

Estimation of Composite Laminate Ply Angles Using an Inverse Bayesian Approach Based on Surrogate Models

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Abstract

A digital twin (DT) relies on a detailed, virtual representation of a physical product. Since uncertainties and deviations can lead to significant changes in the functionality and quality of products, they should be considered in the DT. However, valuable product properties are often hidden and thus difficult to integrate into a DT. In this work, a Bayesian inverse approach based on surrogate models is applied to infer hidden composite laminate ply angles from strain measurements. The approach is able to find the true values even for ill-posed problems and shows good results up to 6 plies.

Keywords: digital twin, inverse problem, simulation-based design, data-driven design, structural analysis

1. Introduction

Digital Twins (DT) offer new possibilities for improving products and enable the development of new products and services like product service systems (PSS). (Stark et al., 2020) Different definitions for the DT can be found, see, for example, (Grieves & Vickers, 2017; Stark et al., 2020; Trauer et al., 2020). One of the first and widely spread definitions is from NASA who defines in (Glaessgen & Stargel, 2012) the DT as

“an integrated multiphysics, multiscale, probabilistic simulation of an as-built vehicle or system that uses the best available physical models, sensor updates, fleet history, etc., to mirror the life of its corresponding flying twin.”

In (Stark et al., 2020) a more precise definition of the DT in the context of product development is given. The DT herein is defined as the digital representation of an instance of the product. It combines models or geometry from the digital master with data from the digital shadow, which includes for example manufacturing process data of a physical product instance. While in the NASA definition the highest possible detail for models and available data should be chosen, in (Stark et al., 2020) the definition of the required model quality is named as a major task. Using detailed data from the physical twin can lead to improved product development and manufacturing processes, see, e.g. (Trauer et al., 2021). Variation simulation and geometric tolerancing benefit from a higher level of detail and therefore a better representation of the physical twin. (Schleich et al., 2017) Particularly applications of composite materials, focusing on endless fiber-reinforced plastics, benefit from a high level of detail. The anisotropic material properties and the layered structure of the laminate determine the structural behavior of the part. Variations from the nominal design have to be measured to obtain an as build instance of the DT. Effects of the variations, like fiber misalignment or gaps, can be considered for the product development through transferring the measurement data to an instance of the DT (Zambal et al., 2018). DTs of composite parts can be used for predictions of

the assembly process (Polini & Corrado, 2020) as well as predictions of the structural behavior (Sayer et al., 2020).

The measurement of the composite part, including the material properties and laminate design parameters, is essential for providing a high quality of the models included in the DT. Non-destructive testing (NDT) methods can be used to characterize composite parts for DT. The difficulty lies in the characterization of not directly observable properties of the composite part, like layer orientation or thickness. To measure these properties, NDT methods like computer tomography, ultrasonic, eddy current, or thermography measurements are available. But they need special equipment and are computationally and time expensive. However, inverse material characterization can provide a way to infer the sought properties by measuring resulting entities such as the structural responses, for example in form of eigenfrequencies or strains, which are easier to measure. Through inverse material characterization material properties can be estimated by solving an inverse problem based on the measurements and surrogate models. (Steuben et al., 2015) During the solving process, the material properties are adjusted so that the results of the surrogate model match the measured data best. The resulting inversely characterized material properties can be used to improve the DT models. The improved simulation models of the DT enable predictions of lifetime or failure that are more precise.

To solve inverse problems two common approaches evolved. On the one hand, the inverse problem can be formulated as a minimization of a least squares formulation which reduces the error between measured data and model predictions with respect to the observed material properties (Gogu et al., 2010). Stable and advanced optimization algorithms have to be applied to minimize those problems, due to challenges like ill-posedness (Daghia et al., 2007; Tarantola, 2005). On the other hand, a probabilistic approach, a Bayesian framework, considers uncertainties in the measurement data and the models. Therefore, it does not compute a single value but a probability distribution (Gogu et al., 2010). Inverse problems described using a Bayesian framework typically cannot be solved analytically. Thus, sampling techniques, such as Gibbs Sampler or Metropolis-Hastings algorithm, can be applied to solve the inverse problem (Tarantola, 2005).

During the solution of the inverse problem, a surrogate model of the physical part simulates the structural behavior. Since the solution of inverse problems is quite expensive in terms of computational effort, it is important to use efficient surrogate models. While the use of finite element analysis (FEA) is very common (Cappelli et al., 2018; Daghia et al., 2007; Euler et al., 2006; Rahmani et al., 2013), the computational effort can be reduced using surrogate models, which are not physics-based. A wide variety of surrogate models is used in inverse characterization, such as the response surface method (Barkanov et al., 2009; Wesolowski & Barkanov, 2014) or Non-Uniform Rational B-Spline (NURBS) (Steuben et al., 2015). Analytical models like the plate laminate theory used in (Zebdi et al., 2009) are computationally efficient but restrict the complexity of the investigated part geometry.

To characterize the material properties, structural data of the parts have to be measured. The direct correlation between the part stiffness and the eigenfrequencies is the reason why they are mainly applied. Besides them, indentation tests or measured strains can as well serve as reference, although they are not as popular as eigenfrequencies.

Applications of inverse approaches in composite structures mainly concentrate on the inverse characterization of composite material properties on different scales. The majority of research concentrates on the characterization of the elastic modulus and shear modulus of the laminate in longitudinal and transverse directions on the macro scale (Daghia et al., 2007; Pedersen & Frederiksen, 1992; Steuben et al., 2015; Wesolowski & Barkanov, 2014; Zebdi et al., 2009). On the mesoscale, the mechanical properties of the single plies are evaluated (Castillo & Kalidindi, 2020) while on the micro-scale the mechanical properties of the fiber and matrix are of interest (Blaheta et al., 2018). More advanced approaches combine the different scales to multi-scale approaches (Cappelli et al., 2018; Cappelli et al., 2019a; Cappelli et al., 2019b) to gain deeper insights into the geometrical features and the material of the microstructure.

The review of the state of the art gives insights into the principles and applications of inverse material characterization especially considering composite materials. Nonetheless, there are still open questions that will be addressed in this contribution:

- While the characterization of mechanical properties of composites is already used on different scales, the characterization of laminate parameters such as layer thickness, layer orientation, or the fiber volume fraction is not applied yet. However, those laminate parameters do not only influence the structural behavior but can help to improve simulation models or be integrated into quality control. Therefore, the question is: How can inverse characterization be used to quantify laminate properties in composite structures?
- To increase the applicability of the inverse characterization approaches the usage of easily accessible experimental data, such as strain data from stiffness measurements, is important. In contrast to, for example, eigenfrequencies, more data is needed to obtain good results. The question arises, where are the limits of inverse characterization of composite structures? How much data is needed to get good predictions? How many composite layers can be characterized? How good are the results of the inverse characterization?
- Inverse material characterization is a data-intense and computationally intense characterization method. Industry 4.0 and the DT are concepts that on the one hand produce and on the other hand need a big amount of data. So, how can potentials of inverse characterization be used in the context of industry 4.0 and DTs?

2. Methods

In order to characterize laminate properties by observing strains, three major problems usually occur:

1. The setup might be ill-posed, with a non-unique solution i.e., more than one set of parameters can lead to the measured strain data,
2. the observation is subject to measurement errors, and
3. the laminate parameters are subject to manufacturing uncertainties.

One method for treating uncertainties and for solving ill-posed problems is Bayesian inference. The result of Bayesian inference is a distribution of the parameters θ given some data d . The Bayes rule is shown in Equation (1), where $\mathcal{L} = p(\mathcal{D} = d|\theta)$ is the likelihood that incorporates how the data d interacts with the parameters θ , $\Pi = p(\theta)$ is the a priori assumed distribution of the parameters θ , which is also called prior, and $\mathcal{P} = p(\theta|\mathcal{D} = d)$ is the posterior which is the distribution of the parameters given the data.

$$p(\theta|\mathcal{D} = d) = \frac{p(\mathcal{D} = d|\theta)p(\theta)}{\int p(\mathcal{D} = d|\theta)p(\theta)d\theta} \quad (1)$$

As the denominator is constant, Equation 1 can be also written as

$$p(\theta|\mathcal{D} = d) \propto p(\mathcal{D} = d|\theta)p(\theta). \quad (2)$$

In general, the posterior can assume different kinds of distributions. In order to determine that posterior distribution \mathcal{P} , the Metropolis-Hastings sampling rule is used (Hastings, 1970). The Metropolis-Hastings sampling strategy is a method for generating samples from any shape of distribution. For each generated sample θ_{i+1} , the current posterior \mathcal{P}_{i+1} is evaluated and compared to the previous one \mathcal{P}_i . The sample is accepted if $\mathcal{P}_{i+1} > \mathcal{P}_i$. If $\mathcal{P}_{i+1} < \mathcal{P}_i$ the sample is accepted with a probability of $\frac{\mathcal{P}_{i+1}}{\mathcal{P}_i}$. This opens the possibility to escape from local maxima. As the posterior takes the prior distribution into account, the method further enables considering prior believes regarding the model parameters.

Before Bayesian inference can be used, the likelihood function \mathcal{L} has to be modeled. In simple laminate configurations, the likelihood function can be modeled with physics-based equations from the classical laminate plate theory (CLPT). For more advanced composite structures, FEA can be applied. In order to reduce the computational time of the sampling strategy, mathematical surrogate models trained on FEA results can be used.

Classical Laminate Plate Theory

The CLPT was developed to model the physical relation of forces and strains on a composite laminate consisting of layers stacked and bonded onto each other. The layered modelling of a composite plate induces the occurrence of in-plane force resultants \mathbf{N} as well as moment resultants \mathbf{M} . The stiffness

matrices are calculated using the mechanical properties of the single plies, such as E-moduli. The resulting matrices are transformed into the global coordinate system, in which the stiffness of the laminate is obtained by summing them up. Equation 3 shows the resulting relation of the force and moment resultants, the stiffness matrix and the strains $\boldsymbol{\varepsilon}$ and curvatures $\boldsymbol{\kappa}$.

$$\begin{Bmatrix} N_{xx} \\ N_{yy} \\ N_{xy} \\ M_{xx} \\ M_{yy} \\ M_{xy} \end{Bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & B_{11} & B_{12} & B_{13} \\ A_{21} & A_{22} & A_{23} & B_{21} & B_{22} & B_{23} \\ A_{31} & A_{32} & A_{33} & B_{31} & B_{32} & B_{33} \\ B_{11} & B_{12} & B_{13} & D_{11} & D_{12} & D_{13} \\ B_{21} & B_{22} & B_{23} & D_{21} & D_{22} & D_{23} \\ B_{31} & B_{32} & B_{33} & D_{31} & D_{32} & D_{33} \end{bmatrix} \begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \gamma_{xy} \\ \kappa_{xx} \\ \kappa_{yy} \\ \kappa_{xy} \end{Bmatrix} \quad (3)$$

The stiffness matrix consist of three submatrices, the extensional stiffness matrix \mathbf{A} , the bending stiffness matrix \mathbf{D} , and the bending-extensional coupling stiffness matrix \mathbf{B} . (Reddy, 2004) The submatrices can be calculated summarizing the stiffness matrix \mathbf{Q} in the global coordinate system over all K plies, as follows

$$A_{ij} = \sum_{k=1}^K Q_{ij}^{(k)} (z_{k+1} - z_k), \quad B_{ij} = \frac{1}{2} \sum_{k=1}^K Q_{ij}^{(k)} (z_{k+1}^2 - z_k^2), \quad D_{ij} = \frac{1}{3} \sum_{k=1}^K Q_{ij}^{(k)} (z_{k+1}^3 - z_k^3) \quad (4)$$

Where the coordinate z_k of the k -th ply is used to consider the thickness and position of the plies. CLPT results in an analytical solution of the continuum-based problem formulation, which is computationally efficient. This makes the CLPT interesting for applications with a high number of computations, like for laminate design in early design stages or the detailed design and analysis of specific part areas and flat panels.

Gaussian Processes

Surrogate models can greatly decrease the computational time especially when using sampling strategies where the model is executed many times. One kind of mathematical surrogate model, which has been used recently by many researchers (Avendaño-Valencia et al., 2020; Franz et al., 2021; Gentile & Galasso, 2020; Kong et al., 2018), are Gaussian processes (GP). Equation 5 shows the definition of a GP consisting of a mean function $m(x)$ and a covariance function $k(x, x')$, which typically consist of some free parameters—also called hyperparameters (Rasmussen & Williams, 2008). These hyperparameters are trained based on input and output data x and y , respectively.

$$f(x) = y \sim \mathcal{GP}(m(x), k(x, x')) \quad (5)$$

The advantage of GPs is that they provide uncertainty estimates for the predicted values. Therefore, they can be used without any adjustments as the likelihood function \mathcal{L} . Referring to Equation 2, the parameters θ and the data \mathcal{d} are the input x and the output y , respectively.

However, other mathematical surrogate models can be also used for Bayesian inference even though they do not provide uncertainty estimates. One possibility is to use a trained mathematical surrogate model as the mean function of a GP. The covariance function can be assumed to be zero for all covariances and to be the squared observation error σ_y^2 for all variances, which can be written as

$$k(x_i, x_j) = \delta_{ij} \sigma_y^2, \quad \text{with } \delta_{ij} = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases}. \quad (6)$$

In the following, the presented Bayesian inference method together with determining the likelihood function are applied to a composite structure.

3. Application

In this section, we first apply Bayesian inference to a composite plate. It is shown how to infer the ply angles of a composite structure and their uncertainty from strain measurements. Second, the limits of the inverse characterization are determined.

3.1. Inverse Characterization of Composite Structures with Bayesian Inference

This subsection explains how to infer the angle and its uncertainty of each ply from strain data. In this paper, we apply the proposed method to a four-layer composite plate (see Figure 1). The plate's parameters are listed in Table 1.

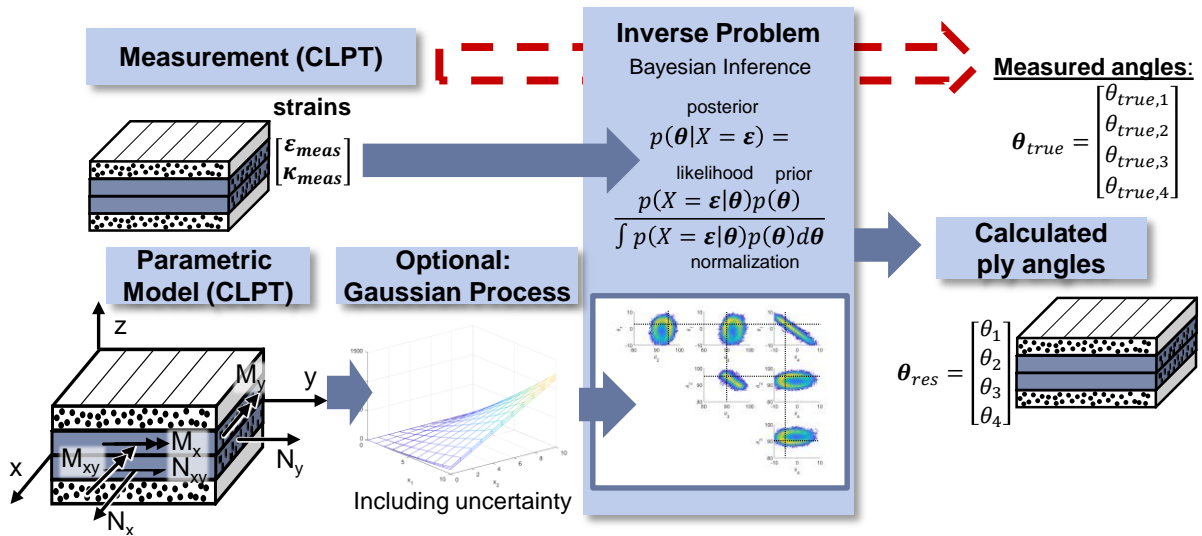


Figure 1. Inverse characterization method for a four layered composite plate.

Table 1. Parameters of composite plate

t in mm	E_x in MPa	E_y in MPa	ν_{xy}	G_{xy} in MPa	θ_{true} in $^\circ$
$[0.2, 0.2, 0.2, 0.2]^T$	120,000	8,000	0.27	5,000	$[31, 48, 20, 58]^T$

In this application example, the plate is loaded with two different load cases, $N_x = 1000$ Nmm and $N_y = 1000$ Nmm. To show the applicability, the measurement data is generated using the CLPT. For each load case, the strains ϵ_{meas} and curvatures κ_{meas} are measured in order to determine the ply angles. A normally distributed measurement error of $\sigma_\epsilon = 0.141$ for all strain and curvature components, ϵ and κ , is assumed, so that

$$\begin{bmatrix} \epsilon \\ \kappa \end{bmatrix} \sim \mathcal{N}_\epsilon(\mu_\epsilon(\theta), \sigma_\epsilon^2 I) \quad (7)$$

With

$$\mu_\epsilon(\theta) = \begin{bmatrix} \epsilon(\theta) \\ \kappa(\theta) \end{bmatrix} = \begin{bmatrix} A(\theta) & B(\theta) \\ B(\theta) & D(\theta) \end{bmatrix}^{-1} \begin{bmatrix} N \\ M \end{bmatrix}. \quad (8)$$

Then the likelihood \mathcal{L} is the probability density for a set of parameters θ evaluated at the measured strains ϵ_{meas} and curvatures κ_{meas} .

As the Bayesian setup enables integrating prior believes regarding the parameters, two different cases are considered:

1. Without prior information and
2. with prior information assuming a normal distribution with $\sigma_\theta = 15^\circ$ for each ply and $\mu_\theta = \theta_{true}$.

For the second case, the prior Π reads

$$\Pi(\theta) = p(\theta) = \mathcal{N}_\theta(\mu_\theta, \sigma_\theta^2 I) \quad (9)$$

and for a new parameter sample θ , a value proportional to the posterior \mathcal{P} can be computed as

$$\mathcal{P}(\theta) \propto \mathcal{L}(\theta) \Pi(\theta). \quad (10)$$

Now, the Metropolis-Hastings sampling strategy explained in Section 2 can be used to determine the posterior distribution.

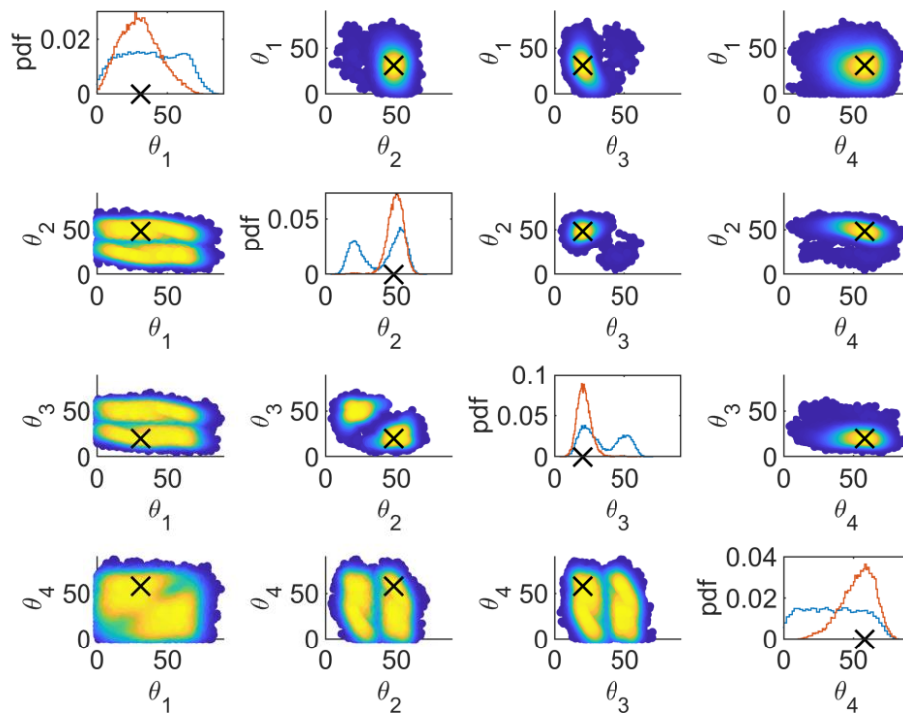


Figure 2. Results of Bayesian inference for a four-layer composite plate without (lower left corner plot & blue line) and with (upper right corner plot & red line) prior information. The color represents the probability density of the samples (dark blue means low & yellow means high).

Figure 2 shows the results of the four-layer composite plate. The main diagonal displays the approximated probability density function (PDF) of each ply. The other subfigures show the samples of the Metropolis-Hastings sampling strategy. The dark blue and the bright yellow color indicates a low and a high posterior value, respectively. The lower left sample plots as well as the blue lines in the main diagonal represent the result without any prior information. The upper right sample plots and the red lines show the result considering prior information. The black cross represents the realized ply angles θ_{true} . Using a mathematical surrogate model leads to similar results.

The lower left corner plot shows multiple high-density regions that indicate an ill-posed problem as the measurement can be achieved by multiple parameter sets. This is also shown by the two peaks in the second and third PDF plots (blue lines). In contrast to that, the upper right corner plot shows only one clear result in this case. By adding prior information, the PDF is dragged towards the prior leading to one clear result in this case. Furthermore, the uncertainty of the result is smaller than the uncertainty without prior information.

Reducing the measurement error leads to more distinct peaks in the posterior distribution. However, when reducing the variance of the assumed measurement error (prior information) too much, the Metropolis-Hastings sampling strategy gets trapped in local maxima and cannot find the full distribution.

3.2. Limits of Inverse Characterization of Composite Structures

Knowing the limits of the inverse characterization method is essential to verify the results. Therefore, two parameter studies are conducted to obtain information about limitations in terms of the characterization of composite structures. The first parameter study scrutinizes the quality of the results respect to the number of different structural observations. The second study investigates the number of layers for which the deviations can be calculated.

3.2.1. Parameter Study 1: Result Quality

While eigenfrequencies include the stiffness properties of the complete part, including all laminate parameters, structural loads do not necessarily lead to an ambiguous result. Therefore, applying several different structural loads increases the detail of information, which leads to increased result quality from the inverse characterization. In order to evaluate the progress in result quality a parameter study with increasing number of load cases is performed.

The parameter study bases on the presented general approach from Chapter 2, using the CLPT model during the inverse characterization, due to its simplicity and good applicability. Moreover, a four-layered laminate with a nominal layup of $\theta_{nom} = (45^\circ/-45^\circ/-45^\circ/45^\circ)$ is set up with reference deviations to the nominal design of $\Delta\theta = (4^\circ/2^\circ/-8^\circ/5^\circ)$. The number of load cases is gradually increased from a single load case to six load cases. The order and force or moment components of the load cases are depicted in Table 2. The order of the load cases is chosen to gain a maximum of information. Therefore, the first three load cases include different directional components and force as well as moment resultants. The resulting strains of the six load cases serve as reference for the inverse characterization of the deviated design, while the nominal layup is used as prior information. To consider the statistical effects in the Metropolis-Hastings sampling every calculation is performed ten times.

Table 2. Load Cases for parameter study 1

Load case number	N_{xx} in Nmm	N_{yy} in Nmm	N_{xy} in Nmm	M_{xx} in N	M_{yy} in N	M_{xy} in N
1	100	0	0	0	0	0
2	0	100	0	0	0	0
3	0	0	0	0	0	100
4	0	0	0	100	0	0
5	0	0	100	0	0	0
6	0	0	0	0	100	0

The root mean square error (RMSE) of the resulting layer angles is calculated for the ten observations. The results are depicted in Figure 3 as box plots. The median of the RMSE values decreases with a rising number of load cases. For more than three different load cases the median shows only minor changes. A similar behavior can be observed for the 25 and 75 percentiles. With a rising number of load cases the distance between both decreases, whereas a convergence for more than three load cases is observed.

The improvement in characterization quality results from the increasing coverage of the stiffness matrix through the different loads. The more information can be obtained about the stiffness matrix, the more a unique layup is likely. Especially the combination of force and moment loads improve the result quality because of the different orders of the distances to the mid-plane in the stiffness matrix. Nonetheless, pre-studies showed that even different levels of the same load component can increase result quality.

3.2.2. Parameter Study 2: Layer Number

The second parameter study investigates whether there are restrictions in the number of layers that can be characterized using the presented method. With a rising number of layers, the number of deviating parameters increases and ill-posedness becomes more likely. Therefore, finding a good solution becomes more difficult.

The second parameter study is designed similar to the first one. Despite of increasing the number of load cases, the number of layers is increased incrementally from 4 layers to 16 layers. All layers are oriented in the same direction, resulting in the layup $\theta_{nom} = (45^\circ)_K$ with the number of layers K. The reference deviations are chosen as random integer values in the range of $[-10;10]$ which results in the following 16 layer deviations $\Delta\theta = (4^\circ / 2^\circ / -8^\circ / 5^\circ / 4^\circ / -1^\circ / -6^\circ / -4^\circ / 8^\circ / -5^\circ / -9^\circ / 2^\circ / 5^\circ / -1^\circ / 6^\circ / -5^\circ)$ which are added to the nominal layer angle. Two load cases with a total of 3 directional components are applied for inverse characterization. Load case 1 consists of the load

component $M_{xy} = 100$ N and load case 2 of a combined load $N_{xx} = 1000$ Nmm and $N_{yy} = 300$ Nmm with all other components being zero. Analogous to parameter study 1 the inverse characterization is performed ten times. The RMSE is considered as result value.

The outcome of parameter study 2 is presented in Figure 3b. The results of the inverse characterization of four layers show a low RMSE value with a median value near 1. This coincides with the good results from parameter study 1. With an increase in layer numbers the RMSE increases to a median value of 9.99° for 7 layers. With a further increase in the layer number, the RMSE median values stabilize between 6.01° and 9.99° .

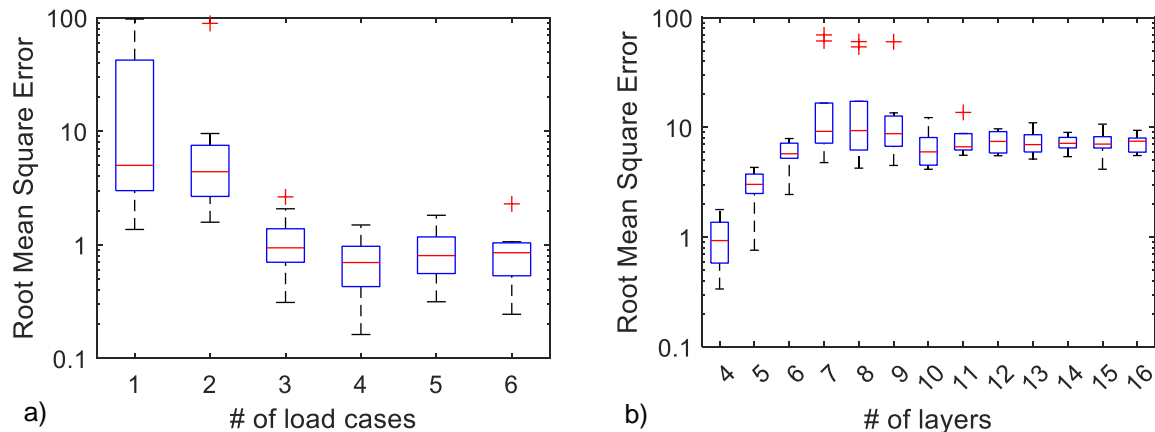


Figure 3. Results of the parameter studies: a) Parameter study 1 shows the RMSE of the layer angles changing with the number of load cases; b) Parameter study 2 shows the RMSE of the layer angles changing with the number of layers. The red crosses represent outliers, the red line shows the median and the blue box defines the 25th percentile and 75th percentile. The whiskers define the non-outlier minima and maxima.

For a small number of layers the inverse characterization of the deviated layer angles shows good results. For higher numbers the result quality decreases severely. On the one hand, the higher number of layers increases the complexity of the inverse problem. Ill-posedness with unambiguity complicates the solution of the inverse problem. On the other hand, the importance of a single layer on the structural response of the plate is reduced when investigating a higher number of layers. Especially small deviations from the nominal angles are more difficult to observe for higher layer numbers. The influence on the structural behavior gets blurred, similar to the effects of homogenization. To counteract this behavior a higher number of degrees of freedom have to be scrutinized. While the CLPT results in six strains, more advanced modelling techniques like the FEA can lead to an improvement.

4. Discussion and Conclusion

The advantage of a DT is, in general, dependent on the model quality and data. As shown in this paper, inverse material characterization of laminate parameters increases the knowledge of the product through data with comparably low measurement effort. On the one hand, this increases applicability in mass production and on the other hand, deviations can be fed to the DT in order to evaluate the structural performance of individual parts. The applications presented in the paper show that the proposed method enables inferring laminate properties such as ply angles from strain measurements. Those laminate properties are “hidden” inside the laminate why non-destructive measurement comes with high effort. The proposed method could reduce time and cost for gaining more precise data.

The general application example shows a positive effect of prior information when solving inverse problems using Bayesian inference. Prior information in terms of nominal design values can be easily integrated in the presented framework and can help to characterize the deviations of the laminate properties. The results also show that the measurement error greatly influences the outcome. When assuming a too small measurement error (prior information) for the Metropolis-Hastings sampling strategy, the algorithm can be trapped in local maxima leading to a wrong posterior distribution.

Therefore, using slightly greater measurement errors than expected can help to find the entire posterior distribution.

Parameter study 1 shows the importance of good measurement data. The more data is available, the better the inverse characterization. Especially when real data is used, further uncertainties occur. Therefore, even more data might be needed to determine the laminate parameters within a certain accuracy. In parameter study 2 good results have been achieved up to 6 layers. This value can be increased by better measurement data and other laminate layups. However, a greater number of layers will decrease the result quality as for composite structures with greater layer numbers the importance of a single deviated layer is lower.

The method was successfully applied and has been compared with measurement data generated by the CLPT. The focus was set on the probabilistic nature of the method. Next steps could include applying the method using experimental data. Especially the needed modeling including its simplifications and measurement errors are further challenges. As mentioned in the paper, mathematical surrogate models such as GPs, which incorporate uncertainties due to their probabilistic formulation, can be trained for more complex structures to reduce computational time. Applying them successfully on real composite structures could be another venue to focus on.

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