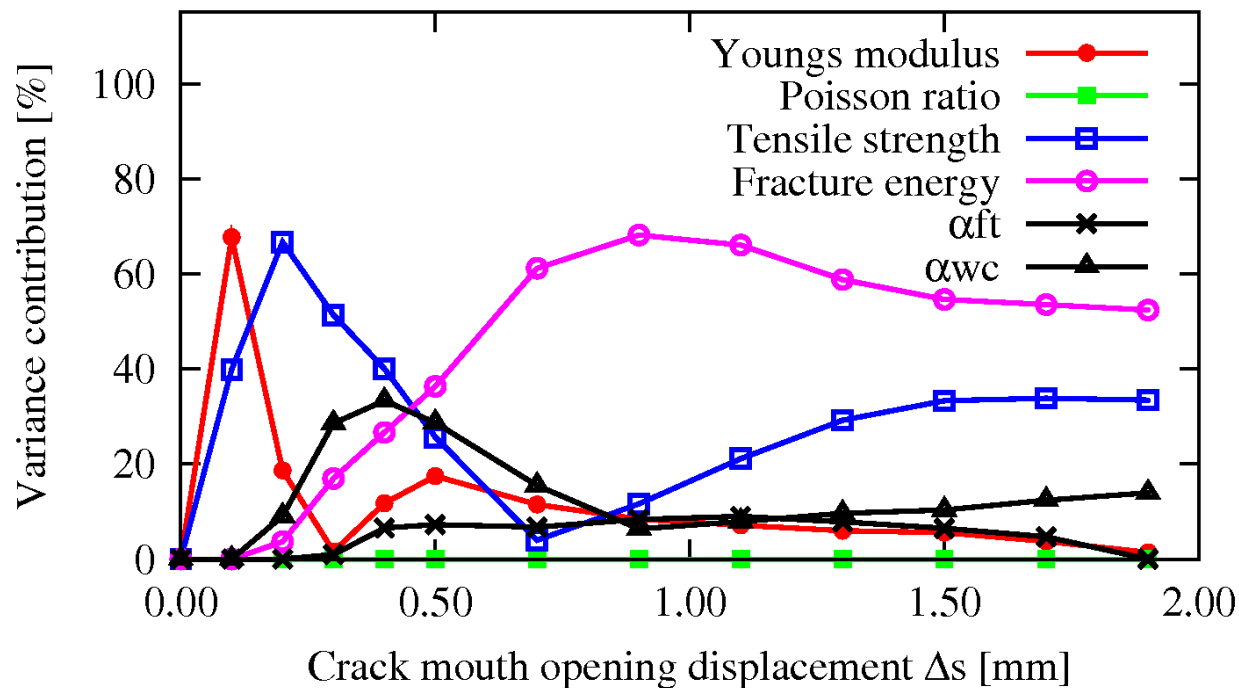
## Sensitivity Analysis



# Wedge Splitting Test

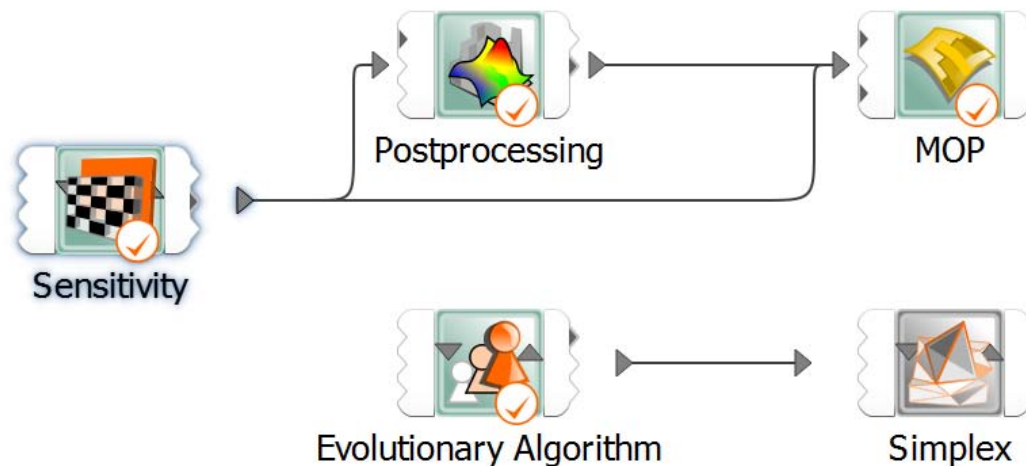
## Sensitivity Analysis

- 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



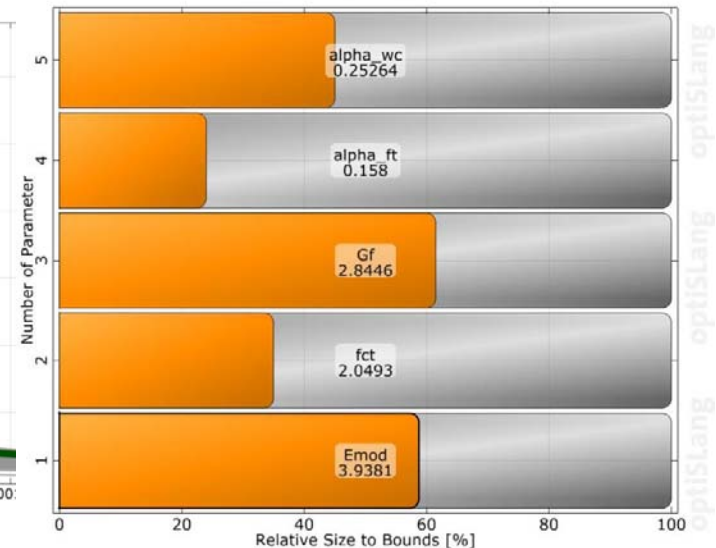
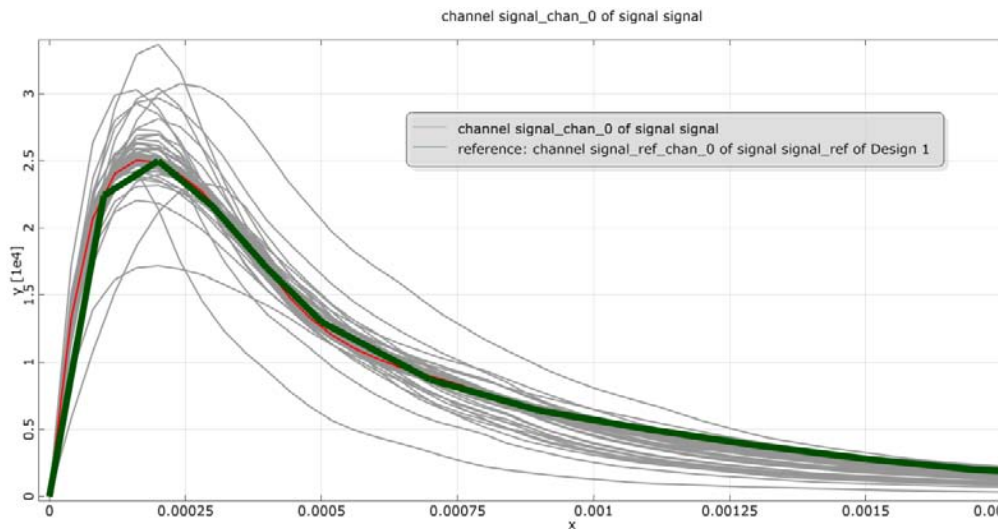
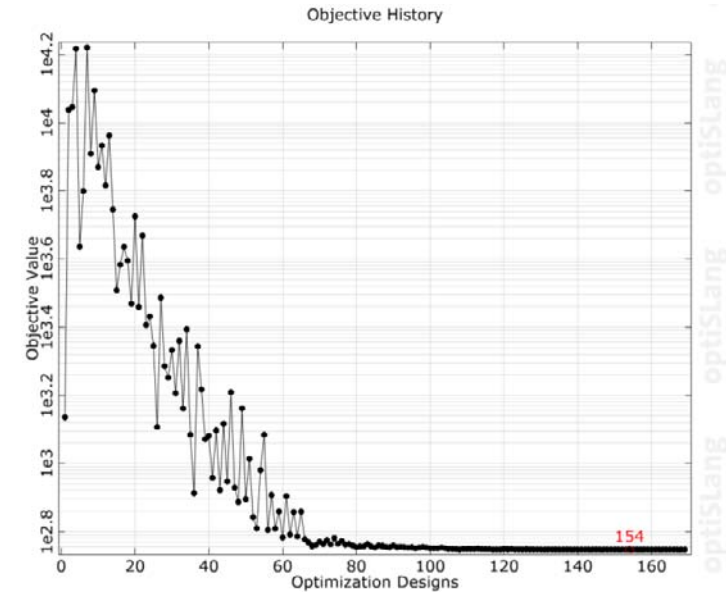
# Wedge Splitting Test Optimization

- 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

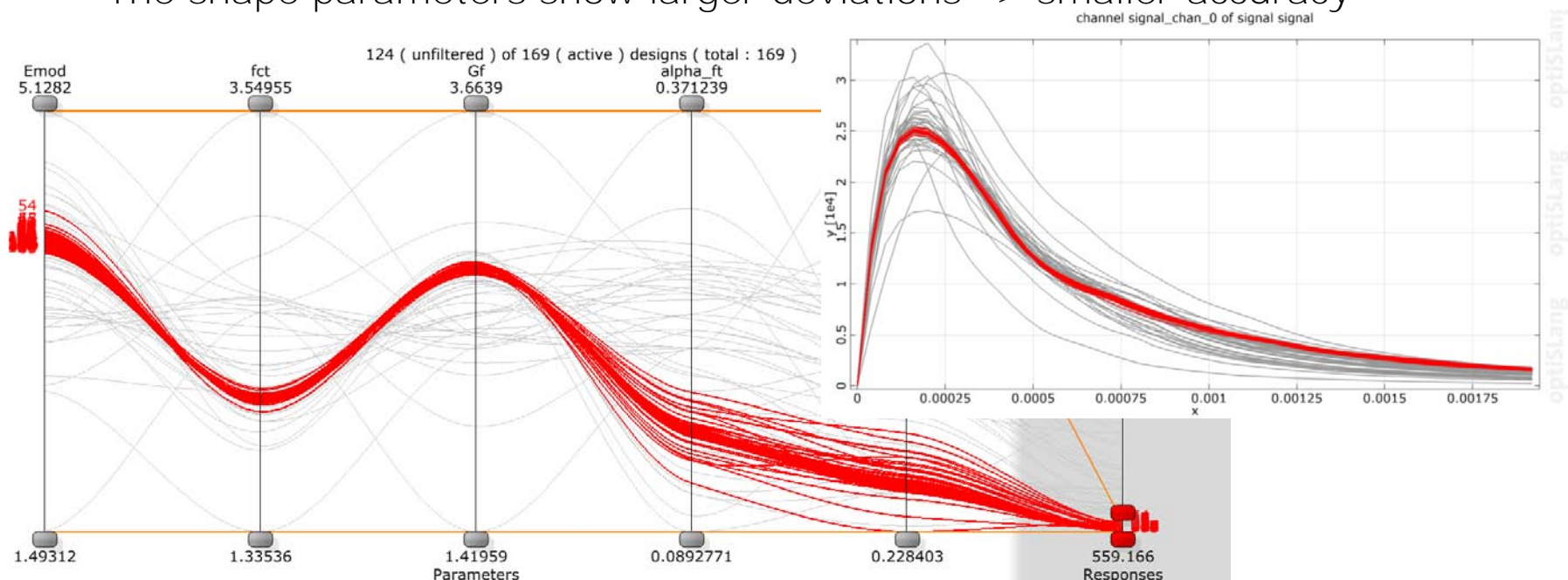
- The signal of the best design agrees very well with the reference
- The unknown parameters are identified by the optimizer



# 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

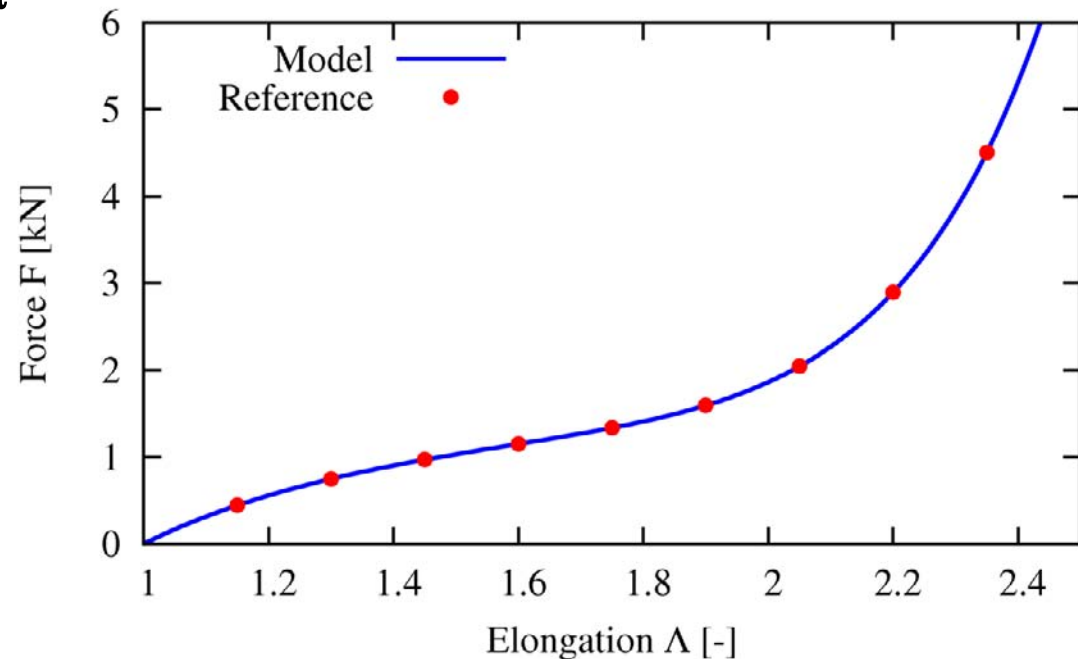


# Ogden Hyperelasticity

## Constitutive Model

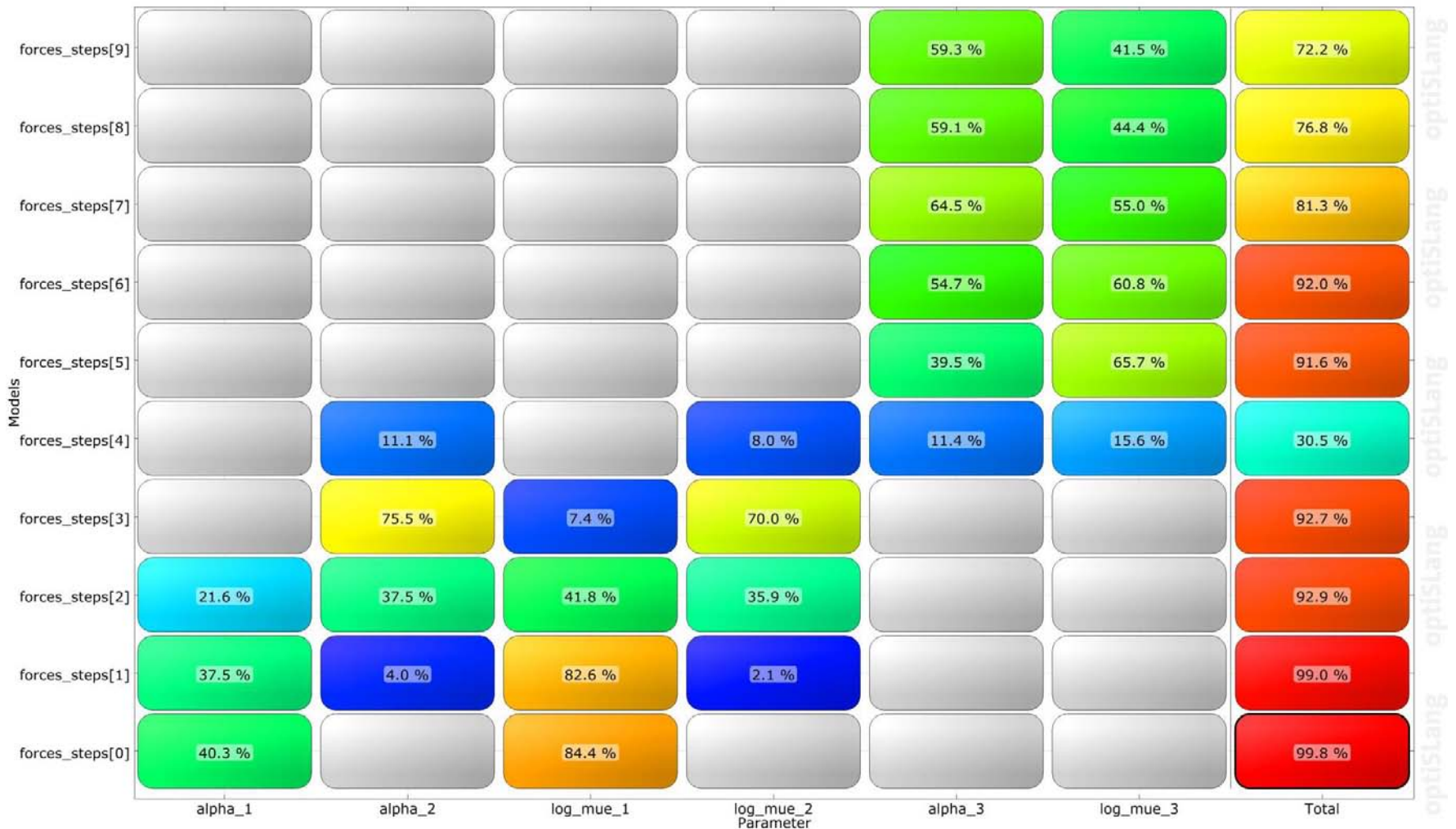
- Hyperelastic model with exponential formulation of Cauchy stress depending on deformation
- One-dimensional case assuming incompressible behavior:
- Often 2 or 3 pairs of  $\mu$  and  $\alpha$  are necessary
- $\mu$  and  $\alpha$  are the unknown parameters in the identification
- How many terms of the OGDEN law are necessary for the given reference ?

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



# Ogden Hyperelasticity

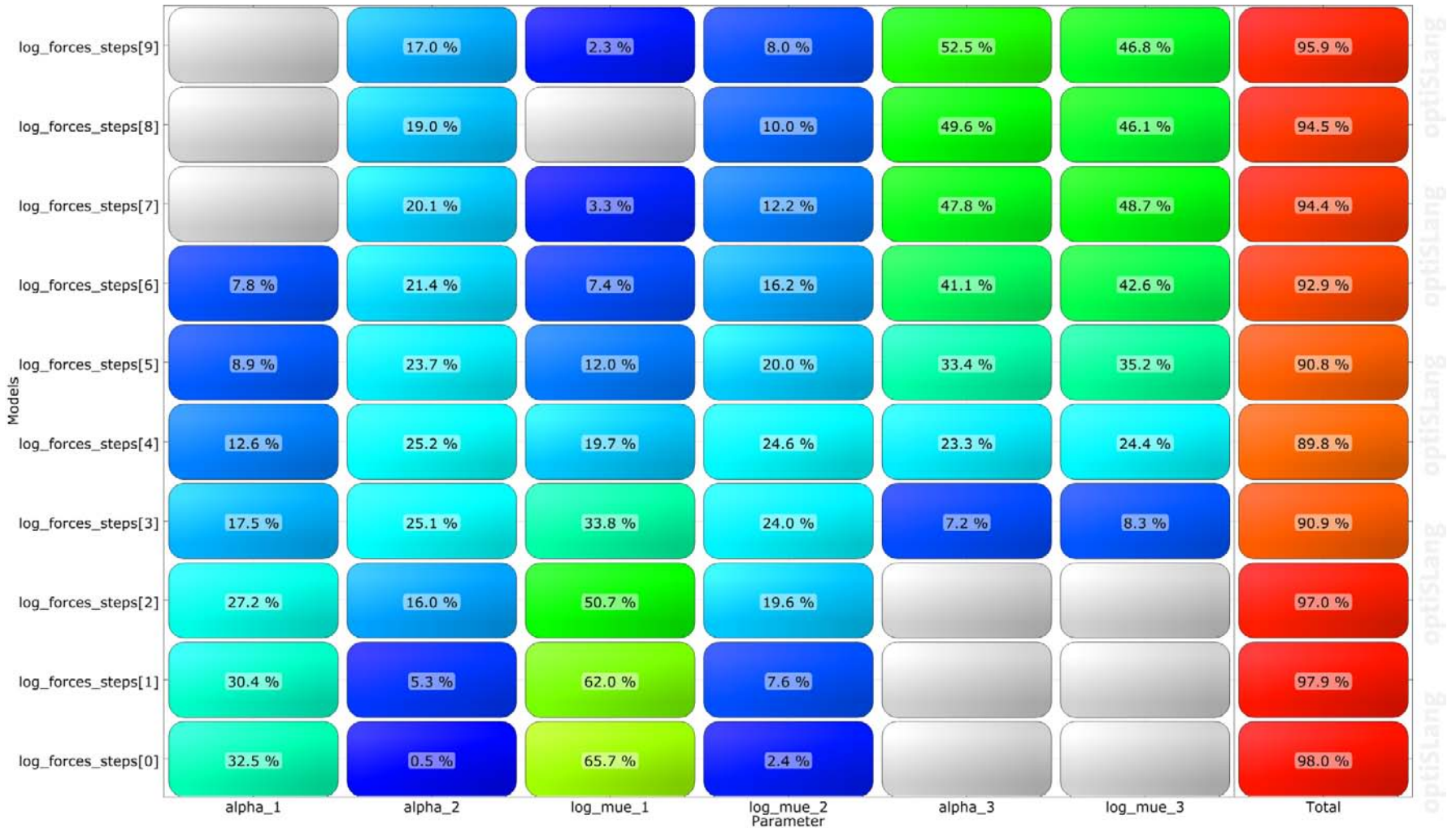
## Sensitivity Analysis – Forces at Reference points





# Ogden Hyperelasticity

## Sensitivity Analysis – Logarithmic Forces at Reference points

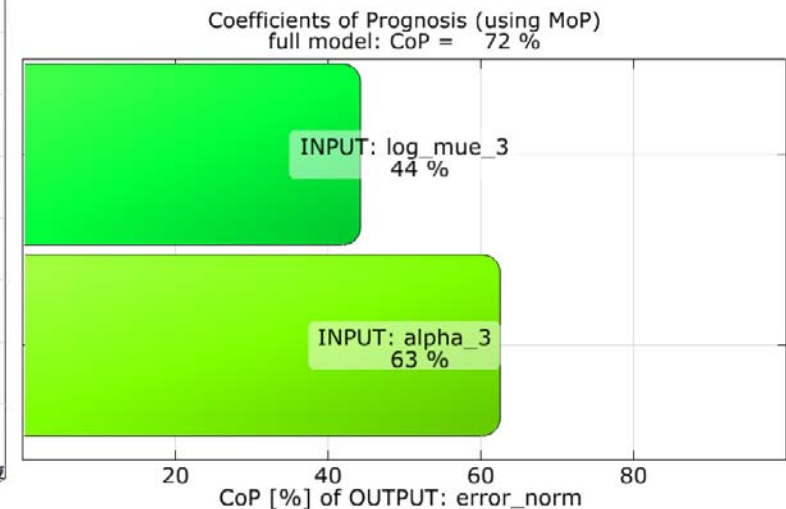
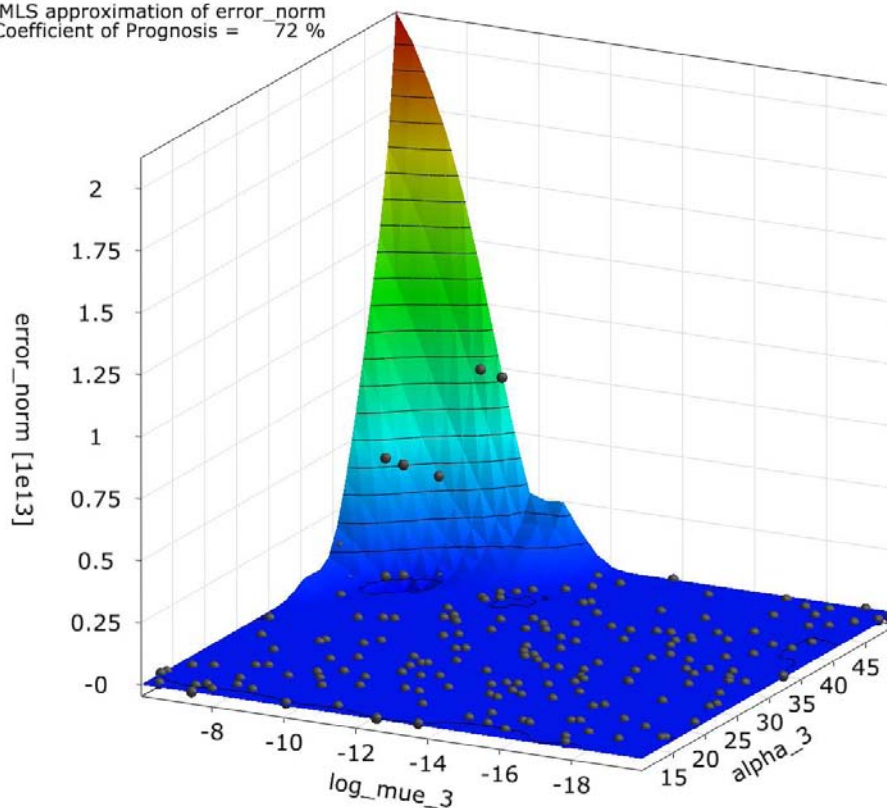


# Ogden Hyperelasticity

## 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

MLS approximation of error\_norm  
Coefficient of Prognosis = 72 %

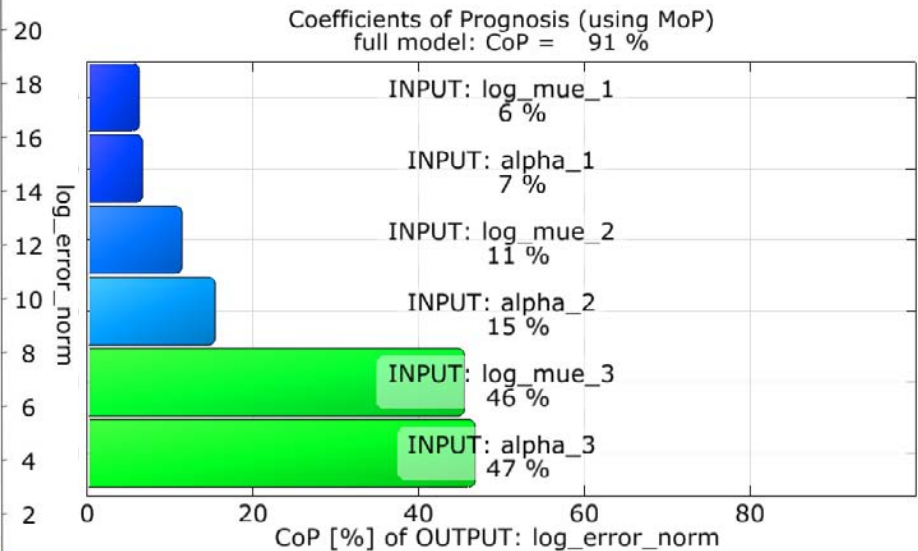
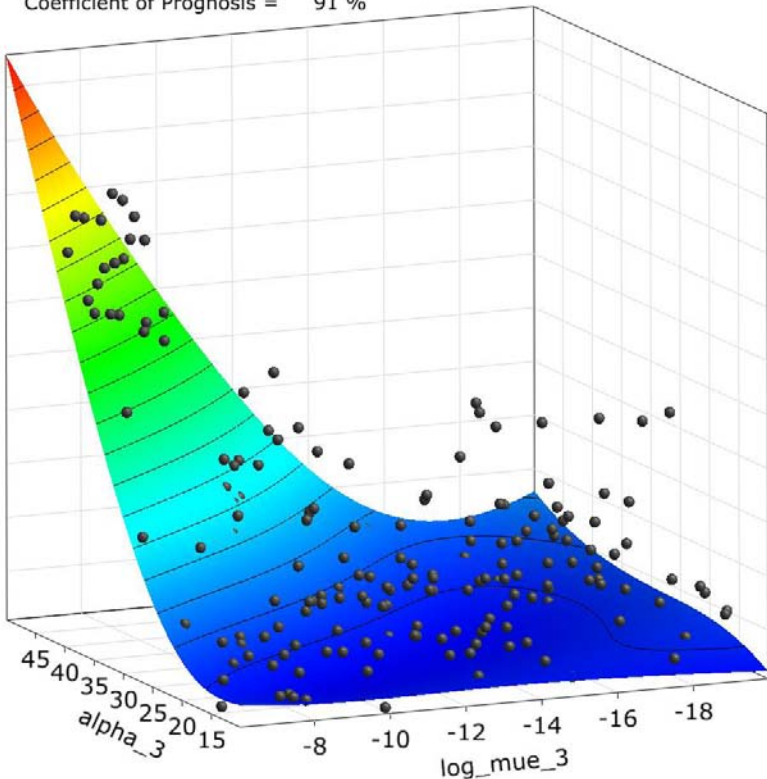


# Ogden Hyperelasticity

## 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

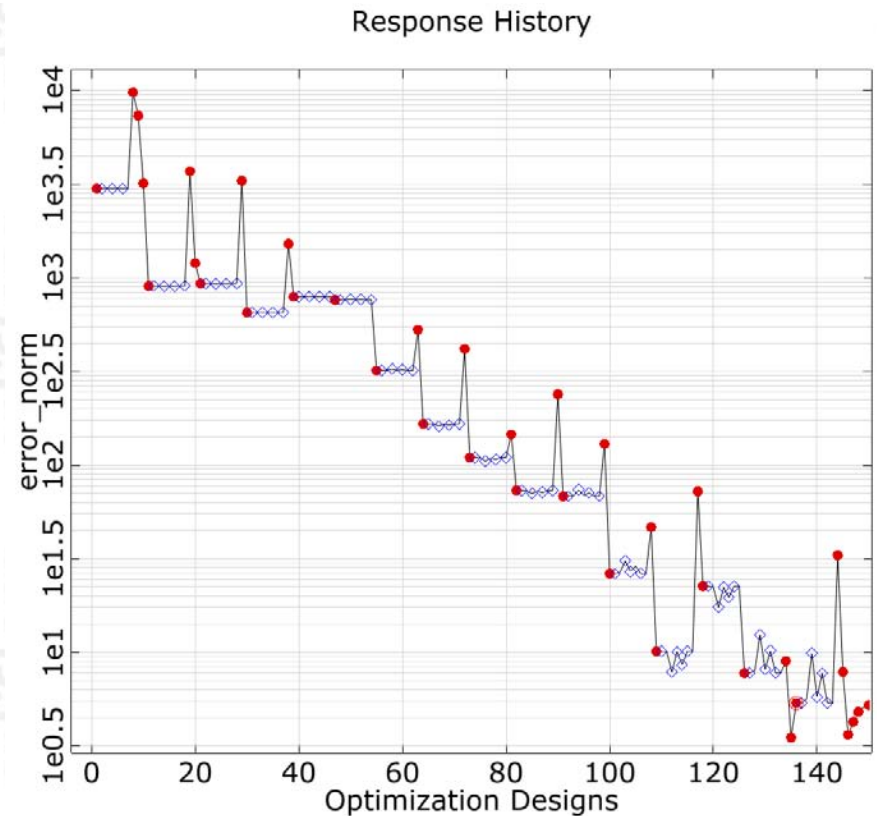
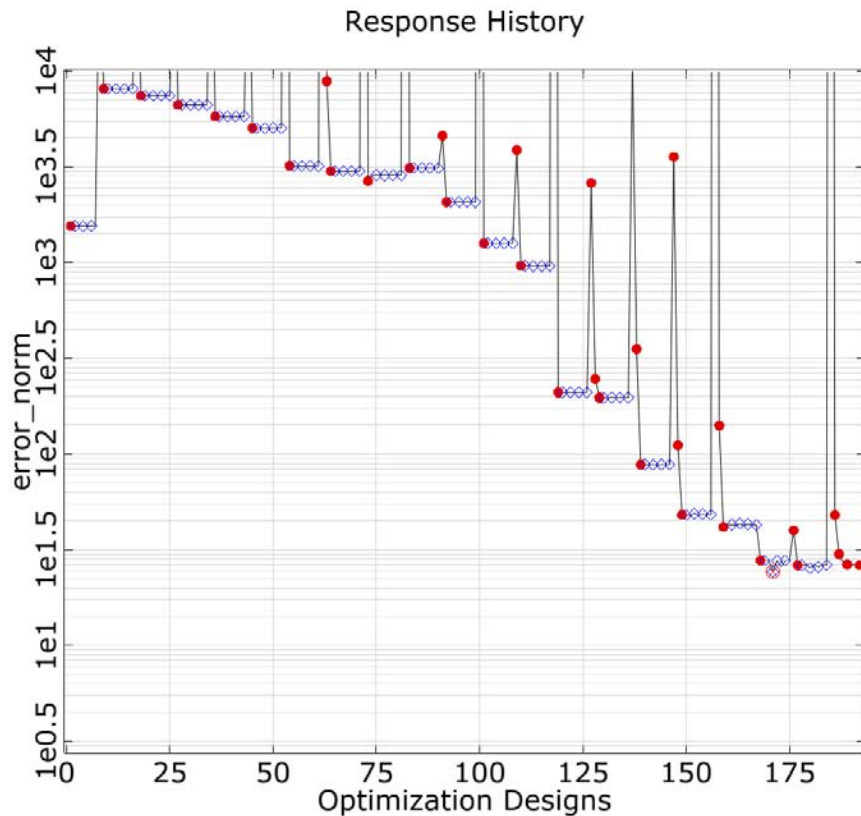
MLS approximation of  $\log\_error\_norm$   
Coefficient of Prognosis = 91 %



# Ogden Hyperelasticity

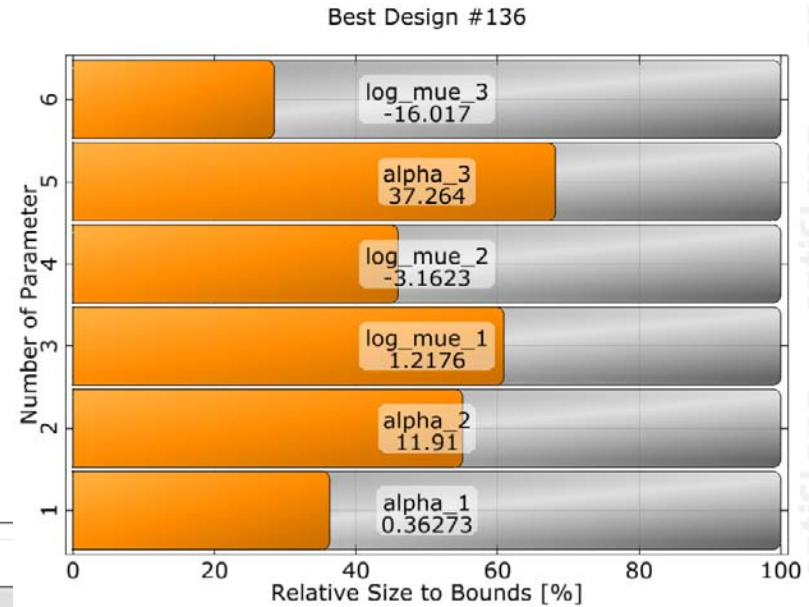
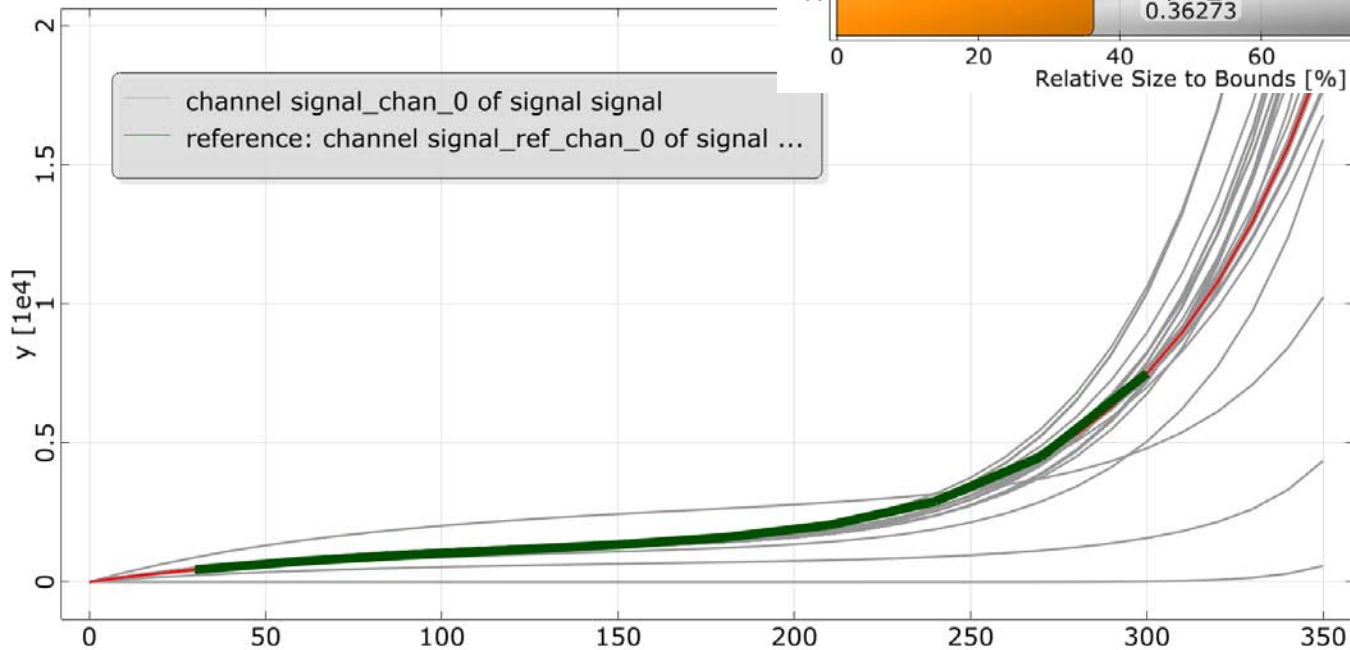
## Least Squares Minimization

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



# Ogden Hyperelasticity Result

- The modulus  $\mu$  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

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

- Estimated covariance of optimal parameters (Markov estimator)

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

- For constant and independent measurement errors we obtain

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

## Posteriori Error Estimation

- Estimated covariance for incorrect models

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

- Variance correction factor

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

- For constant and independent measurement errors we obtain

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



# Wedge Splitting Test

## Estimation of Parameter Accuracy

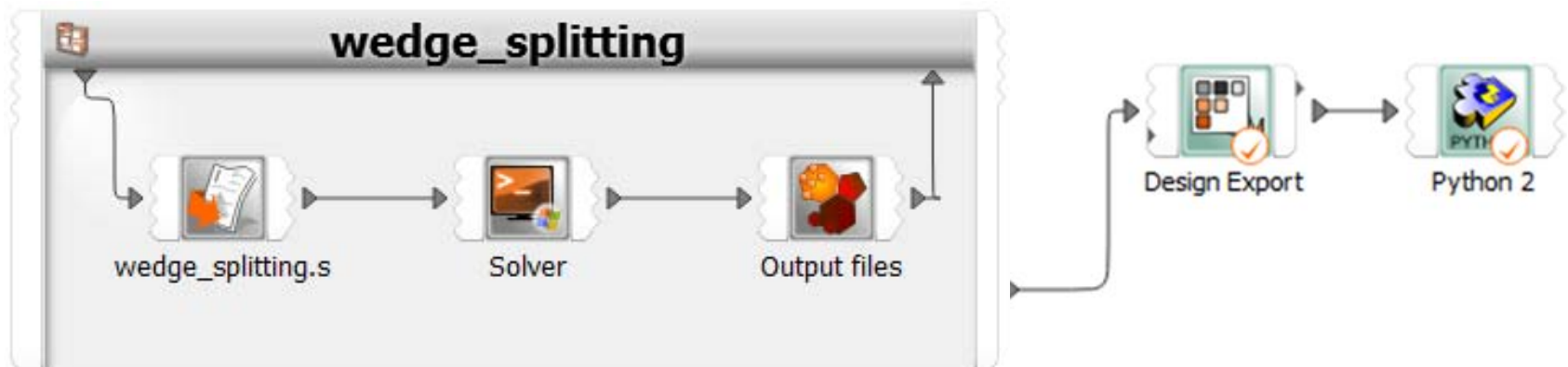
- Define a local sensitivity at the best design
- Add small interval of 0.01 for all identified parameters in the start design table

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