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IDENTIFICATION OF MATERIAL PROPERTIES THROUGH A MARKOV CHAIN MONTE CARLO TECHNIQUE AND A RESPONSE SURFACE APPROXIMATION

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Abstract. *In this work, the problem of identifying a set of model parameters to calibrate a simplified three-dimensional Finite Element (FE) model is addressed, by using data obtained from a three-point bending test. However, the expected computational cost of the forward problem hamper any attempt to perform the inverse analysis. To overcome this problem, the solution of the forward problem via FE is replaced by a metamodel based on a response surface approximation. The inverse problem is solved by using a Markov Chain Monte Carlo method. The proposed methodology reduces the computational cost by several orders of magnitude and results in estimates that allows to accurately reproduce both the synthetic data and the respective output of a FE simulation.*

Keywords: *Inverse Problems, Markov Chain Monte Carlo, Response Surfaces, Material Properties, Aluminum Foam*

1. INTRODUCTION

One of the current challenges in material research in the automotive industry is developing novel cost-effective materials with increased performance and decreasing weights (Duarte *et al.*, 2014; Ghassemieh, 2011). Such is the case of integrating lightweight materials in vehicle designs, in order to make them lighter and more fuel-efficient, without

comprising other key attributes, such as safety, cost-effectiveness and recyclability (Duarte *et al.*, 2015). However, the development of these new materials is only a part of the process of innovation in industry. Another key step in this process is the quantification of several properties, in order to enable engineers to predict its behavior through computer simulations. This quantification process is also performed with the help of computer models, inside an inverse analysis framework. The observed decrease in the past few decades in costs for manufacturing complex material structures and acquiring powerful computers to perform these calculations increased the demand for fast and reliable techniques to identify properties that play a major role in mechanical, electrical or thermal phenomena, among others.

In the particular problem of predicting mechanical behavior, properties such as the Young's modulus, Yield stress and Poisson's ratio are paramount to assess the performance of a given material. This quantification process, done through an inverse analysis, is not without its own adversities, where special techniques and algorithms are needed in order to deal with the ill-posedness of the inverse problem. Also, the observed increase in computational effort in order to obtain more accurate numerical solutions of a given mathematical problem is much larger than the one observed when solving the respective forward problem. This issue, among others, remains a challenge to researchers because, although the problem may be addressed via the Finite Element Method (FEM), the computational cost in an inverse analysis framework is likely to be unfeasible.

Also in the past few years, the interest of researchers in the use of metamodels to replace the typical solution algorithms has increased significantly. These metamodels are designed to reproduce the solution of a mathematical problem with lower accuracy but with very small computational effort and have been used with success in optimization problems (Colaço and Dulikravich, 2011) and also in inverse analysis frameworks (Orlande *et al.*, 2007). Inspired on this, the problem presented in this paper is solved by coupling a metamodel based on a response surface approximation and a Markov chain Monte Carlo method.

2. FORWARD PROBLEM

The goal of this research is to use synthetic measurements obtained from the simulation of a three-point bending experiment to calculate specific material properties in order calibrate a simple FE model. The goal is to allow this simple model to accurately reproduce the behavior of a given material. This synthetic data comprises a set of displacement values and its respective applied forces, and they were inspired on the data presented in Fig. 1 (Duarte *et al.*, 2014).

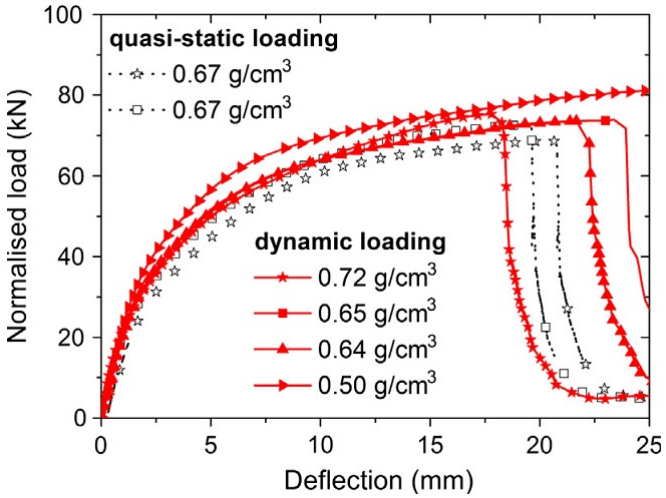
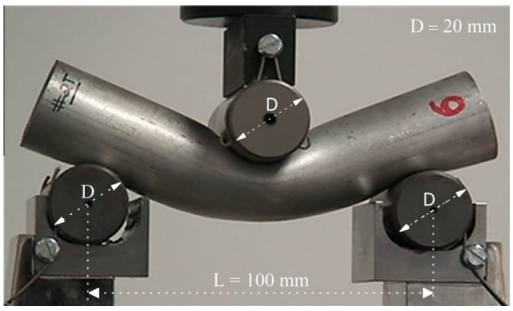


Figure 1: Results from three-point bending tests of the combination of thin-walled Aluminum tube and Aluminum Foam (Duarte *et al.*, 2014).

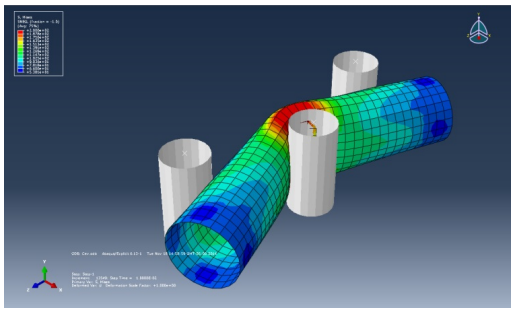
Considering the nature of this physical problem, the general solution approach is to use numerical techniques, such as the Finite Element Method. In the past few years, a number of commercial and open source packages designed to apply this method to several kind of problems have become widely available. The selected software to deal with this problem was Abaqus software, due to its robustness in dealing with solid mechanics problems. A comparison between an experimental (Duarte *et al.*, 2015) and computational set-up can be observed in Fig. 2.

Using this model, one needs to model the material behavior in order to be able to perform simulations. Thus, estimating the parameters that constitute this model is the main goal of the inverse analysis. In this work, seven unknown values were considered: the Young's Modulus, the Poisson's Ratio and five plastic stresses, as presented in Fig. 3. The respective plastic strains are fixed. These pairs of plastic stresses and strains constitute the nonlinear part of the stress-strain curve of the selected material in a piecewise fashion. The expectation is that the accurate estimation of these quantities would

allow for a good reproduction of the synthetic data.



(a) Experimental set-up (Duarte *et al.*, 2015).



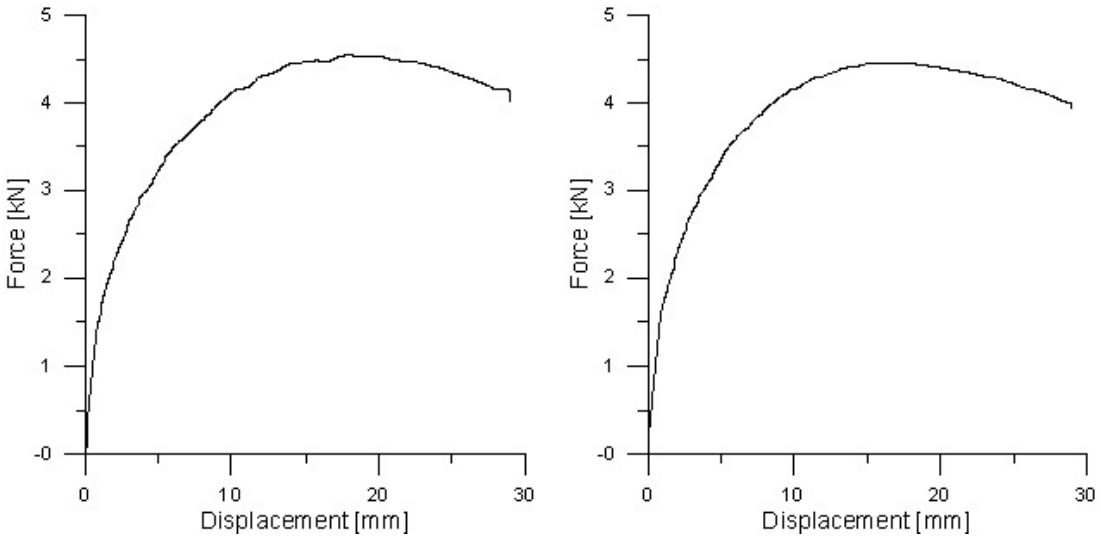
(b) Finite element model in Abaqus.

Figure 2: Experimental and computational set-up for the three-point bending test.

	Yield Stress	Plastic Strain
1	250	0
2	280	0.02
3	300	0.05
4	310	0.1
5	330	0.3

Figure 3: Nonlinear behavior settings in Abaqus.

One very important aspect of using numerical techniques such as FEM was the grid size used to discretize the physical domain. This parameter presents a trade-off between computational time and accuracy of the results. On the particular case of calculating a force-displacement curve, running the solver with a coarse grid led to an inaccurate and non-smooth force-displacement curve. However, as we reduced the grid spacing, the output became more accurate and smooth. Figure 4 shows a comparison between these two cases. This poses a serious difficulty in solving the inverse problem, because such type of analysis usually deals with solving the forward problem several times. As the processing time to solve the forward model increases, the inverse analysis can easily become unfeasible. In order to deal with this problem, the usual Abaqus simulation was replaced by a metamodel.



(a) Coarse grid.

(b) Fine grid.

Figure 4: Experimental and computational set-up for the three-point bending test.

The metamodel used in this work is a response surface approximation. Various response surface methods were tested, including Kriging, Shepard's K-Nearest and Radial Basis Functions (RBF), with the latter providing the most accurate

results. The typical formulation for the RBF is to approximate the output of the objective function as a linear combination of interpolation functions $\phi(\mathbf{x})$, as shown in Eq. (1) (Colaço and Dulikravich, 2011). There are several different types of RBF, and the multiquadric function, shown in Eq. (2) was selected for this work. In this equation, the quantity c is a shape factor, which was considered, for simplicity, as constant and equal to $1/N$, where N stands for the number of measurements.

$$f(\mathbf{x}) \simeq \hat{f}(\mathbf{x}) = \sum_{k=1}^{K} w_k \phi(||\mathbf{x} - \mathbf{x}_k||) \tag{1}$$

$$\phi(\mathbf{x}) = \sqrt{\mathbf{x}^T\mathbf{x} + c^2} \tag{2}$$

The weights w_k are designed to tune the effect of these interpolation functions in order to best reproduce the objective function which, in this case, is the solution of the forward problem. Therefore, in order to calculate these quantities, one needs to obtain a set of K outputs of the original solution of the forward problem, i.e. the Abaqus simulation. These known inputs $\{\mathbf{x}_k\}_{k=1}^K$ and outputs $\{f(\mathbf{x}_k)\}_{k=1}^K$ are called the *training set*. The outputs from this set are organized in a vector $\mathbf{f}$ and the interpolating functions are evaluated according to Eq. (1) and organized into a matrix $\mathbf{\Phi}$. The weights, organized in the vector $\mathbf{w}$, are then calculated by solving the linear system presented in Eq. (3).

$$\mathbf{\Phi w} = \mathbf{f} \tag{3}$$

This approach have a big advantage in comparison with the usual FEM approach, because this calculation of the weights can be performed offline, i.e., before the inverse analysis take place. When the inverse problem solution algorithm starts, the forward problem is solved by just evaluating Eq. (1), resulting in an almost instantaneous calculation.

Having investigated the most accurate method for constructing a response surface, one must also address the distribution of the points used to construct the approximation. This work applies the boundary conforming version of SOBOL's algorithm (Sobol and Levitan, 1976) to uniformly distribute training points through a design space. This version also allows for a user-specified number of points to be placed on the boundary of each variable, leading to the response surface to be accurate up to the variable bounds. Training of the response surface was performed by selecting a set of $K = 400$ materials inside the pre-specified boundaries presented in Tab. 1.

Table 1: Material bounds for the response surface approximation.

Property	Min.	Max.
Young's Modulus [GPa]	60	80
Poisson's Ratio	0.3	0.35
Plastic Stress #1 [MPa]	160	260
Plastic Stress #2 [MPa]	190	290
Plastic Stress #3 [MPa]	210	310
Plastic Stress #4 [MPa]	220	320
Plastic Stress #5 [MPa]	230	340

3. INVERSE PROBLEM

The inverse problem is solved within the Bayesian framework. Besides all the well-known particularities of an inverse problem, this approach is based on four basic principles (Kaipio and Somersalo, 2004):

1. All variables in the model are regarded as random variables;
2. The randomness of these variables describes the degree of information concerning their realizations;
3. The degree of information concerning these values is coded in the form of probability distributions;
4. The solution of the inverse problem is the posterior probability distribution;

The posterior probability density (pdf) $\pi(\mathbf{x}|\mathbf{y})$ is a function of a vector $\mathbf{x}$ containing the desired unknowns (material properties) and a vector $\mathbf{y}$ containing the observations (applied force). According to Bayes' theorem, presented in Eq. (4), the posterior pdf is proportional to two other probability functions, namely the likelihood $\pi(\mathbf{y}|\mathbf{x})$ and the prior $\pi(\mathbf{x})$.

$$\pi(\mathbf{x}|\mathbf{y}) \propto \pi(\mathbf{y}|\mathbf{x})\,\pi(\mathbf{x}) \tag{4}$$

Once we have this pdf, we can manipulate it in order to find out the conditional mean $\hat{\mathbf{x}}_{CM}$ of $\pi\left(\mathbf{x}|\mathbf{y}\right)$, which requires a integration process, described by Eq. (5) (Orlande, 2015).

$$\hat{\mathbf{x}}_{CM} = \mathbb{E}\left[\mathbf{x}|\mathbf{y}\right] = \int_{\mathbb{R}_N} \mathbf{x}\pi\left(\mathbf{x}|\mathbf{y}\right) d\mathbf{x} \tag{5}$$

The main issue with this approach is that it requires a numerical integration in a high-dimensional space of a function that might have a complex form or even be intractable. Such is the case for the proposed problem, once that the solution of the forward problem is not given in the form of an simple analytical expression but rather as a complex combination of functions. On the other hand, the mean and covariance of $\pi\left(\mathbf{x}|\mathbf{y}\right)$ can be approximated via Monte Carlo integration, through Eqs. (6) and (7), where the ensemble $\left\{\mathbf{x}^{(i)}\right\}_{i=1}^{M}$ comprises of samples obtained from $\pi\left(\mathbf{x}|\mathbf{y}\right)$.

$$\hat{\mathbf{x}}_{CM} = \mathbb{E}\left[\mathbf{x}|\mathbf{y}\right] \simeq \frac{1}{M}\sum_{i=1}^{M}\mathbf{x}^{(i)} \tag{6}$$

$$\mathrm{cov}\left(\hat{\mathbf{x}}\right) \simeq \frac{1}{M-1}\sum_{i=1}^{M}\left[\mathbf{x}^{(i)} - \hat{\mathbf{x}}_{CM}\right]\left[\mathbf{x}^{(i)} - \hat{\mathbf{x}}_{CM}\right]^{T} \tag{7}$$

$$\mathbf{x}^{(i)} \sim \pi\left(\mathbf{x}|\mathbf{y}\right), \quad i = 1, \ldots, M \tag{8}$$

Thus, the problem of performing numerical integration in a high dimensional space is replaced by the problem of sampling from a complex probability distribution. In order to perform this sampling, the Metropolis-Hastings algorithm (Metropolis *et al.*, 1953) was chosen. The next step is to construct the posterior pdf, which relies in defining the likelihood pdf $\pi\left(\mathbf{y}|\mathbf{x}\right)$. In this work, this pdf is considered to be a multivariate Gaussian with zero mean, shown in Eq. (9). The measurement errors are considered to be uncorrelated and having the same standard deviation, as shown in Eq. (10). The standard deviation were considered to be of $\sigma = 0.1$kN (Vesenjak, 2014). The prior pdf was modeled as uniform throughout the parameter space.

$$\pi\left(\mathbf{y}|\mathbf{x}\right) \propto \exp\left[-1/2||\mathbf{y} - \mathbf{f}\left(\mathbf{x}\right)||^2_{\mathbf{W}^{-1}}\right] \tag{9}$$

$$\mathbf{W} = \sigma^2\mathbf{I} \tag{10}$$

The goal of using the Metropolis-Hastings algorithm is to construct a Markov chain with $\pi\left(\mathbf{x}|\mathbf{y}\right)$ as its equilibrium distribution (Orlande, 2015). A sample $\mathbf{x}^*$ is obtained from a simple pdf $\pi\left(\mathbf{x}^*|\mathbf{x}^{(i)}\right)$ called proposal distribution, and is tested to measure how likely this sample can also be considered to be a sample from $\pi\left(\mathbf{x}|\mathbf{y}\right)$. If this test is successful, the sample is incorporated as a new state of the Markov chain. Otherwise, the previous state $\mathbf{x}^{(i-1)}$ is accepted as the new state. In this work, the proposal distribution is considered as an uniform pdf, centered at the current state of the present state of the Markov chain, as shown in Eq. (11), resulting in a random-walk model.

$$\mathbf{x}^*|\mathbf{x}^{(i-1)} \sim \mathrm{U}\left[\mathbf{x}^{(i-1)} - \Delta\mathbf{x}, \mathbf{x}^{(i-1)} + \Delta\mathbf{x}\right] \tag{11}$$

After simulating the Markov chain, some post-processing is needed before performing inference on the acquired data. At the beginning of the simulation, the chain presents an initial convergence stage before reaching the equilibrium distribution. This period is called *burn-in* (Orlande, 2015) and samples obtained during this period cannot be used and must be discarded. Furthermore, Eqs. (6) and (7) relies on independent and identically distributed samples and not all of the remaining Markov chains can be used. The calculation of the *Integrated AutoCorrelation Time* (IACT) (Orlande, 2015), symbolized by τ, allows one to determine the interval between two i.i.d. samples inside the remaining Markov chain. The IACT can be calculated by using Eqs. (12)-(14).

$$\tau_j = 1 + 2\sum_{k=1}^{\infty}\rho^j_{ff}(k) \tag{12}$$

$$\rho^j_{ff}(k) = \frac{C^j_{ff}(s)}{C^j_{ff}(0)} \tag{13}$$

$$C^j_{ff}(s) = \mathrm{cov}\left(\mathbf{x}^{(i)}_j, \mathbf{x}^{(i+s)}_j\right) \tag{14}$$

4. RESULTS

In order to assess the functionality of the proposed methodology, a test material, selected at the center of the parameter hypercube presented at Tab. 1, was simulated in Abaqus software. The obtained force values were then corrupted with additive and uncorrelated Gaussian noise with a standard deviation of $\sigma = 0.1$kN, in order to simulate a real experimental framework. The methodology here described was then applied to this set of experimental measurements. One million Markov chains were simulated through this methodology, from which 10^4 were considered to be inside the *burn-in period* and were discarded.

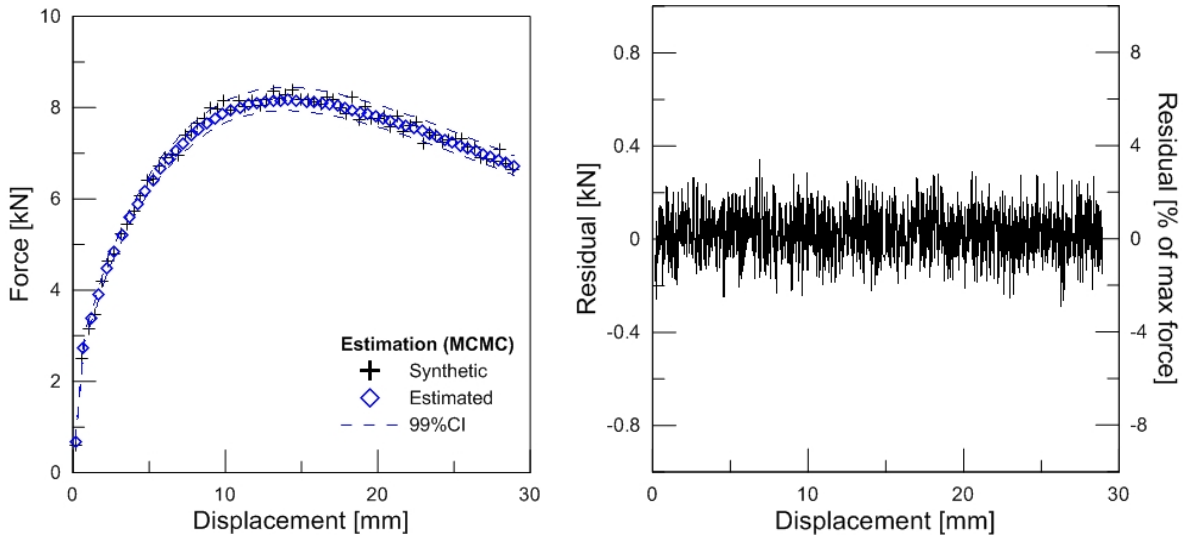
All Abaqus simulations were performed using the cluster from Florida International University. The response surface, the Metropolis-Hastings algorithm and the Integrated AutoCorrelation Time were programmed in Fortran90 and submitted in a single thread of an IntelCore i7-3770 CPU@3.40GHz with 16GB of RAM. The computational time for the inverse analysis was of approximately 2 hours. Direct coupling of Abaqus software in the Metropolis-Hastings algorithm was also considered, but the processing time was unfeasible, leading to 2 weeks of simulation in order to produce less than 10^4 Markov chains. This shows that including the response surface approximation was responsible for decreasing the computational cost by orders of magnitude.

The reference value of the parameters, as well as its estimated values and respective 99% confidence intervals are presented in Tab. 2. Figure 5a shows a comparison between the synthetic measurements and the results of the estimation process. As one can observe, the agreement between synthetic and estimated values is excellent throughout all data points. This is particulary important, because it means that, although some errors are expected because of the RBF approximation, the errors due to the added noise are still dominant.

Figure. 5b shows the obtained residuals, which oscillates around zero with amplitude of the same order of magnitude of σ. These oscillations represent less than 3% of the value of the maximum force observed, and are basically due to the Gaussian noise. This provides another strong evidence of the good quality of the fit.

Table 2: Nominal parameters for simulation of measurements.

Property	Reference	Estimated	99% C.I.
Young's Modulus [GPa]	70	69.709	[67.950; 71.468]
Poisson's Ratio	0.325	0.3289	[0.3211; 0.3367]
Plastic Stress #1 [MPa]	200	196.46	[192.03; 200.90]
Plastic Stress #2 [MPa]	230	236.46	[229.67; 243.26]
Plastic Stress #3 [MPa]	250	243.50	[234.82; 252.19]
Plastic Stress #4 [MPa]	255	254.88	[246.99; 262.76]
Plastic Stress #5 [MPa]	260	260.21	[253.77; 266.64]



(a) Synthetic and estimated forces. (b) Residuals.

Figure 5: Obtained results for the estimation using MCMC.

After estimating the desired quantities, it was necessary to evaluate if these results were meaningful. i.e., check if these properties, when used together with the original forward problem, provided the same output as the one observed

when using the response surface. Thus, Abaqus simulations were once again performed, using the estimated values shown in Tab. 2. Cases using the bounds of the obtained confidence intervals were also considered. These values were compared with the synthetic measurements and the output from the response surface and can be observed in Fig. 6 and the agreement was, once again, excellent. This means that not only the response surface produced a significant reduction on the computational cost, but also did it without presenting noticeable differences from an Abaqus simulation. This is a very interesting result, for it tells that even simple response surface formulations are able to accurately mimic the behavior of the original forward problem and, perhaps, more accurate and complex response surface techniques might not produce significant improvements in the overall results.

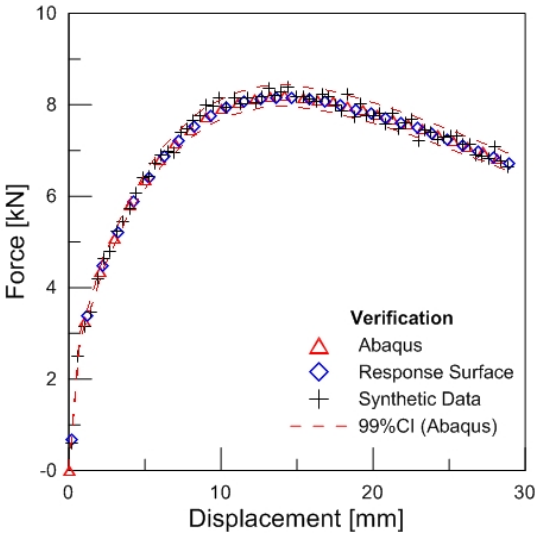


Figure 6: Verification of the results.

5. CONCLUSIONS

The proposed methodology presented results in excellent agreement with the synthetic measurements, while reducing the required computational effort by orders of magnitude. The most intensive calculations are performed in an *offline* manner and can be performed and stored before performing any kind of inverse analysis take place. It is also completely *non-intrusive* and can be applied to any other inverse problem with minimal changes in the computer code. Therefore, it is definitely an alternative for large scale problems, involving large computational efforts for the calculation of the forward problem.

Discarding the uncertainty in the parameters and solving the inverse problem in a deterministic environment results in an even more significant reduction in processing times, but without statistical information that may be helpful in assessing the quality of the results.

The selected mathematical model plays a major role in the whole process, since the presence of modeling errors may produce deviations on the estimates in comparison with complete and very realistic models. Although the obtained estimates accurately calibrate the model to match the synthetic/experimental measurements, they may differ from results available in the literature due for these same parameters.

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