Inverse Characterization of Composite Materials Via Surrogate Modeling

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Abstract

Methods for the inverse characterization of mechanical properties of materials have recently seen significant growth, largely because of the availability of enabling technologies such as automated testing, full-field measurement techniques, and inexpensive computing resources. Unfortunately, as the complexity of the material systems and their associated behaviors increase, even the most advanced methods for inverse characterization require impractically large computation time to produce results. To overcome this limitation we present a method that employs Non-Uniform Rational B-spline (NURBs) based surrogate modeling to generate a very efficient representation of the combined constitutive and structural model response required for inverse characterization. Building on our previous work, we present an inversion method for identifying the constitutive material properties that minimize an appropriate objective function. Verification of this methodology is achieved through synthetic numerical experiments that include material systems of isotropic-elastic, orthotropic-elastic, and orthotropic-hyperelastic with damage nature on selected geometries. Statistical analyses on the effects of experimental noise supplement our analysis. We then proceed to demonstrate the use of this approach to characterize actual specimens tested using a multiaxial robotic system. In conclusion, we discuss the effectiveness and limitations of the surrogate model-based methodology and outline further research required

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to advance this approach.

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1. Introduction

The continuously increasing proliferation of composite materials in manufacturing, along with the associated need for designing composite structures, has further expanded the need for establishing their constitutive behavior and associated material parameters. Unfortunately, recent research [1-5] has shown that the characterization of composite materials can be computationally expensive, especially when specimens are tested using a six degree-of-freedom automated test frame such as the NRL66.3 system developed at the Naval Research Laboratory [3-6]. While the constitutive response models or "forward" models of composite material behavior are well understood, their repeated usage in the optimization loop required to solve the *inverse* problem of determining the material properties from multiple test datasets corresponding to multiple tests, has been shown to require impractically long computation times [6]. To address this problem, we have initiated an effort to explore more computationally efficient representations and methods.

Consequently, in the present work we investigate the potential of increasing the efficiency of conventional physics-based composite material characterization methods, by attempting to replace the structural system model with a physics-agnostic, but numerically accurate representation as is introduced in Section 2. To accomplish this goal we introduce surrogate models that are based on Non-Uniform Rational B-splines (NURBs). Although there is computational cost associated with their construction, the operation is efficient and is an one-time process. On the other hand, querying these surrogates is an extremely efficient activity (equivalent to evaluating a polynomial function) that enables the implementation of an inverse methodology framework that can be used to rapidly recover the material constitutive properties. The implemented nu-

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merical methodology for determining the proposed NURB-based surrogate models is the subject of Section 3.

The effectiveness and efficiency of the proposed method is presented in terms of a series of synthetic test problems in Section 4. We begin with the simple case of an aluminum specimen with a central hole subjected to in-plane loading. The material constitutive behavior is considered to be elastic and isotropic. A laminated composite specimen with an open hole discretized by a 3D finite-element representation that is based on a linear elastic orthotropic constitutive model is the next characterization example. A final synthetic experiment considers also a laminated composite test specimen with dual opposing edge notches and involves an orthotropic hyperelastic material. These results are accompanied by a statistical study on the effects of experimental noise on the accuracy of the recovered material properties. The extension of these synthetic results to the characterization of physical specimens tested in NRL's six degree-of-freedom robotic test frame (NRL66.3) is given in Section 5. Section 6 presents the conclusions drawn from the analysis conducted for these test experiments, as well as future plans.

The findings presented here are an extension of the developmental work found in [7]. The principle novelty of the present work is the mathematically rigorous description of the methodology employed. The details of many minor, but important aspects of the methodology are investigated and explicitly defined. Additionally, the present work extends the methodology into the domain of physical experimentation, and provides concrete support of the merit of this approach.

2. Constitutive Characterization of Composite Materials

2.1. Outline of the forward problem

In the context of continuum mechanics, the complete behavior of a deformable anisotropic elastic body without body forces and inertial terms and for the case of infinitesimal strain theory assumptions, is described by the well known system of equa-

Figure 1: A typical structural continuum system represented by a domain Ω enclosed by a surface S (where S_o is the observable part of the surface and $S - S_o$ is the rest of it), consisting of layup composed by multiple plies each of which typically exhibits transverse isotropic (orthotropic) behavior.

tions [8],

$$\nabla \cdot \sigma = 0, \quad (1a)$$

$$\sigma = C : \varepsilon, \quad (1b)$$

$$\varepsilon = \frac{1}{2} [\nabla u + (\nabla u)^T]. \quad (1c)$$

In this description, Eq. (1a) represents the elastostatic form of the conservation of momentum, while Eq. (1b) represents the linear elastic constitutive law (otherwise known as generalized Hooke's law) and Eq. (1c) the strain-displacement equations for the case of infinitesimal strains and small displacements. The quantities σ , ε and u represent respectively, the two second order tensors of the Cauchy stresses and infinitesimal strains, as well as the displacement vector. The fourth order tensor C contains as its elements all the anisotropic constitutive parameters of the material system and is usually referred to as the elasticity tensor. When these parameters are known for a material system enclosed in some volume Ω and bound by a surface $\partial\Omega = S$ as shown in Figure 1, then this composition of material and geometry is what is usually referred to as a structural system (i.e. a material testing coupon, or a specific structure such as an aircraft or a bridge etc.).

Substitution of Eq. (1c) in Eq. (1b) leads to an expression that when is substituted into Eq. (1a) along with the recognition that the elastic tensor is symmetric, yields the Navier form of the elastostatic system in the form,

$$\nabla \cdot (C : \nabla u) = 0. \quad (2)$$

When a material system described by either of the two equivalent forms of Equations (1) or (2), is exposed to some tractions $\hat{\mathbf{t}}$ and displacements $\hat{\mathbf{u}}$ on the boundary, then $\boldsymbol{\sigma}\mathbf{n} = \hat{\mathbf{t}}$ on $S_t \subseteq S$ ($\mathbf{n}$ is the unit normal vector to the boundary) and $\mathbf{u} = \hat{\mathbf{u}}$ on $S_u \subseteq S$ correspond to the Neumann and Dirichlet boundary conditions respectively. Under those constraints the determination of any of the unknown quantities in Eq. (1) is the solution of a boundary value problem, and it corresponds to the solution of the so-called forward problem. In the general case where closed form solutions of this boundary value problem cannot be found, an approximating solution is usually established by various methods that involve a projection of the continuous system described by Equations (1) or (2) into a finite discrete space referenced by a collection of particular points $\mathbf{x}_i \in \Omega \subset \mathbb{R}^3$. As it is well known, the solution of the problem reduces to the solution of a linear system of equations involving the column vectors $\mathbf{u} = \{\mathbf{u}_i\}$ and $\mathbf{f} = \{\mathbf{f}_i\}$ that collect nodal components of the displacement $\mathbf{u}_i = \{u_x, u_y, u_z\}_i^T$ and force $\mathbf{f}_i = \{f_x, f_y, f_z\}_i^T$ vectors respectively, and has the familiar form,

$$\mathbf{K}\mathbf{u} = \mathbf{f}, \quad (3)$$

where $\mathbf{K}$ is the stiffness matrix. The stiffness matrix $\mathbf{K}$ carries geometry and material parameters and when expression (3) has been derived by applying a standard finite element analysis (FEA) approach [8], then it can be expressed as,

$$\mathbf{K} = \sum_e \int_{V_e} \mathbf{B}_e^T \mathbf{C} \mathbf{B}_e dV_e, \quad (4)$$

where $\sum_e$ denotes the stiffness matrix assembly processes over all elements that the domain has been discretized into, $\mathbf{C}$ is the matrix form of Hooke's tensor, and $\mathbf{B}_e$ is the usual displacements to strain transformation matrix [8]. This transformation is expressed by,

$$\boldsymbol{\varepsilon}^e = \mathbf{B}_e \mathbf{u}^e, \quad (5)$$

where $\boldsymbol{\varepsilon}^e$ is the column array containing the components of strain of element e with its nodal displacements stored in the column array $\mathbf{u}^e$.

It is now a matter of simple array partitioning to collect to a subarray any quantities related to the system of Eq. (1) that may relate to quantities that can be potentially

measured by an experiment during for example a mechanical test of a material coupon or structural component. If displacements at discrete points can be measured then the solution of Eq. (3) can be used to collect the proper model predictions as a subset of the total column array $\mathbf{u}$ in order to compare them with the experimental values. With the advent of full field strain measurement techniques a similar approach would be followed to collect an array of strain component values predicted by the model at an observable subset of surface points of the structure. It is a matter of simple algebraic substitutions, to demonstrate that the strain components vector associated with an arbitrary point i shared by N_i elements that belongs onto the observable surface of the deformable body can be represented by,

$$\boldsymbol{\varepsilon}_i = \mathfrak{X}_e^{N_i} \left(\Phi_e \left\{ \left[\mathbf{K}^{-1} \mathbf{f} \right]_e \right\} \right), \quad (6)$$

where Φ_e represents the matrix transforming the apex nodal displacements to apex nodal strains and $\mathfrak{X}_e^{N_i}$ is an operator that returns some aggregate average of the contributions of all elements sharing the node and in the most common case can be considered to be described by the traditional averaging operator as $\mathfrak{X}_e^{N_i} = \frac{1}{N_i} \sum_e^{N_i}$. Furthermore $\left\{ \left[\mathbf{K}^{-1} \mathbf{f} \right]_e \right\}$ represents the collection of the displacement values of the nodes of element e into and appropriate vector. It should be noted that the inversion of $\mathbf{K}$ is usually implicitly realized through appropriate direct or iterative solvers. Alternatively, and after introducing Eq. (4) this relation can be written as,

$$\boldsymbol{\varepsilon}_i = \mathfrak{X}_e^{N_i} \left(\Phi_e \left\{ \left[\left(\sum_e \int_{V_e} \mathbf{B}_e^T \mathbf{C} \mathbf{B}_e dV_e \right)^{-1} \mathbf{f} \right]_e \right\} \right), \quad (7)$$

to indicate that the material parameters are inside $\mathbf{C}$. Furthermore systemic behavior is captured in Eq. (7) from the perspective of what is observable as a function of both the nature of the material (through the material parameters in $\mathbf{C}$) and the excitation on the system through the applied forces as they are represented in the vector $\mathbf{f}$.

2.2. Outline of the inverse problem

Alternatively, when the material parameters are not known, but experiments can be made to measure the response of the material system under controlled loading, then one faces the challenge of solving the continuous or discrete form of the equations

describing the behavior of the system inversely, aiming into the determination of the material parameters. This is the reason that the mathematical activity for achieving this is called inverse solution of the elastostatic problem, or material characterization.

When the form of the constitutive model is assumed to be known (in our case the constitutive model is that of linear anisotropic elasticity), the goal of material characterization is to calculate the values of the unknown constitutive parameters, which in the materials community are known as the constitutive properties. Decades of advances in force, displacement, and strain measurement techniques in general, and full-field strain measurement techniques in particular, have enabled the collection of very rich data sets from mechanical tests [9-19]. Having acquired these data, an integrated approach that combines experimental with numerical methods to recover the elastic parameters is very prevalent. With this strategy the elastic constants are recovered minimizing an objective function, expressing some vectorial measure of the distance (usually the L_2 norm) between the full experimental measurements and the corresponding analytical model predictions, via an iterative optimization procedure [1-5, 20-23]. Since the numerical model usually takes the form of a Finite-Element Analysis (FEA) that exploits the constitutive response of the model, this optimization procedure is computationally costly [6,23] as it essentially involves solving a form of Eq. (7) inversely to determine the material parameters embedded in $\mathbf{D}$.

In order to improve the computational efficiency of material characterization, alternative approaches have been developed. Virtual field methods [24,25] avoid the use of FEA simulation by finding virtual fields and inversely solving for parameters by substitution of full-field measurements. The weakness of this method is that it is limited to cases where such fields are derivable. Another recent technique utilized data acquired using the meshless random grid method (MRGM) [26]. This reduces the problem to that of finding the pseudoinverse of a matrix formed using the forward material model. Energy-based characterization methods using total and dissipated strain energy density determination [27, 28], that take advantage of the total potential energy [29] have also been demonstrated. Nonparametric constitutive models of anisotropic materials have also been used to identify elastic constants. The use of stochastic corrections to parameter estimates using Kalman filtering is shown in [30]. Another approach based on the

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Figure 2: Illustration of mixed numerical/experimental material characterization.

use of artificial neural networks [31] is presented in [32] and further demonstrated in [33]. As neural networks may be considered a physics-agnostic surrogate model, their utilization is most closely related to our earlier work utilizing NURBs-based surrogates [7].

In the present work we focus on the acceleration of the FEA-in-the-loop characterization approach (as opposed to defining a new method for characterization) as it is conceptually straightforward. Figure 2(a) illustrates this technique: a physical experiment produces an experimental dataset and is associated with a material system model (finite element or otherwise) of the tested specimen. From an initial state, an optimization algorithm iteratively adjusts this model until the model response matches the experimental data. Once this has been achieved, the model parameters are extracted and reported.

Our aim is to remove the computationally expensive combination of the FEM model with the constitutive model from the optimization loop and replace it with an efficient surrogate, as seen in Figure 2(b). Generally speaking, surrogate models are computationally efficient but physics-agnostic representations of more expensive physics-specific models which are generated by sampling the underlying model and subsequently fitting some functional form to the sampled data. They can also be conceptualized as a model of another model. This is the reason the term *metamodel* is frequently found in the literature, especially in the field of design engineering. We avoid the use of this term however, as it conflicts with an existing definition in the field of mathematical logic.

A wide variety of surrogate models exists. They can be broadly grouped into three families [34]:

- Geometric Models
 - Response Surface Models (RSMs) [35]
 - * Linear RSMs
 - * Quadratic RSMs
 - Spline Models
 - * Cubic Splines [36, 37]
 - * Non-Uniform Rational B-Splines (NURBs) [38]
 - * Multivariate Adaptive Regression Splines [39, 40]
- Stochastic Models
 - Kriging Models
 - * Geostatistical Kriging [41]
 - * Design and Analysis of Computer Experiments (DACE) Kriging [42]
 - Radial Basis Functions (RBFs) [43, 44]
 - * Single RBF Models
 - * Extended RBF Models

- Heuristic Models
 - Support Vector Machines [45]
 - Neural Networks [46, 31]
 - Frequency Domain Methods
 - * Fourier Series
 - * Wavelet Approaches

Rigorous comparisons of the different aspects of these surrogate modeling techniques are presented in [34, 47]. Generally, there are tradeoffs associated with the selection of a surrogate model type; for instance, a technique capable of approximating highly non-linear data may be more computationally expensive than other alternatives. In this work we use NURBs-based surrogates of material constitutive models composed with the shape of structural components. This choice is driven by the generality and computational efficiency of the NURBs formulation, as well as their established ability to represent non-linear black box functions. In the next section, we turn to the discussion of how these surrogate models are used to characterize materials.

3. Surrogate Characterization Methodology

Our approach proposes a composite material characterization methodology that employs a mixed experimental-numerical methodology. We assume a known model of the material system that operates over a physical domain $\Omega \subset \mathbb{R}^3$ (i.e. a test specimen), and we approach characterizing this system as the task of determining a set of independent constitutive parameters in $\mathbf{a}$ such that,

$$\mathbf{t}^e(\mathbf{x}_t, \mathbf{f}_t) + \boldsymbol{\epsilon}_e + \boldsymbol{\epsilon}_r = \mathbf{c}^e(\mathbf{a}, \mathbf{x}_c, \mathbf{f}_c) + \boldsymbol{\epsilon}_m, \quad (8)$$

where $\mathbf{t}^e$ is a vector field function that collects experimentally observed strain tensor components at a set of points $\mathbf{x}_t \in S_o \subseteq \Omega \subset \mathbb{R}^3$ and $\mathbf{c}^e$ is likewise a system model vector function of strain tensor components that can be given in discrete form by Eq. (7), which are functions of a constitutive model. The specimen's response is sampled at locations $\mathbf{x}_c \in S'_o \subseteq \Omega'$. The domain Ω' is the computational domain the system model evaluates into. The subdomains S_o and S'_o serve the purpose of providing an

optimization space for the inverse problem that is compatible with the capabilities of experimental measurement techniques. The parameters $\mathbf{f}_c$ dictate the specific loading of the test specimen. Given a well-designed experimental/numerical setup, it is reasonable to assume that $\forall \mathbf{x} \{ \mathbf{x} \in \Omega \Leftrightarrow \mathbf{x} \in \Omega' \}$ and hence $\mathbf{x}_t$ can be taken to coincide with $\mathbf{x}_c$. Similarly, the loading of the experimental and numerical forms can be considered to be approximately equal $\mathbf{f}_t \approx \mathbf{f}_c$. The terms ϵ_e , ϵ_r , and ϵ_m represent respectively systematic experimental errors, random experimental errors, and errors due to system model formulation. In a well designed experiment and a properly constructed computational system model, these errors should be relatively small in magnitude.

We note at the outset that $\mathbf{c}^e$ is typically computationally expensive to formulate and to evaluate. In some simple cases, analytical constitutive models are available, but $\mathbf{c}^e$ is more typically formulated via the solution of a FEA model. In order to achieve a more computationally efficient characterization, we introduce a surrogate model, $\mathbf{m}^e$, of the original strain response model $\mathbf{c}^e$ that involves the original constitutive model. Therefore, Eq. (8) becomes,

$$\mathbf{t}^e(\mathbf{x}_t, \mathbf{f}_t) + \epsilon_e + \epsilon_r = \mathbf{m}^e(\bar{\mathbf{a}}, \mathbf{x}_c, \mathbf{f}_c) + \epsilon_m + \epsilon_s \quad (9)$$

where $\bar{\mathbf{a}}$ are the approximated material parameters of the surrogate model and ϵ_s denotes additional error introduced by the surrogate model. Successful characterization depends on constructing $\mathbf{m}^e$ such that it

- represents $\mathbf{c}^e$ sufficiently well, i.e. ϵ_s is small;
- can be evaluated with minimum computational expense;
- is robust with respect to experimental noise in the sampling of $\mathbf{t}^e$, i.e. increases in ϵ_e or ϵ_r have little effect on the results produced;
- does not require *a priori* assumptions on the values of $\bar{\mathbf{a}}$ or the structure of $\mathbf{c}^e$.

If the physical experiment, underlying model, and surrogate model are all well designed, then all of the error terms will be small. Combined with the choice of common measurement locations, geometry and loadings between the experiment and model, Eq.

(9) can be expressed compactly as,

$$\mathbf{m}^\varepsilon(\bar{\mathbf{a}}, \mathbf{x}) \approx \mathbf{t}^\varepsilon(\mathbf{x}) \quad (10)$$

3.1. Definition of the Surrogate Model

The development and definition of the surrogate model are largely driven by experimental considerations. We assume that the test specimen is represented by a domain $\Omega \in \mathbb{R}^3$ with a surface boundary S . Since mechanical elements of physical test apparatus (e.g. the grips) typically do not permit experimental measurements on the entirety of S , we define the observable subset of $S_o \subset S$ as shown in Figure 1. The experimental measurement locations are thus restricted to $\mathbf{x} \in S_o$.

Because FEA based system models evaluate to a set of domain nodes we also assume that our sampling occurs on a discrete number of such points represented as vectors $\mathbf{x}_i \in S_o, i = 1 \dots n_m$. Consequently, our data consists of a set of n_m individual surrogate models, $\mathbf{m}_i^\varepsilon$, each of which approximates $\mathbf{c}^\varepsilon$ at a single point i represented by a vector $\mathbf{x}_i$.

$$\mathbf{m}_i^\varepsilon(\bar{\mathbf{a}}) = \mathbf{m}^\varepsilon(\bar{\mathbf{a}}, \mathbf{x}_i), i = 1 \dots n_m \quad (11)$$

The purpose of each of these surrogates is to generate a vector of scalars measurable at a point on the material specimen, that depend on the constitutive parameters. Since these surrogates are meant to replace actual models of the form given by Eq. (6) or Eq. (7), we have decided to use a full field strain measurement methodology and therefore, construct these surrogates to consist of the measured surface strain tensor components of the form,

$$\mathbf{m}_i^\varepsilon(\bar{\mathbf{a}}) = \left\{ {}^i_m \varepsilon_{xx}, {}^i_m \varepsilon_{yy}, {}^i_m \varepsilon_{xy} \right\}^T, i = 1 \dots n_m \quad (12)$$

Similarly, we define a set of experimental observations at corresponding locations,

$$\mathbf{t}_i = \mathbf{t}(\mathbf{x}_i), i = 1 \dots n_m, \quad (13)$$

where the individual observations $\mathbf{t}_i$ have the same form as $\mathbf{m}_i$,

$$\mathbf{t}_i = \left\{ {}^i_t \varepsilon_{xx}, {}^i_t \varepsilon_{yy}, {}^i_t \varepsilon_{xy} \right\}^T, i = 1 \dots n_m \quad (14)$$

While any of a number of well established interpolation techniques could be used to construct the functional relationship of $\mathbf{m}_i$ in this research we utilize NURBs. both [48]

and [49] are excellent references on the mathematics and development of these splines. NURBs are recursively defined parametric blended polynomials. The case of a single independent variable u is given by,

$$\mathbf{p}(u) = \frac{\sum_{i=1}^{n_c} \mathbf{b}_i w_i N_{i,k}(u)}{\sum_{i=1}^{n_c} w_i N_{i,k}(u)} \quad \text{for } u_{min} \leq u \leq u'_{max}, \quad (15)$$

where $\mathbf{b}_i$ is a vector defining the location of the i^{th} of n_c control points, w_i is a positive scalar weight associated with the i^{th} control point, and $N_{i,k}(u)$ is the B-spline basis function given as a parametric function of u . The parameter u defines a position along the curve length which is equivalent to a point on the curve defined by the vector $p(u)$. The B-spline basis function is a recursive function defined by,

$$N_{i,k}(u) = \left(\frac{u - x_i}{x_{i+k-1} - x_i} \right) N_{i,k-1}(u) + \left(\frac{x_{i+k} - u}{x_{i+k} - x_{i+1}} \right) N_{i+1,k-1}(u), \quad (16)$$

$$N_{i,1}(u) = \begin{cases} 1 & \mathbf{x}_i \leq u \leq \mathbf{x}_{i+1} \\ 0 & \text{otherwise} \end{cases} \quad (17)$$

where x_i is the i^{th} component of the knot vector $\mathbf{x}$, a monotonic sequence of parameter values defining the regions of influence of the control points within the NURBs curve. For the i^{th} control point that region of influence is defined by the curve order k . The B-spline basis functions are subject to,

$$0/0 \equiv 0 \quad (18)$$

$$\text{subject to } 2 \leq k \leq n_c \quad (19)$$

and therefore exhibit the property,

$$\sum N_{i,k}(u) \equiv 1 \quad \forall \quad k \text{ and } u. \quad (20)$$

The division of Eq. (18) is undefined, but it is used as a convenient method to prevent divide-by-zero errors in the implementation of NURBs-based software. It does not affect the validity of the NURBs curve as 0 over 0 occurs in the basis function definitions only when the basis function is inactive in the region queried [48]. In the present work, we take $k = 3$, which is to say that we use quadratic NURBs surrogates.

Figure 3: NURBs representations

A uniform knot vector is employed (see [48] for precise details on knot vector construction), which in the univariate case has the form $(0, 0, 0, 1, \dots, n_c, n_c, n_c)$ where n_c is the number of control points defining the surrogate. Uniform unitary weights are also applied, $w_i = 1$ for all i .

NURBs generalize to higher dimensions by use of a tensor product, for instance a NURBs surface of two variables has the form given by,

$$\mathbf{p}(t, u) = \frac{\sum_{i=1}^n \sum_{j=1}^m b_i w_i N_{i,k}(t) N_{j,k}(u)}{\sum_{i=1}^n \sum_{j=1}^m w_i N_{i,k}(t) N_{j,k}(u)} \quad \text{for} \quad \begin{matrix} t_{min} \leq t \leq t_{max} \\ u_{min} \leq u \leq u_{max} \end{matrix} \quad (21)$$

where m and n are the dimensions of the rectangular control point grid. Similarly, a NURBs object of 3 independent variables has the form given by,

$$\mathbf{p}(s, t, u) = \frac{\sum_{i=1}^n \sum_{j=1}^m \sum_{l=1}^v b_i w_i N_{i,k}(s) N_{j,k}(t) N_{l,k}(u)}{\sum_{i=1}^n \sum_{j=1}^m \sum_{l=1}^v w_i N_{i,k}(s) N_{j,k}(t) N_{l,k}(u)} \quad \text{for} \quad \begin{matrix} s_{min} \leq s \leq s_{max} \\ t_{min} \leq t \leq t_{max} \\ u_{min} \leq u \leq u_{max} \end{matrix} \quad (22)$$

In this case n , m , and v are the dimensions of a three-dimensional rectangular hexahedral control point lattice. A parametric NURBs function of one independent and two dependent variables is shown in Figure 3.

3.2. Construction of the Surrogate Model

The primary challenge of constructing each of the $\mathbf{m}_l^e$ in Eq. (11) is the construction of each of the individual NURBs-based surrogate models m^e such that they reproduce the behavior of $\mathbf{c}^e$ for a fixed load/geometry at a predetermined point. In order to do so, it is necessary to sample or evaluate $\mathbf{c}^e$ at combinations of values for the elements of $\mathbf{a}$. We use a space filling grid technique to sample $\mathbf{c}^e$: each element of $\mathbf{a}$ is varied in even increments between some minimum and maximum value. This technique does require *a priori* determination of upper and lower bounds of the constitutive parameters, but in practice these bounds are very loose and can span several orders of magnitude.

For each of the nodes $\mathbf{x}_i \in S_o$ the system model $\mathbf{c}$ is sampled for l combinations of the constitutive parameters $\mathbf{a}_q, q = 1 \dots l$. Depending on the dimensionality of the vector space of $\mathbf{a}$ this sampling can be performed on an 1D line a 2D planar grid, a 3D cubic lattice or a higher dimensional hyperrectangle lattice. This sampling results in a set of vector valued elements $\mathbf{s}_j(\mathbf{a}_k)$ that correspond to the response of $\mathbf{c}^e$ at a particular location on S_o with a predetermined combination of constitutive material parameters and loading conditions.

Once $\mathbf{c}$ has been sampled, there are several techniques which could be employed to fit the NURBs-based surrogate models to this data. We use a direct method which produces an exact interpolation of the acquired data. In the case where $\mathbf{a}_q \in \mathbb{R}^1$ (hence $\mathbf{a}_q = a_q$) this can be formulated as the solution to a set of simultaneous linear equations of the form,

$$\mathbf{s}_j(a_q) = \mathbf{m}_j(u_q) = \mathbf{p}_j(u_q) = \sum_{i=1}^{n_c} {}^j\mathbf{b}_i N_{i,k}(u_q), \quad j = 1 \dots n_m \text{ and } q = 1 \dots l \quad (23)$$

where ${}^j\mathbf{b}_i$ are the unknown control point locations. for the single variable case. The j^{th} surrogate model $\mathbf{m}_j$ is defined to be equal in value to the corresponding dataset $\mathbf{s}_j$ at each of the parametric coordinate values u_q . The values of u_q are chosen according the the values of a_q used to generate $\mathbf{s}_j$, and in a fashion so as that u_q takes on a range of $[0,1]$,

$$u_q = \left(\frac{a_q - a_{min}}{a_{max} - a_{min}} \right) \quad (24)$$

The system of equations defined in Eq. (23) can be extended to the multivariate case in the same manner shown in the progression from Eq. (15) to Equations (21) and (22). For instance, the two-variable case takes takes the form,

$$\mathbf{s}_j(\mathbf{a}_q) = \mathbf{p}_j(u_q, v_q) = \sum_{i=1}^n \sum_{l=1}^m j \mathbf{b}_i N_{i,k}(u_q) N_{l,k}(v_q), \quad j = 1 \dots n_m \text{ and } q = 1 \dots l \quad (25)$$

Once the linear system has been formed, it may be solved using any technique. Typically these systems are small; involving no more than a few thousand equations. The uniform grid sampling approach also avoids a numerical issue that can arise with other NURBs fitting methods; the “stacking” of control points at identical coordinates induces poor conditioning in the linear system. In this research we use routines built into the Mathematica computer algebra system to invert the linear system and fit the NURBs-based surrogates. For the interested reader, further information on the use of splines as interpolators can be found in [50-52], and some recent research into the use of NURBs for the same purpose can be found in [53-55]. At the conclusion of the fitting process, $\mathbf{m}_i^\varepsilon$ are expressed as a set of interpolating functions,

$$\{\mathbf{m}_1^\varepsilon(\bar{\mathbf{a}}), \mathbf{m}_2^\varepsilon(\bar{\mathbf{a}}), \dots, \mathbf{m}_{n_m}^\varepsilon(\bar{\mathbf{a}})\} = \{\mathbf{p}_1(\bar{\mathbf{a}}), \mathbf{p}_2(\bar{\mathbf{a}}), \dots, \mathbf{p}_{n_m}(\bar{\mathbf{a}})\} \quad (26)$$

3.3. Characterization by Optimization

As indicated earlier, the characterization process can be formed as an inverse problem that seeks to minimize the difference between the experimentally observed and computationally calculated strain tensor components on the surface of a specimen. Based on Eq. (10) such a problem can be formulated as,

$$\min h(\bar{\mathbf{a}}) = \int_{S_o} \|\mathbf{m}^\varepsilon(\bar{\mathbf{a}}, \mathbf{x}) - \mathbf{t}^\varepsilon(\mathbf{x})\| dS \quad (27)$$

However, we recall that $\mathbf{m}^\varepsilon$ decomposes into n_m surrogate models at particular locations i . If $\mathbf{c}^\varepsilon$ is built by a finite-element model as Eq. (7) indicates, then we take $\mathbf{x}_i$ to be the vectors that represent the nodal locations of that model that lie within S_o . If $\mathbf{c}^\varepsilon$ is built by a closed-form analytic solution, then $\mathbf{x}_i$ can be chosen arbitrarily, e.g. a radial pattern of samples on a plate-with-hole test specimen. Recalling the recasting of $\mathbf{t}$ from Eq. (13) and $\mathbf{m}$ from Eq. (26), the minimization problem of Eq. (27) can be

Figure 4: Visual demonstration of the characterization algorithm.

expressed in a discrete form as,

$$\begin{aligned} \min. \quad & f(\bar{\mathbf{a}}) = \sum_{i=1}^{n_m} \|\mathbf{p}_i(\bar{\mathbf{a}}) - \mathbf{t}_i\| \\ \text{s.t.} \quad & a_{\min_j} \leq \bar{a}_j \leq a_{\max_j} \quad \forall \quad j \in 1 \dots n_a \end{aligned} \quad (28)$$

where n_a is the number of constitutive parameters (i.e. $\bar{\mathbf{a}} \in \mathbb{R}^{n_a}$). Figure 4 demonstrates this algorithm in a visual fashion.

For the sake of generality, the minimization problem of Eq. (28) is unconstrained. It is conceivable that we could use constraints expressing certain properties of the material model that are known *a priori*. Examples of such relationships are those among the elements of the elasticity tensor which ensure that this tensor either exhibits a certain material symmetry or remains positive definite. However, in our case this is not necessary for two reasons. On one hand, $\mathbf{t}$ implicitly satisfies the positive definiteness of the elasticity tensor constraints because of the fact that the data used for its determination refer to the behavior of a system that exhibits a linear elastic response and therefore, the objective function effectively penalizes invalid combinations of $\bar{\mathbf{a}}$. This ensures that the minimum value of f corresponds to a valid combination of parameters, provided that $\mathbf{p}$ is sufficiently representative of $\mathbf{c}^{\mathcal{E}}$. On the other hand, we aim to

determine the unknown material parameters for the most general (and therefore unconstrained) case, prior to restricting the problem with *a priori* knowledge that may be valid from a physical perspective but computationally expensive and unnecessary.

The presence of experimental noise complicates efforts to analyze the properties of f . In practice, any reasonably powerful non-linear optimization routine can be employed. In the present research we have elected to use either simulated annealing [56, 57] or Nelder-Mead downhill simplex algorithms [58-60] which do not require derivative information. Before further discussion of the optimization procedure, it is important to discuss the experimental noise factor in greater detail.

3.4. Mitigating Experimental Noise

In the formulation of Eq. (9), we can now assume that the noise terms can be aggregated into a single error term ϵ , which will be considered to represent a random or pseudo-random Gaussian noise with a mean $\mu_\epsilon = \mathbf{0}$ and variance of s_ϵ . The Law of Large Numbers dictates that the mean $\bar{X}$ of n samples from a distribution X tends to μ ($\bar{X} \rightarrow \mu$) as $n \rightarrow \infty$ [61]. This implies that a sufficiently large n_m will reduce the effect of experimental noise.

This allows us to conclude that increasing the sampling of the experimental / analytical model pair will reduce the effects of experimental noise on the recovery of $\bar{\mathbf{a}}$. This could be achieved by using a finer mesh in the FEA constitutive model and sampling the experimental at the new nodal locations. However, the computational complexity of such additional sampling is above linear, due to the finite element formulation. There is another option for increasing sampling which maintains linear complexity, however. The surrogate model formulation of the characterization problem can be used to combine several experimental *frames* of data, each of which, features the same geometry, sampling locations, and underlying constitutive model, while a different loading is applied in each frame. This is shown in the following equation,

$$\begin{aligned} \min. \quad & f(\bar{\mathbf{a}}) = \sum_{i=1}^{n_m} \left(w_1 \|\mathbf{m}_{1,i}^\epsilon(\bar{\mathbf{a}}) - \mathbf{t}_{1,i}\| + w_2 \|\mathbf{m}_{2,i}^\epsilon(\bar{\mathbf{a}}) - \mathbf{t}_{2,i}\| + \dots \right) \\ \text{s.t.} \quad & a_{\min_j} \leq \bar{a}_j \leq a_{\max_j} \quad \forall \quad j \in 1 \dots n_a \end{aligned} \quad (29)$$

where w_n is a weight parameter associated with the n^{th} load case. There is no fundamental reason that Ω or $\mathbf{x}$ could not be varied between frames of data; although we do not do so in order to reflect typical automated test regimes. Specimens of identical geometry are tested under varying load cases, and the surface strains are computed in the same locations and compared to the same constitutive model. This also gives confidence in the assumption that $\epsilon_1 \approx \epsilon_2 \approx \dots \approx \epsilon_n = \epsilon$. The computational cost of combining experiments in this fashion grows linearly with the number of frames of data.

There is an additional benefit that is realized from the use of multiple load cases. For many strain response models it is often difficult to determine a single loading that produces a response which is sensitive to the values of all of the constitutive parameters. By allowing the combination of several or many load cases it is possible to make f sufficiently sensitive to the values of all of the constitutive parameters and hence avoid an ill-posed formulation [62]. Additionally, the premise of $\mu_\epsilon = \mathbf{0}$ can be tested by examining the minimal value of f . If $\min(f) \gg 0$ it is likely that one or more frames of data contain noise with $\mu_\epsilon \neq \mathbf{0}$ which may be the result of experimental bias, error in the formulation of $\mathbf{c}$, or poor representation by $\mathbf{m}$.

4. Verification with Numerical Experiments

To verify the functionality of the method proposed in the previous section we conducted a series of synthetic numerical experiments. Three experiments were conducted; the first case used an analytical model while the second and third used FEA models. These experiments were:

- An infinite plate of isotropic material with a round hole subjected to in-plane loading at infinity;
- An orthotropic composite material test specimen of plate-with-hole geometry subjected to multiaxial loading; and
- A finite anisotropic composite material specimen of double-notch geometry subjected to multiaxial loading

The details of each of these synthetic experiments are laid out in the sections below. In each case the primary goals were to establish the accurate recovery of constitutive parameters using our surrogate-based methodology, especially in the presence of experimental noise. Towards this end, the following procedure was employed:

1. Begin: build the surrogate model $\mathbf{m}_i^\epsilon$ of the constitutive model $\mathbf{c}_i^\epsilon$ as described in Section 3.2.
2. Generate a synthetic experimental data set $\mathbf{t}_i^\epsilon$ by running the full FEA or closed-form analytical solution model using reference values of the constitutive parameters as inputs.
3. Add noise to the synthetic experimental data set. The noise should be applied to the different responses (ϵ_{xx} , ϵ_{yy} , and ϵ_{xy}) independently, in a normally distributed fashion, with a mean $\mu_\epsilon = 0$ and a standard deviation s_ϵ .
4. Recover the parameters from the noisy experimental dataset using the optimization procedure outlined in Section 3.3.
5. Repeat steps 2-4 20 times in order to collect statistical data on the effect of experimental noise at a level of s_ϵ on the accuracy of the recovered constitutive parameters.
6. Increase s_ϵ . Repeat steps 2-5 until s_ϵ has reached a maximum value.
7. Terminate: plot the mean accuracy of each parameter's recovery as a function of s_ϵ .

Based on the existing physical apparatus available for automated multiaxial testing [6] we set an accuracy goal of parameter error not exceeding 2.5% in the presence of $s_\epsilon = 100\mu\epsilon$ (microstrain) noise. To verify that this goal was met we ran the synthetic experiments for $s_\epsilon = 0$ to $200\mu\epsilon$, in increments of $10\mu\epsilon$. The results of testing using this procedure are given in the following three sub-sections.

4.1. Infinite Domain Numerical Experiment for Isotropic Material

A well-known analytical solution of Eq. (1) in terms of the stress fields of an infinite isotropic material specimen with a hole is given by [26]. Figure 5 illustrates the domain, the coordinates and parameters used, as well as the sampling locations $\mathbf{x}_i$.

Figure 5: An infinite isotropic domain with a hole of radius a subjected to in-plane loading σ_∞ . Only a subset of the actual sampling locations x_T are shown.

Specifically, and according to [26], given some far-field stress σ_∞ the stress field is calculated in polar coordinates by,

$$\begin{aligned}\sigma_{\theta\theta} &= \frac{\sigma_\infty}{2} \left(1 + \frac{a^2}{r^2} - \left(1 + \frac{3a^4}{r^4} \right) \cos(2\theta) \right) \\ \sigma_{rr} &= \frac{\sigma_\infty}{2} \left(1 - \frac{a^2}{r^2} + \left(1 - \frac{4a^2}{r^2} + \frac{3a^4}{r^4} \right) \cos(2\theta) \right) \\ \sigma_{r\theta} &= -\frac{\sigma_\infty}{2} \left(1 + \frac{2a^2}{r^2} - \frac{3a^4}{r^4} \right) \cos(2\theta).\end{aligned}\tag{30}$$

The frame reference transformation from the polar to the Cartesian coordinate system is implemented by using the well known transform,

$$\begin{aligned}\sigma_{xx} &= \frac{1}{2} (\sigma_{rr} + \sigma_{\theta\theta} + (\sigma_{rr} - \sigma_{\theta\theta}) \cos(2\theta) - 2\sigma_{r\theta} \sin(2\theta)) \\ \sigma_{yy} &= \frac{1}{2} (\sigma_{rr} + \sigma_{\theta\theta} + (-\sigma_{rr} + \sigma_{\theta\theta}) \cos(2\theta) + 2\sigma_{r\theta} \sin(2\theta)) \\ \sigma_{xy} &= \sigma_{r\theta} \cos(2\theta) + (\sigma_{rr} - \sigma_{\theta\theta}) \cos(\theta) \sin(\theta).\end{aligned}\tag{31}$$

The strains are then computed from the stresses using the inverse form of Hooke's constitutive law as shown in (1b).

$$\boldsymbol{\varepsilon} = \boldsymbol{C}^{-1} : \boldsymbol{\sigma}\tag{32}$$

Table 1: Sampling data for the first numerical experiment

Parameter	True Value	Minimum value	Maximum Value	Sampling Increment
E	69 GPa	34.5 GPa	103.5 GPa	17.25 GPa
ν	0.333	0.2	0.8	0.15

which for the isotropic case takes the matrix form

$$\begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ 2\varepsilon_{yz} \\ 2\varepsilon_{xz} \\ 2\varepsilon_{xy} \end{bmatrix} = \frac{1}{E} \begin{bmatrix} 1 & -\nu & -\nu & 0 & 0 & 0 \\ & 1 & -\nu & 0 & 0 & 0 \\ & & 1 & 0 & 0 & 0 \\ & & & 2(1+\nu) & 0 & 0 \\ (sym) & & & & 2(1+\nu) & 0 \\ & & & & & 2(1+\nu) \end{bmatrix} \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} \quad (33)$$

This strain model was evaluated on 1600 locations $\mathbf{x}_i$ in a uniform radial pattern around the hole ($r = 1$), a subset of which are seen in Figure 5. The samples were taken with values of $\theta = 0$ to 2π in increments $\frac{\pi}{40}$ and $r = 1$ to 3 in increments of 0.1. A single frame of data was used, with $\sigma_\infty = 50\text{MPa}$. Table 1 shows data regarding the sampling of the constitutive parameters E and ν (Young's modulus and Poisson's ratio, respectively). The true parameter values in Table 1 reflect the properties of Al-6061-T6. With 1600 values of $\mathbf{x}_i$, at each of which the model of Equations (30-33) was evaluated at 25 combinations of constitutive parameter values, the constitutive model was evaluated 40,000 times in total. The experimental procedure of the previous section was applied, both the generation of the surrogate models and the subsequent optimization were performed on a computer with a quad-core Intel i7 processor and 16 GB of memory. A simulated annealing optimizer, built into the Mathematica computer algebra system, was used to recover the constitutive parameters. Generation of the surrogate models required less than 0.5 seconds of computation time in total, and recovering the parameters required, on average, 0.39 seconds for each trial. The accuracy of the elastic parameter recovery as a function of experimental noise is presented in Figure 6. The error quantity visualized in this figure, and subsequent figures, is

$$Error = 100 \left(\frac{|\mathbf{a} - \bar{\mathbf{a}}|}{a_{max} - a_{min}} \right) \quad (34)$$

Figure 6: Mean error in the recovery of constitutive parameters E and ν (plot markers) and the associated standard deviation (whiskers) as a function of noise level for the first numerical experiment.

where $\mathbf{a}$ and $\bar{\mathbf{a}}$ are the true parameter value and recovered parameter value, respectively. a_{max} and a_{min} are the maximum and minimum values of a used during the sampling to create the associated surrogate models, as in the discussion surrounding Eq. (24). Figure 6 clearly shows that the recovery of E is satisfactory even up to experimental noise magnitudes of $200 \mu\epsilon$. The error in ν is also acceptable at a noise magnitude of $100 \mu\epsilon$. However, given that this is the simplest test case possible, this result seemed relatively poor.

In order to improve this result two further steps were taken. The first step involved the adoption of a second optimization routine, the Nelder-Mead descending simplex optimizer [58-60]. This algorithm is both conceptually and computational simple, and there are only four parameters which must be determined to utilize it. The reflection (α), expansion (γ), contraction (β) and shrinkage (ρ) coefficients are typically assigned the values $\alpha = 1$, $\gamma = 2$, $\beta = \frac{1}{2}$ and $\rho = \frac{1}{2}$ [59]. Because of the relatively short time required to recover the constitutive parameters, we experimented with perturbations from these recommendations and evaluated performance gains in terms of the number of algorithm iterations required for convergence. We found that the recommended parameters performed sufficiently well, but a small decrease in optimization effort can be achieved with the adjustments $\beta = 0.6$ and $\rho = 0.6$. It is also well known that general non-linear optimization using the Nelder-Mead method requires a multi-start approach. In this case we used 50 starts of the optimization algorithm with randomly-generated initial simplexes in order to capture the global objective function minimum. For both

optimizers, the input variables were normalized to the range of $[0, 1]$ to eliminate any effects associated with the different scales of the unknown parameters.

In addition to adopting a second optimization routine, as a second step we employed the noise mitigation strategy outlined in Section 3.4. The density of sampling locations $\mathbf{x}$ was doubled in both the radial and angular dimensions in order to increase noise rejection. The surrogate models were constructed on this denser set of locations in the same fashion described previously. The results of applying both optimizers against both sets of surrogate models is given in Figure 7. These results indicate clearly that the optimizers produce results of roughly equivalent accuracy. Additionally, it is seen that the methodology for reducing the effect of experimental noise given in Section 3.4 is effective. The mean error in the recovery of ν is reduced to 2.55% at $200 \mu\epsilon$ of simulated noise. We also found that the normalization of the input variables had no effect on the results produced; the commercial optimizers employed are therefore performing such rescaling internally.

Generally, the computational performance of the Nelder-Mead optimizer is superior to that of the simulated annealing optimizer. For the dense set of sampling locations shown in Figure 7 the Nelder-Mead method required approximately $\frac{1}{3}$ the compute time of the simulated annealing method. For this reason, we maintain the use of the Nelder-Mead method in the remaining test problems.

Figure 7: Comparison of mean errors in the recover of E and ν , using both the Nelder-Mead (NM) and simulated annealing (SA) optimizers on the coarse (c) and fine (f) sets of surrogate models.

Figure 8: Geometry, layout, and mesh for the second numeric experiment. The inset shows detail of the central hole and composite layup. The different shades indicate lamina of different fiber orientation angles, as measured from the y-axis.

4.2. Finite Domain Numerical Experiment for Orthotropic Material

A more demanding numerical experiment was developed for a three-dimensional linear-orthotropic composite specimen. No analytical model was available to describe the strain fields on the surface of the specimen, thus we turned to a finite-element constitutive model of the specimen. Such a model has the property that it can capture strain states that may manifest in out of plane loading and hence depend on properties that are otherwise inactive in the constitutive law. In this case we used the ANSYS finite element code. A 8-node brick element (Solid185) was used for the finite element model. Figure 8 shows the test specimen geometry, composite layup, and finite-element mesh. In this case, the constitutive relationship which underlies the finite element analysis is again Hooke's law, which now has the matrix form,

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ & c_{22} & c_{23} & 0 & 0 & 0 \\ & & c_{22} & 0 & 0 & 0 \\ & & & \frac{c_{22}-c_{23}}{2} & 0 & 0 \\ (sym) & & & & c_{66} & 0 \\ & & & & & c_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{xz} \\ \epsilon_{xy} \end{bmatrix}, \quad (35)$$

Table 2: Sampling data for the second numerical experiment

Parameter	True Value	Minimum value	Maximum Value	Sampling Increment
c_{11}	6.8×10^{-6}	4.5×10^{-6}	8.0×10^{-6}	8.75×10^{-7}
c_{22}	9.71×10^{-5}	6.5×10^{-5}	1.0×10^{-4}	1.375×10^{-5}
c_{12}	-1.84×10^{-6}	-5.0×10^{-6}	-1.0×10^{-6}	1.0×10^{-6}
c_{23}	-2.67×10^{-5}	-5.0×10^{-5}	-1.0×10^{-5}	1.0×10^{-6}
c_{66}	1.4×10^{-4}	1.0×10^{-4}	4.0×10^{-4}	7.5×10^{-5}

where c_{11} , c_{22} , c_{12} , c_{23} , and c_{66} are the independent constitutive parameters which must be recovered through the surrogate model characterization process. The sampling data associated with these parameters are given in Table 2.

The true parameters listed in Table 2 reflect the properties of AS4/3506-1, a widely studied carbon/epoxy composite system. For this experiment two different surrogate models were built for two different loading cases, and two synthetic experimental datasets were produced using the real constitutive parameters. The loading for $\mathbf{m}_{1,i}$ was a tension load of 80 kN along the positive y-axis and an in-plane shear load of 9 kN along the positive x-axis. The loading for $\mathbf{m}_{2,i}$ was 200 kN compression load along the negative y-axis and a 2 kN out-of-plane shear load. Since the constitutive model consists of five parameters, there are 3125 parameter combinations which must be sampled, both for the construction of $\mathbf{m}_{1,i}$ and $\mathbf{m}_{2,i}$. The location vectors $\mathbf{x}_i$ were taken as the 1824 observable nodes on the surface of the finite-element model. As the finite element model takes roughly 3-5 seconds to run on the modest computing hardware used, several hours were required to produce the surrogate models. The Nelder-Mead optimizer described in the previous section was employed to recover the values of the constitutive parameters. On average this recovery required approximately 30 seconds.

We also performed several experiments to determine the effect of the relative values of the weights w_1 and w_2 (associated with the different frames of data) on the accuracy of the recovered constitutive parameters. The best results were achieved with $w_1/w_2 = 2$. The full results for this case are shown in Figure 9, in a manner analogous to that seen in Figure 6. The effect of the relative magnitudes of w_1 and w_2 are given in Table 3. The particular quantity reported in this table is the mean of the error in the five recovered constitutive parameters at an experimental noise level of $100 \mu\epsilon$. Although

Figure 9: Mean error in the recovery of constitutive parameters (plot markers) and the associated standard deviation (whiskers) for the second numeric experiment. Note that the dependent axis of each plot shows the level of experimental noise, in microstrain ($\mu\epsilon$).

the 2:1 mixing provides the best results by this metric, the variance between 4:1 and 1:1 is small, and indicates that the accuracy is not overly sensitive to the choice of weights. The ideal choice of 2:1 produces good results, with all parameters recovered within our target of 200 $\mu\epsilon$ of noise (excepting a_{23} which meets the target at up to 190 $\mu\epsilon$).

4.3. Finite Domain Double Notched Experiment with Damage

The primary goal of the final numerical experiment was to verify the function of the surrogate model characterization method on constitutive models which are not linear-elastic in nature and can account for strain-induced damage. To do so we consider a hyperelastic (or Green elastic) constitutive model, which has previously been used to

Table 3: The effect of w_1 and w_2 on the accuracy of constitutive parameter recovery

w_1/w_2	Error at $100\mu\epsilon$
4	0.71 %
3	0.62 %
2	0.62 %
1	0.97 %
0.5	1.53 %

characterize composite materials [6]. A finite strain formulation (FSF) is employed that is nonlinear from both the material and the geometrical perspectives, which can be expressed as an additive decomposition of volumetric (W_v) and distortional (W_d) strain energy density and it was introduced in [63], i.e.

$$U = (1 - d_v)W_v(J) + (1 - d_d)W_d(\bar{\mathbf{C}}, \mathbf{a} \otimes \mathbf{a}, \mathbf{b} \otimes \mathbf{b}), \quad (36)$$

with the damage parameters [64] $d_k \in [0, 1]$, $k \in [v, d]$ defined as,

$$d_k = d_{ka}^\infty \left[1 - e^{\left(-\frac{a_k(t)}{\eta_{ka}} \right)} \right], \quad (37)$$

where $a_k(t) = \max_{s \in [0, t]} W_k^o(s)$ is the maximum energy component reached so far, and d_{ka}^∞, η_{ka} are two pairs of parameters controlling the energy dissipation characteristics of the two components of the strain energy density (SED). In this formulation, $J = \det \mathbf{F}$ is the Deformation Gradient, $\bar{\mathbf{C}} = \mathbf{F}^T \mathbf{F}$ is the right Cauchy Green (Green deformation) tensor, $\mathbf{a}, \mathbf{b}$ are constitutive material directions in the undeformed configuration, and $\mathbf{a} \otimes \mathbf{a}, \mathbf{b} \otimes \mathbf{b}$ are microstructure structural tensors expressing fiber directions. Each of the two components of the SED are defined as,

$$\begin{aligned} W_v(J) &= \frac{1}{d}(J - 1)^2 \\ W_d(\bar{\mathbf{C}}, \mathbf{a} \otimes \mathbf{a}, \mathbf{b} \otimes \mathbf{b}) &= \sum_{i=1}^3 a_i(\bar{I}_1 - 3)^i + \sum_{j=1}^3 b_j(\bar{I}_2 - 3)^j + \sum_{k=1}^6 c_k(\bar{I}_4 - 1)^k + \\ &\quad + \sum_{l=2}^6 d_l(\bar{I}_5 - 1)^l + \sum_{m=2}^6 e_m(\bar{I}_6 - 1)^m + \sum_{n=2}^6 f_n(\bar{I}_7 - 1)^n + \\ &\quad + \sum_{o=2}^6 g_o(\bar{I}_8 - (\mathbf{a} \cdot \mathbf{b})^2)^o \end{aligned} \quad (38)$$

Figure 10: Geometry, layup, and mesh for the final numeric experiment. The inset shows detail of the notch-tips and composite layup. The different shades indicate lamina of different fiber orientation angles, as measured from the y-axis.

where the strain invariants are defined as follows,

$$\begin{aligned}\bar{I}_1 &= \text{tr} \bar{\mathbf{C}}, \quad \bar{I}_2 = \frac{1}{2}(\text{tr}^2 \bar{\mathbf{C}} - \text{tr} \bar{\mathbf{C}}^2) \\ \bar{I}_4 &= \mathbf{a} \cdot \bar{\mathbf{C}} \mathbf{b}, \quad \bar{I}_5 = \mathbf{a} \cdot \bar{\mathbf{C}}^2 \mathbf{b} \\ \bar{I}_6 &= \mathbf{b} \cdot \bar{\mathbf{C}} \mathbf{b}, \quad \bar{I}_7 = \mathbf{b} \cdot \bar{\mathbf{C}}^2 \mathbf{b}, \quad \bar{I}_8 = (\mathbf{a} \cdot \mathbf{b}) \mathbf{a} \cdot \bar{\mathbf{C}} \mathbf{b}.\end{aligned}\tag{39}$$

In this case there are seven constitutive parameters which must be recovered, denoted d , a_1 , b_1 , c_1 , e_1 , d_a^∞ , and η_a . Again, we employ the ANSYS finite element solver to exploit this constitutive model. The experimental geometry, composite material layup, and finite element mesh are shown in Figure 10. For this experiment, three different loading cases were used, as outlined in Table 4. We considered 1014 observable nodes of each frame for the location vectors $\mathbf{x}_i$. In this experiment there were $5^7=78125$ combinations of parameter values, which are summarized in Table 5. The FEA model required approximately 13 seconds to run, thus construction of the surrogate models required several weeks of computing time. Each of the frames of data was weighted equally ($w_1 = w_2 = w_3$) and recovery of the elastic parameters required approximately 120 seconds. The Nelder-Mead optimization routine described in the previous section was used without modification. The results achieved using this technique are given in Figure 11. The results of the hyperelastic numeric experiment are promising at low noise levels; very accurate recovery of the constitutive parameters can be achieved. However, these results break down and begin exhibiting excessive error at noise levels well below the target of $100 \mu\epsilon$. This, combined with the results of the previous two numeric experiments indicates that the surrogate-based characterization methodology

Table 4: Load cases for the hyperelastic numerical experiment, Forces (F) are in Newtons and moments (M) are in Newton-millimeters.

Frame	F_x	F_y	F_z	M_x	M_y	M_z
1	0	0	0	3000	10000	10000
2	0	-3000	0	3000	10000	10000
3	0	0	0	-3000	10000	10000

Table 5: Sampling data for the third numerical experiment

Parameter	True Value	Minimum value	Maximum Value	Sampling Increment
d	7.01×10^{-5}	5×10^{-5}	1.0×10^{-4}	1.25×10^{-5}
a_1	1.61×10^3	1.0×10^3	2.0×10^3	2.5×10^2
b_1	7.13×10^2	3.0×10^2	1.0×10^3	2.0×10^2
c_1	2.92×10^5	2.0×10^5	5.0×10^5	5.0×10^4
e_1	-4.59×10^2	-5.0×10^2	-2.0×10^2	7.5×10^1
d_a^∞	0.90	0.50	1.50	0.25
η_a	1.80	1.0	2.0	0.25

Figure 11: Mean error in the recovery of constitutive parameters (plot markers) and the associated standard deviation (whiskers) for the final numeric experiment. Note that the dependent axis of each plot shows the level of experimental noise, in microstrain ($\mu\epsilon$).

Table 6: Recovery of constitutive properties from physical test data. The reference values for the parameters are taken from [65], in engineering form.

	E_1 (GPa)	E_2 (GPa)	ν_{12}	ν_{23}	G_{12} (GPa)
Recovered	148.5	10.8	0.277	0.280	9.86
Reference	147.0	10.8	0.270	0.280	7.0

is theoretically sound, but still requires some practical improvements. This is discussed further in Section 6.

5. Validation with Physical Experiments

As a followup to the numeric experiments described in the previous section, we present some characterization results achieved using physical test data. An experimental campaign was carried out using the automated test system NRL66.3 [6] to characterize a series of AS4/3506-1 specimens. From this test campaign 20 frames of data were chosen, one per specimen. The frames were taken from the load-path history of each experiment at a point where linear-orthotropic responses were dominant. The constitutive model used for characterization was implemented in the ANSYS FEA code in a manner identical to that seen in Section 4.2, except for the use of double-notch specimen geometry (see Figure 10) and the associated stackuo sequence defining the composite layup angles. The Nelder-Mead optimizer implemented previously was employed here as well to recover the material constitutive properties. The results achieved from this process are shown in Table 6. These results indicate that the surrogate model based characterization can indeed be used to recover the anisotropic elastic properties of a composite from actual experimental data under realistic conditions. This was done despite the various sources of noise introduced in the data by camera sensor and electronics as well as the rest of the optical setup.

6. Conclusions

In this paper we have developed, verified and validated a technique for the characterization of composite materials which is based on the use of NURBs-based surrogate

models. The principle advantage of this technique is computational efficiency. By replacing the expensive constitutive model with an efficient surrogate in the optimization loop which drives the characterization process material properties can be recovered in seconds, as opposed to the hours or days previously required. We have also shown that the expense of building the surrogate models is a one-time expense, and that a single surrogate model can be used to characterize multiple material systems . Additionally, we have demonstrated that the NURBs-based surrogates offer a convenient method for data fusion, and allow the results from many experiments to be combined in order to achieve characterization. Finally, we have demonstrated that this algorithm meets our expectations of accuracy in the presence of experimental noise, and can also properly characterize physical specimens using data acquired during a robotic test campaign. We believe that the strength of these justifies further investigation into techniques for material characterization enabled by surrogate models.

6.1. Performance Comparison

In order to assess the merit of the surrogate-enabled characterization methodology, a performance comparison is warranted. Because the surrogate model construction process is expensive, but can then be used to characterize multiple specimens, we analyze the break-even point at which the surrogate model approach becomes more computationally efficient overall when compared to the traditional inverse approach with the full system model. This is defined as

$$\min [n_{be}] | n_{be} c_f > c_{sc} + n_{be} c_s, n_{be} \in \mathbb{Z} \quad (40)$$

where n_{be} is the number of specimens which must be characterized to break even in terms of computational effort, c_f is the cost of characterizing one specimen using the full system model, c_{sc} is the cost of constructing the surrogate models, and c_s is the cost of characterizing one specimen using the surrogate methodology. In the case of the 7-parameter hyperelastic experiment from Section 4.3, and taking computational runtime as the cost metric, $c_{sc} = 1015600$ seconds and $c_s = 120$ seconds. In a previous work [6], we found that $c_f = 104400$ seconds. Therefore $n_{be} = \lceil \frac{1015600}{104400-120} \rceil = \lceil 9.74 \rceil = 10$, where $\lceil \cdot \rceil$ is the ceiling operator. Given that even small experimental campaigns will

test more than ten specimens, and the campaigns associated with [6] tested more than a thousand specimens, this is strong evidence that the surrogate-enabled methodology has practical value.

6.2. Improvements and the Path Forward

The results of the numerical experiment involving a non-linear elastic material with damage that is traditionally modelled by using a finite strain formulation indicate that additional research is required in order to advance the techniques proposed in this paper. Although the material properties are recovered correctly in cases where experimental noise is small, the accuracy of recovered parameters decreases rapidly as experimental noise increases. This decrease in accuracy is much greater than that observed in the preceding simple numerical experiments involving the infinite isotropic and finite anisotropic elastic models. This could be indicative of several issues:

1. Insufficient sampling of the underlying constitutive model, either in terms of the physical space or the parameter space;
2. Applied loads which do not excite all of the material constitutive parameters, producing an objective function which is not sensitive to perturbations of these values;
3. Breakdown in the performance of the Nelder-Mead optimizer in higher-dimensional spaces;
4. Failure of NURBs to represent the non-linearity of the constitutive model.

We believe that the first two of these issues are the primary reasons for the relatively poor performance experienced in the hyperelastic numerical experiment. If the optimization algorithm was failing to converge in higher-dimensional spaces, we would expect to see parameter errors even in cases where experimental noise is small. Because of the general formulation of NURBs, and their proven ability to represent highly non-linear data, we do not anticipate that they are the culprit. We believe that the first issue, insufficient sampling, is driving the relatively poor performance seen for higher-dimensional constitutive models. The uniform grid scheme used to sample the parameter space is very inefficient in high dimensional cases, the cost of sampling increases geometrically with the number of parameters in the constitutive model. As a result,

limits on computation enforce sparse sampling which may not capture the response of the constitutive model. Furthermore, as it was evident in the case in the isotropic test problem, a small number of sample points in the spatial domain may be producing unacceptable sensitivity to experimental noise. Compounding these difficulties, the time required to produce the surrogate model is often extensive. This in turn limits the number of frames of data which can be considered, since a set of surrogate models must be built for each frame. This brings the second issue listed above to the forefront. It may well be the case that due to limitations on time and computational effort load cases which sufficiently excite all of the elastic parameters of the hyperelastic constitutive model with damage, have not been identified.

In order to redress the issue of sampling, we propose the adoption of adaptive sequential sampling techniques to build the surrogate models. These techniques, such as those of [53, 66] use various metrics in order to decide where to sample the underlying model based on the results of earlier samplings. They typically allow more efficient exploration and sampling of high-dimensional functions using fewer samples overall. Adoption of these methodologies will allow surrogates of higher-dimensional constitutive models to be constructed in an time-effective manner. Additionally, it may be beneficial to examine the use of different surrogate model formulations. As we outlined in Section 2 many well-developed surrogate model formulations are available, further investigation into which of these alternatives provide the best combination of computational performance and model fidelity is needed.

Another avenue for future research lies in the field of parallel computing. It is obvious from the form of Equations (28-29) that each of the individual surrogates could be constructed independently. Additionally, each term in the series of Eq. (28) or (29) can be calculated in parallel. Since there may be many thousands of values of $\mathbf{x}_i$, and the same number of individual surrogate models, highly parallel computing architectures may be utilized. We believe that General Purpose Graphics Processing Unit (GPGPU) computing [67] may be very useful in this capacity. The finely grained parallelism in this problem is well suited for GPGPU computing, and one of the original features of many GPUs is the efficient handling of NURBs using special hardware. The adoption of GPGPU parallel computing methodologies will reduce the time required

for material characterization significantly, allowing for more rigorous testing of greater numbers of specimens within a finite experimental budget. This may in turn improve the state of design using composite materials in diverse engineering fields.

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