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(U) Survey of DAKOTA's V&V Capabilities in the Simulation of Residual Stresses in a Simple Composite Structure

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Abstract

Process-induced residual stresses occur in composite structures composed of dissimilar materials. As these residual stresses can result in fracture, their consideration when designing composite parts is necessary. However, the experimental determination of residual stresses in prototype parts can be time and cost prohibitive. Alternatively, it is possible for computational tools to predict potential residual stresses. Therefore, a process modeling methodology was developed and implemented into Sandia National Laboratories' SIERRA/SolidMechanics code. This method can be used to predict the process-induced stresses in any composite structure, regardless of material composition or geometric complexity. However, to develop confidence in these predictions, they must be rigorously validated. Specifically, sensitivity studies should be completed to define which model parameters are critical to the residual stress predictions. Then, the uncertainty associated with those critical parameters should be quantified and processed through the model to develop stress-state predictions encompassing the most important sources of physical variability. Numerous sensitivity analysis and uncertainty quantification methods exist, each offering specific strengths and weaknesses. Therefore, the objective of this study is to compare the performance of several accepted sensitivity analysis and uncertainty quantification methods during the manufacturing process simulation of a composite structure. The examined methods include simple sampling techniques as well as more sophisticated surrogate approaches. The computational costs are assessed for each of the examined methods, and the results of the study indicate that the surrogate approaches are the most computationally efficient validation methods and are ideal for future residual stress investigations.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the assistance provided by Kevin Nelson and Brian Werner in procuring the validation test specimens and completing the residual stress measurements. The authors also gratefully acknowledge Ari Frankel for his technical expertise and guidance in the development of the surrogate models.

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1. INTRODUCTION

1.1. Technical Problem and Project Goals

Fiber-reinforced composite materials lend themselves to many modern structural applications. Materials such as these offer superior strength-to-weight and stiffness-to-weight ratios when compared to metals. However, when considering the utilization of composite materials, perhaps in place of a metal, unique and complex material behaviors must be considered. Specifically, given a composite structure's lamination and the global interaction of a composite's constituent components, interlaminar delamination, or the debonding of adjacent composite plies, is a mode of failure common to composites, but uncommon in structures composed of metallic materials. Therefore, the loading scenarios and material characteristics related to the potential for interlaminar delamination within fiber-reinforced composites must be well understood and accounted for during the structural design process.

One material phenomenon that has been observed to effect the delamination behavior of a laminated composite is the presence of manufacturing process induced residual stresses [1-2]. These residual stresses form during the elevated temperature curing cycles required of most composite material systems due to differences in the composite materials' coefficients of thermal expansion, as well as the shrinkage upon cure exhibited by most thermoset polymer matrix materials. While experimental methods can be used to quantify the post manufacturing stress state of a composite component, an experimental approach becomes less practical as the composite structure under examination becomes progressively more complex. As an alternative, validated computer simulations, which model the composite materials' elevated temperature cure cycles, can instead be used to predict the post-fabrication stress state of a composite part. This approach represents not only a cost and time savings when compared to physical experimentation, but it also presents the ability to understand the residual stress state in any structure, regardless of complexity.

In order for representative predictions of a post-fabrication stress state to be made, finite element methods, which sufficiently account for the physical changes undergone by a composite during its curing process, are necessary. Upon review of the existing literature, two common residual stress modeling approaches were found. The first method attempts to simulate the complete evolution of the composite material's mechanical properties functionally dependent upon the cure state. Specifically, both White, et. al., and Tavakol, et. al., present highly detailed modeling methodologies and constitutive models, which incorporate most of the physics relevant to the polymer curing process, including cure kinetics, polymer shrinkage, thermal strains, and the effect of the tool-to-part interface [3-5]. Alternatively, the second method observed in the literature for the simulation of a composite's curing process is much simpler, as all of a composite's fabrication processing details are accounted for through the experimental determination of the stress-free temperature, which is related to the temperature at which the polymerization reaction occurs. As discussed by Jumbo, et. al., Hanson, et. al., and Nelson, et. al., it can be assumed that a composite's final residual stress state depends only upon the composite materials' coefficients of thermal expansion (CTE) and thermal excursions from the stress-free temperature [6-8]. Interestingly, regardless of the modeling method's fidelity, the predictions associated with both the complex and simple finite element approaches discussed in literature were well validated experimentally.

Regardless of the complexity of the process modeling approach, many input parameters will be required to completely define the constitutive models and boundary conditions governing the predicted response. These parameters, which are generally related to the thermal and mechanical behaviors of the modeled composite material, can be determined experimentally. Although, as the number of required parameters for analysis increases and considering potential constraints in experimental budgets, facilities, and expertise, the complete physical characterization of the required input for a model can become prohibitive. Alternatively, sensitivity analysis methods can be used to understand which of a finite element model's required inputs are most influential to the final prediction. Then, experimental resources need only be expended in characterizing those critical parameters, while approximate values can be used to define the less influential model inputs. Examples exist in the literature demonstrating the value of parametric sensitivity studies in understanding various physical phenomena, particularly those related to composite materials. Namely, Radebe, et. al., and Daneshpayeh, et. al., demonstrated the use of sensitivity analyses in their studies of the effect of material property uncertainty on the performance of nanostructures and nano-composites [9-10], Vu-Bac, et. al., utilized a sensitivity analysis to assess the effect of uncertain material parameters on mechanical properties determined through multi-scale modeling [11], and Islam, et. al., utilized a sensitivity study in the process of optimizing manufacturing parameters for particleboards [12].

Furthermore, fiber-reinforced composite materials exhibit a significant amount of inherent material property variability. Since the majority of modern composite structures are in some part manufactured by humans and by hand, certain physical characteristics, such as void content, fiber volume fraction, ply thickness, and ply orientation, are uncontrollable, and small variations can have significant impact on the composite's elastic and fracture properties. Therefore, in order to properly validate a process model's predictions of a composite's post-fabrication residual stress state, this inherent material property variability must be considered. Examples exist in the literature demonstrating the value of uncertainty quantification techniques in the process of properly accounting for the effects of material property variability on the performance of composite structures. Particularly, Zhang et. al., demonstrated the negative effect that material porosity can have, due to the variability that such material inconsistencies can create in the composite's mechanical properties [13], and Nelson, et. al., presented an uncertainty quantification in the process of predicting the response of flexurally-loaded composite beams for which a complete material characterization was not possible [14].

Examples from literature have indicated that accurate predictions of a composite's post-fabrication stress state can be made with a simple approach, dependent only upon thermal expansion coefficients and the stress-free temperature, and that verification and validation methods can be applied in understanding the response of structures characterized by material variability. However, while there is certainty in the optimal approach for simulating the formation of process-induced residual stresses, there are many accepted sensitivity analysis and uncertainty quantification methods. These methods range in complexity, from very simple, such as Monte Carlo sampling, to very complex, such as a Polynomial Chaos expansion, and each technique offers unique trade-offs between computational cost and implementation difficulty. Therefore, the objective of this study is to assess the performance of several common sensitivity analysis and uncertainty quantification techniques considering the simulation of composite

residual stresses. It is desired that a validation procedure that is optimized for computational efficiency be defined for future simulations measuring the performance of fiber-reinforced composite structures.

1.2. Approach for Technical Work

As discussed in the preceding section, a composite structure's post-fabrication residual stress state must be considered during the structural design process due to the implications these stresses have on the potential for interlaminar delamination. Therefore, the simplified process modeling method, which was recommended by Hanson, et. al., and Nelson, et. al. [7-8], will be employed to simulate the residual stresses formed during the curing process of a bi-material, carbon composite/aluminum strip. Specifically, utilizing Sandia National Labratories' SIERRA/SolidMechanics code, the developed finite element approach will account for the formation of stresses within the bi-material strip immediately following the composite's birth during the polymerization reaction at elevated temperature, which are primarily due to differences in the composite and aluminum coefficients of thermal expansion.

Since the proposed modeling method requires the definition of many input parameters, sensitivity analyses will be completed to guide characterization efforts to only include the examination of the most critical parameters. Particularly, utilizing Sandia National Laboratories' DAKOTA toolkit, which provides an interface between the SIERRA/SolidMechanics simulation code and iterative analysis methods, a survey of several sensitivity analysis methods will be completed. Six of the sensitivity analysis methods available within DAKOTA will assess the criticality of the bi-material strip model's input parameters. The methods will include both simple techniques, such Monte Carlo and Latin Hypercube sampling, as well as more sophisticated approaches, such as a polynomial chaos expansion and a Gaussian process. The relative computational cost and critical parameter lists will be assessed in the process of recommending an ideal sensitivity analysis approach for future residual stress investigations.

Following the completion of the sensitivity study survey and the subsequent determination of the bi-material strip model's critical model parameters, a similar survey of DAKOTA's uncertainty quantification methodologies will be completed. As discussed in the preceding section, composite materials are characterized by inherent material property variability. Therefore, given a list of critical parameters, the expected uncertainty in those parameters must be determined and accounted for in predictions of the composite's performance. Likewise to the sensitivity study survey, five of DAKOTA's uncertainty quantification techniques will be examined that range in complexity from very simple to complex. The computational cost associated with each of the methods in determining a converged mean prediction will be determined and used to make a recommendation of the ideal validation procedure.

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2. VALIDATION EXPERIMENTS

A simple, yet representative, process-induced residual stress experiment was developed to provide validation data for a finite element model. Specifically, a bi-material, carbon composite/aluminum strip was developed that would exhibit post-fabrication residual stresses visually, through measurable deformations at ambient temperatures, and would also be efficient and low-cost to model. Bi-material strips were manufactured and their room temperature deformations were quantified for comparison with analysis.

2.1. Composite Strip Manufacturing

The bi-material strips were composed of a carbon fiber/epoxy composite, which consisted of an AS4C, 8-harness satin weave fabric pre-impregnated with a TCR 3362 resin, and 6063-T6 aluminum. These materials were selected for their dissimilar coefficients of thermal expansion, which guaranteed the development of significant and measurable residual stresses. Since the residual stresses developed within the structure would exist at the composite-to-aluminum interface, interlaminar delamination was a potential concern. As this type of fracture is difficult to quantify experimentally and capture in a finite element model, practical steps were taken during the composite manufacturing process to minimize the likelihood of delamination. Particularly, prior to the strips' manufacturing, the bonding surface of the plain aluminum was anodized and primed to promote bonding with the carbon composite. Then, a flat, uncured laminate of the composite material was placed on a rigid caul plate and the prepared aluminum strips were placed on top of the uncured laminate. The uncured composite then underwent a standard vacuum bagging process within an autoclave. Upon completion of manufacturing, excess carbon composite was removed from the edges of the aluminum strips with a combination of rough cutting on a vertical bandsaw and precision filing to the final desired dimension. Figure 2.1 shows a representative strip after manufacturing.

Figure 2.1: Manufactured bi-material strip

A total of three strips were prepared for testing and had in-plane measurements of 25.4 mm by 304.8 mm with an approximate thickness of 1.6 mm. This total thickness was comprised of the aluminum, which had an individual thickness of 0.8 mm, and a two-ply laminate of the carbon composite with a stacking sequence of $[0^o]_S$. A symmetric stacking sequence was purposefully chosen such that only the residual stresses developed at the strips' bi-material interface would need to be considered. Specifically, the symmetric composite laminate guaranteed that

unbalanced thermal strains would not develop within the laminate itself and contribute significantly to the measured residual stresses.

2.2. Residual Stress Measurement and Results

The manufactured bi-material strips were designed to exhibit significant residual stresses visually through physical deformation. As shown in figure 2.1, following a cooling cycle from the composite curing temperature to ambient conditions, significant out-of-plane warpage, or curling along the strip's length, was observed. Two primary mechanisms are thought to contribute to the development of this deformation. First, the carbon composite's and aluminum's dissimilar coefficients of thermal expansion lead to unbalanced thermal strains within the structure; and, second, polymer shrinkage creates an irreversible strain component in the composite during the curing process that is not recoverable upon re-heating.

To quantify the observed process-induced deformation, the strips were placed on a granite table and a digital height gage was used to measure the out-of-plane displacements at two locations along the strips' lengths (figure 2.2). The first out-of-plane displacement measurement was made at a location 152.4 mm from the strip's end, or at the strip's center. A total of three strips were measured and the range of deformation was recorded as 26.41 mm ± 0.21 mm. This measurement was meant to validate simulations of the full length strip during the uncertainty quantification methods survey. Alternatively, while consideration of the full length strip is practical for an uncertainty quantification, which generally requires hundreds of simulations, a shorter, less expensive strip geometry was desired for the sensitivity study survey, which was anticipated to require thousands of simulations. Therefore, a second out-of-plane displacement measurement was made at a location 50.8 mm from the end of one strip and was recorded as 15.4 mm. The difference in the two measured displacements, 26.41 mm versus 15.4 mm, is 11.01 mm, and this value approximates the center deflection of a shorter, 203.2 mm long strip, assuming the strip's radius of curvature is independent of its length. Note that limited experimental rigor (i.e., repeated measurements) was expended in determining the displacement value associated with the 203.2 mm long strip, since the sensitivity study survey was not an exercise in model validation. Rather, the qualitative nature of the experiment would simply be used to judge whether or not a nominal finite element model could currently capture the physical trend.

Figure 2.2: Experimental set-up to measure process-induced deformations

3. FINITE ELEMENT METHODS

To facilitate the survey of sensitivity analysis and uncertainty quantification methods, and to determine an ideal validation approach when considering the process modeling of composites, a finite element model of a structure exhibiting the phenomena of interest and optimized for computational efficiency was necessary. Therefore, utilizing the process modeling methods presented by [7-8], a computational model of the bi-material strip discussed in the previous section was created. Furthermore, as it was anticipated that the DAKOTA surveys would require a model to be processed thousands of times, a rigorous mesh study was undertaken to find the model discretization providing the best combination of cost effectiveness and accuracy.

3.1. Methods

3.1.1. Analysis Software

The bi-material strip simulations utilized Sandia National Laboratories' SIERRA/ SolidMechanics code, Adagio. Adagio is a Lagrangian, three-dimensional code for the finite element analysis of solid structures and is suitable for implicit, quasi-static analyses, such as these manufacturing process simulations. Adagio makes use of a multi-level solver, which is built upon a nonlinear, conjugate gradient algorithm that can iteratively find a solution that is within some user-defined tolerance of equilibrium. Use of the multi-level solver assists in the solution of problems, like the composite/aluminum strip, which models materials with non-linear responses or extreme differences in stiffness [15].

Also, DAKOTA was used to facilitate the sensitivity study and uncertainty quantification surveys. The DAKOTA toolkit provides a flexible and extensible interface between the SIERRA/SolidMechanics analysis code and iterative analysis methods. It specifically contains algorithms that may be used to exercise computational models in an iterative manner, such as with sensitivity analysis, uncertainty quantification, and gradient and non-gradient based optimization [16]. For the current study, DAKOTA was utilized to facilitate sensitivity and uncertainty studies based upon sampling, design of experiments, stochastic expansions, and parameter study methods.

3.1.2. Element Formulation

The bi-material strip model was simulated exclusively with eight-noded hexahedral elements. For efficiency, the element formulation default to Adagio was used. This formulation conducts the volume integration with single point Gaussian quadrature and, although it is computationally inexpensive, it exhibits zero energy, or "hourglassing," modes. However, a simple method of controlling this undesirable behavior is the application of a small elastic stiffness that can stop the formation of any anomalous modes without affecting the global response. Sierra Adagio is automatically equipped with a default "hourglassing" stiffness of 0.05 and this value was used in all of the completed analyses [15].

3.1.3. Material Models and Nominal Property Values

The bi-material strip model required the definition of three separate materials, the uncured carbon/epoxy composite, the cured carbon/epoxy composite, and the aluminum alloy, and these three materials were defined in simulation with just two materials models.

First, as no plastic deformation was expected for the aluminum, it was modeled with Sierra Adagio's elastic material model. This model describes a simple linear-elastic behavior and the only material properties required for its use are: a thermal strain function related to the material's coefficient of thermal expansion, Young's modulus, and Poisson's ratio [15]. Table 3.1 summarizes nominal material properties for the 6063 aluminum alloy [17].

Table 3.1: Elastic material properties of the aluminum alloys

Density, ρ (kg/m^3)	2,700
Young's Modulus, E (GPa)	68.9
Poisson's Ratio, ν	0.33
Coefficient of Thermal Expansion, CTE (1/ºC)	23.4e-06

Second, in the uncured state, the composite's epoxy matrix material can flow and its response is dominated by the adjacent aluminum component, which behaves isotropically. Therefore, the uncured carbon composite was modeled as a compliant and incompressible, isotropic-elastic solid with that same elastic material model used to define the response of the aluminum. Table 3.2 summarizes the properties defining the uncured composite material.

Table 3.2: Elastic material properties of the uncured composite

Density, ρ (kg/m^3)	1,600
Young's Modulus, E (GPa)	0.1
Poisson's Ratio, ν	0.499
Coefficient of Thermal Expansion, CTE (1/ºC)	23.4e-06

Lastly, the cured carbon composite material was defined with Adagio's elastic orthotropic material model, which simulates linear-elastic, orthotropic material behaviors without failure. The model's nominal parameter values, which are summarized in table 3.3, are related to the composite's elastic and thermal behaviors and were determined from a combination of tests and micromechanical representative volume models. Specifically, all in-plane elastic properties (E_{11}, E_{22}, G_{12}, and ν_{12}) were determined experimentally with methods based upon ASTM test standards D3039 and D3518. The out-of-plane properties (E_{33}, ν_{13}, ν_{23}, G_{13}, and G_{23}) were determined from micromechanical representative volume models of the composite, which are described in [18]. The thermal properties (T_g, CTE_{11}. CTE_{22}, and CTE_{33}) were determined with thermomechanical analysis experiments, and lastly, the stress-free temperature was determined with the experiment discussed in [8].

Table 3.3: Elastic orthotropic material properties for the cured composite

Density, ρ (kg/m^3)	1,600	
Elastic Moduli, E_{11}, E_{22}, E_{33} (GPa)	63.86, 62.74, 8.59	
Poisson's Ratios, ν_{12}, ν_{13}, ν_{23}	0.0480, 0.4075, 0.0548	
Shear Moduli, G_{12}, G_{13}, G_{23} (GPa)	3.44, 3.27, 3.25	
Glass Transition Temperature, T_g (ºC)	125.1	
Stress-Free Temperaure, T_{sf} (ºC)	128.8	
	Glassy Region	Rubbery Region
Coefficient of Thermal Expansion, CTE_{11} (1/ºC)	3.40e-06	1.13e-06
Coefficient of Thermal Expansion, CTE_{22} (1/ºC)	3.36e-06	1.13e-06
Coefficient of Thermal Expansion, CTE_{33} (1/ºC)	7.20e-05	2.83e-04

3.1.4. Model Geometry and Boundary Conditions

Three-dimensional geometries and discretized meshes were created for the bi-material strip (figure 3.1 show a representative geometry) using Cubit, which is a robust software toolkit capable of creating both two- and three-dimensional geometries and meshes. In the developed model, the aluminum and composite materials were modeled as separate, homogenized material layers with the dimensions specified in Section 2.1. As discussed, discretized models of strips with lengths of either 203.2 mm or 304.8 mm were created for use during the sensitivity study and uncertainty quantification surveys, respectively. Also, the strip models assumed symmetry along two planes for computational efficiency. As shown in figure 3.1, symmetry conditions were assumed across both the 13- and 23-planes.

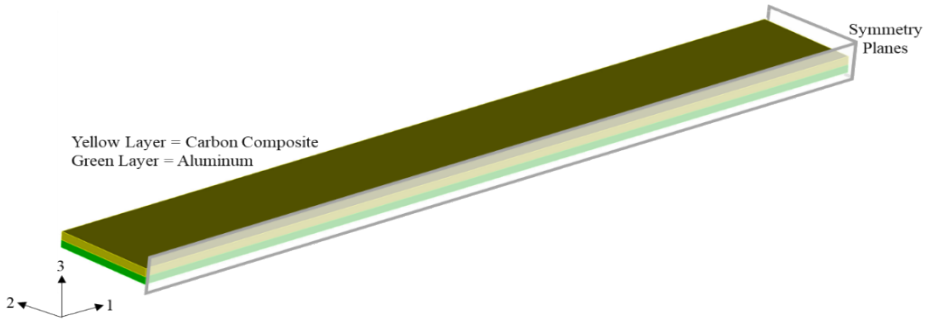

Figure 3.1: Bi-material strip model (shown without mesh lines)

In addition to symmetry conditions, boundary conditions were applied to simulate the composite's curing process, which included heating to and cooling from the stress-free temperature. Specifically, the complete simulation of the bi-material strip's curing took place in two steps. In the first step, the uncured composite was virtually heated from ambient conditions to the stress-free temperature to simulate the polymerization reaction conditions and, in the second step, the finished strip was virtually cooled back to room temperature to manifest the residual stresses. Details regarding this process of simulating a composite's curing process are provided in the following section.

3.1.5. Element Activation

The manufacturing process model of the bi-material composite strip simulates the matrix material's stiffness change during the polymerization reaction. This physical phenomenon is approximated within Sierra Adagio with element "activation," and the transferring of stress, strain, and displacement states between subsequent simulations. With these techniques, an initial simulation can be completed in which one or more component representing the uncured composite is modeled with very compliant material properties until a temperature indicative of the polymer's curing conditions is reached. Any component in this initial simulation modeled with the compliant properties will deform according to the non-compliant components without affecting the behavior of the stiffer parts. Once the specified temperature is reached, the simulation can be ended and stress, strain, and displacement data can be saved to an output file. Then, a new simulation can be performed in which the input geometry, displacements, and states of stress and strain are transferred from the output of the previous simulation. At the onset of this second simulation, the material parameters of the initially compliant parts can be set to their actual values, "activating" the previously compliant components and simulating the stiffness change undergone by a curing polymer.

The element activation process was applied to approximate the composite strip's manufacturing in two simulations. In the first simulation, the strip was virtually heated from ambient conditions to the stress-free temperature with the uncured composite's behavior defined with the properties given in table 3.2. Then, once the stress-free temperature was reached, this initial simulation ended and the stress, strain, and displacement states were written to an output file. Then, a second simulation was initiated with the input transferred from the previous simulation's output file. The boundary conditions applied in this second simulation virtually cooled the composite strip from the stress-free temperature back to the ambient conditions with the composite's behavior switching from compliant to stiff. Table 3.4 provides a detailed description of the material properties and boundary conditions defining the two simulations of the composite strip's manufacturing process. Refer to [8] for a detailed description of the element activation process, as well as discussion regarding the stress-free temperature and its determination.

Table 3.4: Summary of composite strip manufacturing process simulations

Simulation #	Components Modeled with Actual Material Properties	Components Modeled with Compliant Material Properties	Applied Temperature Boundary Conditions
1	Aluminum Layer	Composite Layer	Heating from 20ºC to 128.8ºC
2	Aluminum Layer, Composite Layer	None	Cooling from 128.8ºC to 20ºC

3.2. Mesh Convergence Study and Nominal Model Validation

As it was anticipated that the planned sensitivity and uncertainty studies would require the bi-material strip model to be processed many times, an efficient mesh was desired. Therefore, a mesh convergence study was completed considering not only the effect of a hexahedral element's size on the simulated predictions, but also the effect of the element's aspect ratio. Particularly, the mesh study was undertaken to verify the analysis methods described in the

preceding sections, as well as to determine the maximum permissible element size and aspect ratio that could confidently be used during the sensitivity study and uncertainty quantification simulations.

Richardson's extrapolation, which is an extrapolation based error estimation technique, was used to form an approximation of a higher order estimate of the model's continuum solution given a series of lower order, discrete solutions [19-20]. As shown in equation 1, with this technique, a discrete solution, f_k, can be thought of as the exact solution plus some error terms:

$$f_k = f_{exact} + g_1 h_k + g_2 {h_k}^2 + g_3 {h_k}^3 + \cdots \quad (1)$$

Where g_i represents the i-th term error coefficient and h_k represents a measure of the grid spacing, or element size. Then, if a second order method is assumed ($g_1 = 0$) for the above equation and if the discrete solutions exist for at least two different mesh sizes, the above equation can be solved for the exact, or continuum, solution with equation 2:

$$f_{exact} \approx f_1 + \frac{f_1 - f_2}{r^2 - 1} \quad (2)$$

Where r is the ratio of grid sizes, ${}^{h_2}/_{h_1}$, and f_k represents the two discrete solutions. Then, the Richardson extrapolation given by the above equation can be generalized for any p-th order method (equation 3):

$$f_{exact} \approx f_1 + \frac{f_1 - f_2}{r^p - 1} \quad (3)$$

In equation 3, p is the order of convergence, or the order of accuracy, and it is related to the behavior of the solution's error. Given at least three solutions corresponding to three different mesh sizes, the value of p can be estimated through the solution of equation 4, in which r is again the ratio of discrete solution mesh sizes and ε_{ij} represents the differences in the discrete solutions, or f_i-f_j.

$$\frac{\varepsilon_{23}}{r_{23}^p - 1} = r_{12}^p \left(\frac{\varepsilon_{12}}{r_{12}^p - 1} \right) \quad (4)$$

Following the above described process, the geometry shown in figure 3.1 representing the 203.2 mm long strip was discretized with three uniformly refined mesh sizes, 0.88 mm, 0.44 mm, and 0.22 mm, as well as three different aspect ratios, 1:1:1, 1:2:2, and 1:4:4. The resulting 9 models were processed with the finite element methods discussed in the preceding sections. Figure 3.2 shows a representative portion of the three model discretizations associated with the coarsest element size, 0.88 mm, and the three different aspect ratios.

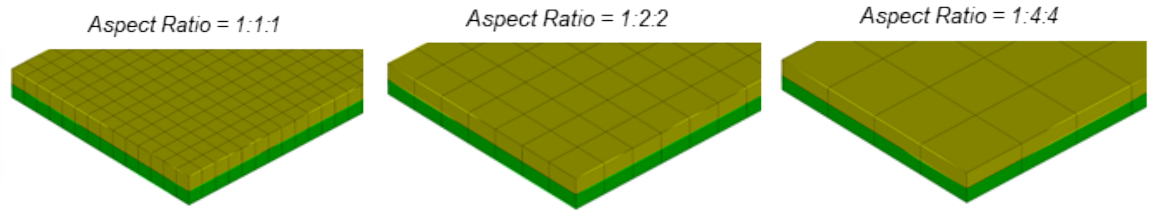

Figure 3.2: Representative mesh convergence study models

The metric upon which mesh convergence was measured was the peak out-of-plane displacement observed at ambient conditions. The three aspect ratios were considered as three separate mesh convergence studies, each consisting of three uniformly refined meshes (0.22 mm, 0.44 mm, and 0.88 mm), and three Richardson's extrapolated exact solutions were found. These continuum solutions, as well as the associated discretization errors (equation 5) and required computational solution times, are presented in table 3.5.

$$discretization\ error = \frac{f_{exact} - f_k}{f_{exact}} \cdot 100 \tag{5}$$

Table 3.5: Mesh convergence study results

Aspect Ratio	Mesh Refinement Level	Run Time (min) /Solution Cores	Predicted Deflection (mm)	Error (%)	Exact Solution (mm)
1:1:1	Coarse	01:14.3/1	14.02	20.2	11.666
	Medium	04:51.7/4	12.16	4.3	
	Fine	24:32.7/36	11.77	0.9	
1:2:2	Coarse	00:33.7/1	12.75	9.4	11.652
	Medium	01:04.4/4	11.90	2.2	
	Fine	03:24.3/36	11.71	0.5	
1:4:4	Coarse	00:25.2/1	9.33	20.3	11.702
	Medium	00:40.1/4	10.94	6.5	
	Fine	00:59.7/36	11.46	2.1	

As shown in table 3.5, the extrapolated exact solutions corresponding to the three aspect ratios do not differ significantly from each other, indicating that a ratio as great as 1:4:4 could safely be used with a reasonable expectation of model accuracy. However, when also considering solution time, required computational resources, and the discretization error, the medium mesh size associated with the 1:2:2 element aspect ratio seems to offer the best combination of computational efficiency and model accuracy. Particularly, this discretization level provided the lowest discretization error, 2.2%, with fewer than 36 solution cores; and it was selected for the sensitivity study survey. Alternatively, the fine mesh size associated with the 1:2:2 element aspect ratio was selected for use during the uncertainty quantification methods survey. This refinement provided the lowest discretization error of the nine examined models, 0.5% and, since uncertainty quantification is an exercise in validation and is assumed to require fewer simulations than the sensitivity study survey, the selection of a computationally more expensive model is justifiable.

Before undertaking any further analyses, the accuracy of the selected discretizations' predicted deformations, 11.90 mm and 11.71 mm, was assessed. Given the experimental discussion provided in Section 2, the magnitudes of the predicted out-of-plane displacements and the simulated shape of deformation (figure 3.3) agree well enough with the physical observations (figure 2.1) to assume that the model represents the physics of the curing process, and this permits the sensitivity and uncertainty surveys.

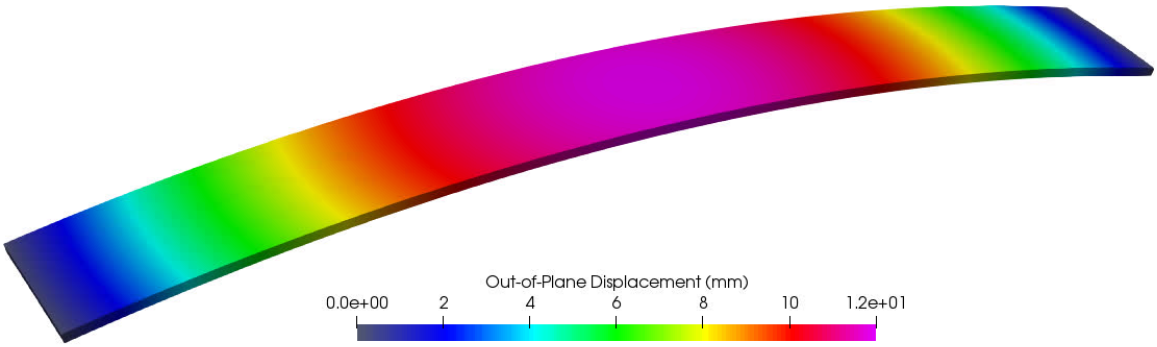

Figure 3.3: Nominal composite strip model prediction

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4. SENSITIVITY ANALYSIS METHODS SURVEY

As discussed in the preceding sections, the aluminum and cured composite material properties presented in tables 3.1 and 3.3 were determined from a combination of experimentation, computational methods, and literature survey. Hence, the characterization of the modeled materials is only approximate. The inexactness of the material descriptions, particularly in those parameters determined through micromechanical modeling or from literature, require an assessment of uncertainty that can be processed through the finite element model and accounted for in the final prediction. However, given sparse experimental resources, the rigorous characterization and uncertainty quantification of each of the 20 parameters described in the tables is not practical. Therefore, in an effort to prioritize characterization activities, sensitivity surveys were completed to understand which of the model parameters most significantly affect the simulated response.

Many sensitivity study methods exist, offering potential benefits and trade-offs related to computational complexity and cost. Therefore, utilizing the mesh optimized bi-material strip model discussed in the preceding section, a survey of several of DAKOTA's sensitivity analysis methods was completed to understand, first, which of the strip's model parameters most profoundly affect the residual stress predictions and, second, to determine the most effective sensitivity analysis approach when considering the process modeling of composites. Specifically, six common sensitivity analysis methods available within DAKOTA were exercised. The selected methods were of four types: parameter studies, design of computer experiments, sampling methods, and surrogate methods. These methods are discussed in detail in the ensuing sections.

After the sensitivity analysis methods of interest were selected. Plausible minimum and maximum values for each of the parameters of interest were specified, such that the explored parameter space could be bounded by realistic minimum and maximum values. Therefore, engineering judgement was used to created upper and lower values for each of the model parameters described in tables 3.1 and 3.3, with the nominal values provided in these tables acting as the means of the specified ranges. As an example, most of the ranges associated with the composite material were based on the mean value plus-or-minus three times the experimental or modeled standard deviation, and the ranges for the aluminum properties were taken as the provided average plus-or-minus some percentage of the mean value, such as 20%. These ranges are given in table 4.1. Provided the data described in this table, the developed parameter space was sampled according to the six different sensitivity analyses methods. Upon completion of the survey, the primary metric that was used to compare the methods was the minimum number of samples necessary to provide a converged list of critical model parameters, which was determined via a multiway analysis of variance (ANOVA) [21].

4.1. Sensitivity Analysis Methods

Six of DAKOTA's sensitivity analysis methods were analyzed to determine the most efficient sensitivity analysis approach when considering the process modeling of composites and predictions of a bi-material strip's residual stress driven, out-of- plane displacement. The examined methods include a centered parameter study, a Box-Behnken design of computer experiments, both Monte Carlo and Latin Hypercube sampling, and two surrogate methods, a polynomial chaos expansion and a Gaussian process.

Table 4.1: Model parameter ranges sampled during sensitivity studies

	Parameter	Minimum Value	Maximum Value
Composite Properties	E_{11} (GPa)	57.5	70.2
	E_{22} (GPa)	56.5	69.0
	E_{33} (GPa)	7.7	9.4
	ν_{12}	0.043	0.053
	ν_{13}	0.367	0.449
	ν_{23}	0.367	0.448
	G_{12} (GPa)	3.1	3.8
	G_{13} (GPa)	2.9	3.6
	G_{23} (GPa)	2.9	3.6
	T_g (ºC)	110.9	141.8
	T_{sf} (ºC)	140.6	146.1
	CTE_{11} (1/ºC, rubbery)	0.294e-6	1.913e-6
	CTE_{22} (1/ºC, rubbery)	0.357e-6	2.794e-6
	CTE_{33} (1/ºC, rubbery)	268.1e-6	290.9e-6
	CTE_{11} (1/ºC, glassy)	3.060e-6	3.708e-6
	CTE_{22} (1/ºC, glassy)	2.585e-6	4.165e-6
	CTE_{33} (1/ºC, glassy)	67.8e-6	76.5e-6
Aluminum Properties	E (GPa)	57.0	85.6
	ν	0.264	0.396
	CTE (1/ºC)	18.7e-6	28.1e-6

4.1.1. Parameter Study Method

A single parameter study method was selected for consideration, a centered parameter study. While DAKOTA has the capability for centered, multi-dimensional, and vector parameter studies, the centered approach is much less computationally expensive than the multi-dimensional method, which is full factorial, and it can quantify the relationship between multiple input parameters and a simulated response, while the vector parameter study is generally only used for single-coordinate parameter studies.

DAKOTA's centered parameter study (CPS) executes multiple coordinate-based parameter studies, one per input parameter, centered about a specified set of initial values. Specifically, DAKOTA treats each of the parameter space's dimensions independently, as "steps" are taken along each of the parameter space's orthogonal directions, thereby varying each parameter one-at-a-time. For example, considering a two-dimensional parameter space, beginning with the initial value set, "steps," and their corresponding simulations, are processed along the first parameter's dimension in the parameter space, while the value defining the second model parameter is held constant. Then, "steps" are processed along the second parameter's dimension, while the value defining the first parameter is held constant at its initial value. This process

creates two, independent parameter studies, one for each of the model's input parameters, centered at the initial point of interest [16].

To generate a centered parameter study within DAKOTA, four variables must be defined: the model parameters to be varied, the initial value set, the "step" size to be taken along each of the parameter space dimensions, and the number of steps to be taken in each dimension. Equation 6 represents the number of samples required for a centered parameter study as a function of the parameter space size and the "step" size.

$$Samples_{CPS} = 1 + 2\sum_{i=1}^{s} n_s \tag{6}$$

Where: s= Number of steps along each dimension
n= Number of dimensions, or parameters

For the centered parameter study of the bi-material strip, the model parameters of interest were as described in table 4.1, and the initial value set was specified as the nominal properties provided in tables 3.1 and 3.3. The number of "steps" taken in each of these dimensions was incrementally increased, starting with a value of one, until a converged list of critical model parameters was found with the ANOVA. Regarding "step" size, the parameter values were systematically increased, or decreased, so that the maximum, or minimum, parameter value, as shown in table 4.1, was reached by the final step in each direction of the model's 20 dimensions.

4.1.2. Design of Computer Experiments

One classical design of experiments method was selected for consideration in this study, Box Behnken Design (BBD). Although DAKOTA has the capability for other computer experiment designs, the BBD approach has a highly stable sampling scheme, as it does not sample outside of the defined parameter space, and it generally requires fewer overall samples to develop trends between the model input parameters and the simulated output when compared to other similar methods (e.g., centered composite design). Specifically, equation 7 describes the number of samples required for BBD as a function of the parameter space size.

$$Samples_{BBD} = 1 + 2k(k-1) \tag{7}$$

Where: k= Number of dimensions, or parameters

To generate a Box Behnken design within DAKOTA, three, equally spaced levels must be defined for each of the model variables, or parameters, of interest. These three levels, which generally correspond to a parameter's minimum, maximum, and mean values, define the edges and center of the process space. Then, BBD systematically creates parameter combinations at the center and midpoints of the resulting process space's edges. Figure 4.1 graphically depicts a three-dimensional parameter space and the 13 parameter combinations making up its Box Behnken design [22].

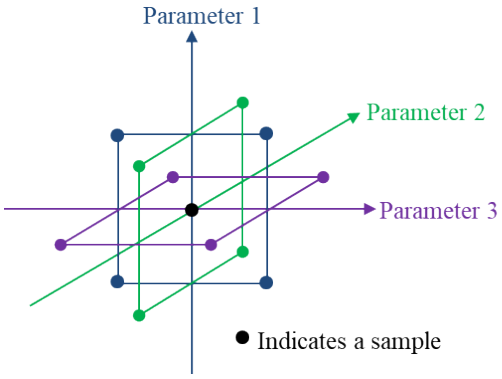

Figure 4.1: Sample Box-Behnken parameter space

For the BBD sensitivity study of the bi-material strip, the parameter space was defined with the 20 model variables described in table 4.1. The three levels required for each of the parameters were taken as the minimum and maximum values provided in table 4.1, as well as the mean, or nominal, values for each variable as given in tables 3.1 and 3.3. The corresponding 20-dimensional parameter space was sampled through BBD and the resulting 761 parameter combinations generated 761 simulated predictions, which were processed through an ANOVA to determine the critical parameter list.

4.1.3. Sampling Methods

Two sampling methods were examined as part of this sensitivity analysis survey: Monte Carlo sampling and Latin Hypercube sampling. The Monte Carlo approach was selected for consideration as it is simple and relatively easy to implement into different analysis codes. Alternatively, while Latin Hypercube sampling is slightly more technically complex, it represents a stratified sampling technique and provides more complete coverage of the process space with fewer samples than Monte Carlo.

4.1.3.1. Monte Carlo Sampling (MC)

The Monte Carlo approach represents purely random sampling. Therefore, all that is required for its use within DAKOTA is the parameter space to be sampled and the number of desired samples. Although MC is simple, because it is completely random, there is no guarantee that any number of samples will fully cover a parameter space. As a result of this uncertainty, MC methods can require a prohibitive number of samples before model convergence is demonstrated [16].

To generate a Monte Carlo based sensitivity study for the bi-material strip model, a process space was first defined with the parameters given in table 4.1 along with their minimum and maximum values. The resulting process space was initially sampled 22 times, and then, the number of samples was systematically doubled until a convergent list of critical model parameters was found through the ANOVA.

4.1.3.2. Latin Hypercube Sampling (LHS)

Unlike the Monte Carlo approach, which is completely random, LHS is a stratified sampling technique. Specifically, given a desired number of samples, *N*, the ranges defined by the

minimum and maximum values for each of a model's input parameters are divided into *N* segments of equal probability. The relative "length" of each of these segments is determined by the probability distribution describing each of the model parameter's ranges. For example, material parameters defined with uniform distributions will feature segments of equal length, while normal distributions will result in smaller, more densely spaced segments near the mean and wider, sparser segments near the tails of the distribution. Then, given a segmented, or grid-like, parameter space, the *N* desired samples can be randomly placed within the grids. However, with LHS, the samples are placed within the grids, or bins, of the process space in such a fashion that one, and only one, sample is placed in each bin [16]. This sampling technique guarantees more complete and uniform coverage of the process space, given a set number of samples, when compared to MC methods. This process of creating bins and selecting samples is graphically shown in figure 4.2 for a two-dimensional parameter space subjected to four samples.

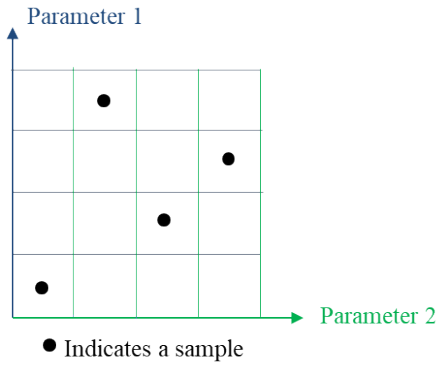

Figure 4.2: Example Latin Hypercube sampling scheme

To develop an LHS based sensitivity study with the bi-material strip model, a process space was defined with the 20 material parameters described in table 4.1, and, for each of the 20 variables, a uniform distribution was defined ranging between the provided minimum and maximum values. The resulting process space was stratified and initially sampled 22 times. The number of samples was then systematically doubled until a convergent list of critical model parameters was found through the ANOVA.

4.1.4. Surrogate Methods

Two commonly utilized surrogate modeling methods were selected for consideration: polynomial chaos expansion (PCE) and Gaussian process (GP). With a surrogate method, a parameter space is sampled a minimum number of times in the process of finding a numerical function, or surrogate model, that defines the relationship between the desired model output and the design variables. Then, once a surrogate model has been defined and validated, it can be evaluated thousands of times over a process space with a negligible computational cost.

4.1.4.1. Polynomial Chaos Expansion (PCE)

A polynomial chaos expansion (PCE) represents a stochastic expansion method, which forms an approximation, or surrogate model, of the functional relationship between a response function and its random inputs. PCE specifically employs multivariate orthogonal polynomials that are tailored to represent the specific input parameter distribution types. As an example, in

DAKOTA's implementation of PCE, Hermite and Legendre polynomials are applied to normal and uniform parameter distributions, respectively. The coefficients of these polynomials can be evaluated using either a spectral projection approach, such as with Smolyak sparse grid quadrature, or with a regression, such as with the least squares approach [16]. Spectral projection approaches are preferred, as they best represent high-dimensional functions, but the number of samples required by these methods to develop a surrogate increases exponentially with the dimension of the parameter space. Therefore, sparse grid quadrature can become prohibitively expensive when considering greater than four model parameters. Alternatively, while regression approaches are perhaps more ambiguous, requiring the definition of both the desired polynomial order and a set of response functions to which a regression can be fit, they are computationally less expensive. Specifically, by systematically varying the user-defined polynomial order and response function set size, a converged surrogate can be found with minimal sampling of the parameter space.

In order to build a PCE surrogate for the bi-material strip model and its 20-dimensional parameter space, the regression approach for approximating the polynomial's coefficients was applied. Specifically, 21, or $n+1$, LHS samples of the parameter space were processed through the composite strip model to develop a set of response functions to which a regression could be fit. Then, polynomials of orders one through five were fit to the response function data with cross-validation methods determining the most appropriate polynomial order. Particularly, with cross-validation, 90% of the response function data is used to generate the surrogate and the remaining 10% of data is used to test, or validate, the surrogate. Next, once a surrogate was built and validated, it was subjected to 10000 samples of the parameter space, and the ANOVA was applied to the resulting 10000 surrogate evaluations to develop a critical parameter list. This process of building a response function set, creating and validating a surrogate, and processing 10000 function evaluations through an ANOVA was repeated with increasing response function set sizes until a converged list of critical parameters was found. The response function set size corresponding to the surrogate providing the converged critical parameters list was the metric for comparison with the other considered sensitivity analysis techniques.

4.1.4.2. Gaussian Process (GP)

Alternatively, a surrogate built upon a Gaussian process (GP) utilizes a Gaussian correlation function with parameters that are selected via a Maximum Likelihood Estimation (MLE), which is simply a method of estimating the parameters of a statistical model, given several observations, or function evaluations. A fundamental aspect of a Gaussian process is that all of the finite dimensional distributions must have a multivariate normal, or Gaussian, distribution. Particularly, the distribution associated with each observation must be normally distributed. As an example, given a stochastic process in which X is a function of the variables within a set T, for any choice of distinct values of T, the corresponding vector $\boldsymbol{X}$ must have a multivariate normal distribution. This implies that, given the distribution's mean and covariance functions, the normal distribution can be effectively described and a Gaussian process is completely determined through the definition of these two functions. [16, 23]

In order to build a Gaussian process-based surrogate for the bi-material strip model, the function evaluations necessary for the Gaussian correlation function were assembled. Specifically, the finite element model was processed with 21, or $n+1$, LHS samples of the 20-dimenstional

parameter space. Then, assuming the resulting evaluations adhered to a Gaussian distribution, mean and covariance functions, as well as the surrogate were determined. Also, similarly to the PCE approach, cross-validation methods were applied during the development of the surrogate to measure its accuracy. Once a surrogate was built and validated, it was subjected to 10000 samples of the parameter space, and the ANOVA was applied to the resulting 10000 surrogate evaluations to develop a critical parameter list. This process of gathering the Gaussian function evaluations, creating and validating a surrogate, and processing 10000 surrogate evaluations through an ANOVA was repeated with an increasing number of initial function evaluations of the bi-material strip model until a converged list of critical parameters was found. The number of function evaluations corresponding to the surrogate providing the converged critical parameters list was the metric for comparison with the other considered sensitivity analysis techniques.

4.2. Sensitivity Survey Results and Discussion

Sensitivity analyses measuring the criticality of the input parameters to the residual stress predictions of the bi-material strip manufacturing process model were completed with the six methods described in the preceding sections. As described, for all but the Box Behnken design of experiments, the examined methods were processed with increasing sample sizes until converged critical parameter lists were found. Table 4.2 describes the results for each of the completed sensitivity studies.

Table 4.2: Summary of sensitivity analysis methods survey. (A filled grid space indicates criticality and bold text indicates convergence.)

		Model Parameters																			
Method	Sample #	E_{11}	E_{22}	E_{33}	ν_{12}	ν_{13}	ν_{23}	G_{12}	G_{13}	G_{23}	$\alpha_{11,G}$	$\alpha_{22,G}$	$\alpha_{33,G}$	$\alpha_{11,R}$	$\alpha_{22,R}$	$\alpha_{33,R}$	T_g	T_{sf}	E_{AI}	ν_{AI}	α_{AI}
CPS	41	■									■			■			■	■	■		■
	81	■	■								■			■			■	■	■		■
	121	■	■								■			■			■	■	■		■
MC	22	■	■	■	■	■	■		■	■	■	■	■	■	■	■	■	■	■	■	■
	44	■						■			■			■		■	■	■	■	■	■
	88	■	■								■			■			■	■	■		■
	176	■						■			■			■		■	■	■	■		■
	352	■						■			■			■			■	■	■		■
	704	■	■		■				■		■			■		■	■	■	■		■
	1408	■	■								■			■			■	■	■		■
	2816	■	■		■						■	■		■			■	■	■	■	■
	5632	■	■		■						■	■		■			■	■	■	■	■
LHS	22									■	■						■	■			■
	44	■	■							■	■			■			■	■	■		■
	88	■	■								■			■			■	■	■		■
	176	■	■								■			■			■	■	■	■	■
	352	■	■								■	■		■			■	■	■		■
	704	■	■		■						■			■			■	■	■	■	■
	1408	■	■		■						■	■		■			■	■	■	■	■
	2816	■	■		■						■	■		■			■	■	■	■	■
BBD	**761**	■	■		■						■	■		■			■	■	■		■
PCE	21	■	■			■			■		■			■			■	■	■		■
	42	■	■		■	■		■	■	■	■	■	■	■			■	■	■		■
	84	■	■								■	■		■			■	■	■	■	■
	168	■	■		■						■	■		■	■		■	■	■		■
	336	■	■		■						■	■		■	■		■	■	■	■	■
	672	■	■		■						■	■		■	■		■	■	■	■	■
GP	21				■		■					■	■	■		■					■
	42	■						■	■			■		■	■	■		■		■	■
	84	■	■	■	■	■	■	■	■	■	■	■	■	■		■	■	■	■		■
	168	■	■	■	■	■		■	■	■	■	■		■	■		■	■	■	■	
	336	■	■		■						■	■		■	■		■	■	■	■	■
	672	■	■		■						■	■		■	■		■	■	■	■	■

Several conclusions can be drawn from the information provided in the table concerning the examined sensitivity analysis methods, as well as the critical parameters themselves. First, regarding the six sensitivity analysis techniques exercised in this study, four observations can be made:

- The surrogate methods (PCE/GP) require the fewest samples for a converged list of critical parameters, and, of the two examined surrogate methods, GP may be the preferred approach, as it does not require a user-defined polynomial order.
- The sampling methods (MC/LHS) are the least efficient approaches, as they require the most samples for a converged list of critical parameters, in some cases four to eight times as many samples as the surrogate methods.
- A centered parameter study (CPS) provides a reasonable list of critical parameters at a low number of samples, but seems to omit some of the less influential critical parameters. This could perhaps imply that a CPS should be employed when a measure of sensitivity is required, but only a handful of samples are computationally affordable.
- While a Box Behnken design (BBD) requires far fewer samples than the sampling methods, it is just over twice as expensive as the surrogate methods, and, although BBD is more expensive than either PCE or GP, it is much less technically complex.

Therefore, according to a user's computational resource limitations and technical expertise, a design of experiment approach could be appropriate.

Next, several observations can also be made regarding the critical parameters themselves:

- All of the examined methods selected E_{11}, E_{22}, $\alpha_{11,G}$, $\alpha_{11,R}$, T_g, T_{sf}, E_{Al}, and α_{Al} as influential. Furthermore, except for CPS, all of the methods additionally selected ν_{12} and $\alpha_{22,G}$. This indicates first that, as previously mentioned, the CPS, while computationally inexpensive, seems to omit some of the less influential critical model parameters, and second, that the model parameters selected as influential to the residual stress predictions seem intuitively correct. Specifically, the in-plane mechanical and thermal properties of the composite (E_{11}, E_{22}, $\alpha_{11,G}$, $\alpha_{11,R}$, ν_{12}, and $\alpha_{22,G}$), as well as the parameters associated with the aluminum (E_{Al} and α_{Al}), would be expected to significantly impact predictions, since differences in the two materials' in-plane contractions during the simulated cooling cycle govern the development of the residual stress state. Furthermore, the glass transition temperature (T_g) and the stress-free temperature (T_{sf}) are justifiably important, as they indicate at what temperatures and with what rates the thermal strains should begin to develop.
- All of the examined methods, except for CPS and BBD, selected ν_{Al} as critical. Likewise, only the two surrogate approaches selected $\alpha_{22,R}$. This could indicate that these two parameters are less influential to the simulated response when compared to the other critical model parameters.

In addition to the ANOVA, PCE also permits the determination of Sobol indices, or sensitivity indices, which are useful in ranking the influential model parameters in terms of their criticality. Specifically, a percentage weight is applied to each of the examined model parameters, which represents the relative influence of each input parameter to the simulated response. The Sobol indices were determined through sampling of the converged PCE surrogate and are shown below in table 4.3.

Table 4.3: Sobol Indices from the converged PCE surrogate

Parameter	Sobol Index	Parameter	Sobol Index
α_{Al}	98.003763%	$\alpha_{22,G}$	0.000295%
T_{sf}	1.091548%	$\alpha_{22,R}$	0.000018%
T_g	0.363556%	ν_{13}	0.000000%
$\alpha_{11,G}$	0.354474%	E_{33}	0.000000%
E_{Al}	0.059520%	$\alpha_{33,R}$	0.000000%
$\alpha_{11,R}$	0.056149%	G_{23}	0.000000%
E_{11}	0.027971%	$\alpha_{33,G}$	0.000000%
E_{22}	0.001954%	ν_{23}	0.000000%
ν_{12}	0.000305%	G_{13}	0.000000%
ν_{Al}	0.000301%	G_{12}	0.000000%

Several interesting observations can be made from the data provided in this table:

- The parameters shown in table 4.3 that were selected as critical by some, but not all, of the examined methods (ν_{12}, $\alpha_{22,G}$, $\alpha_{22,R}$, and ν_{Al}) have some of the lowest

sensitivity indices. This confirms the likelihood than these parameters were overlooked by some of the examined sensitivity analysis methods due to their threshold values.

- The parameters with the most significant indices (α_{Al}, $\alpha_{11,G}$, T_g, and T_{sf}) govern the development of thermal strains. This seems intuitively correct, since the modeling process employed to approximate the composite's curing relies upon a simulated cooling cycle from the stress-free temperature.
- The Sobol index associated with α_{Al} is much greater than all other indices. This indicates that the response of the bi-material strip is governed by the thermal expansion of the aluminum. This is somewhat intuitive, however, since the in-plane coefficient of thermal expansion of the composite material is much less than the aluminum's CTE. Therefore, the thermal contractions of the aluminum would be significantly greater than that of the composite and would likely drive the residual stress development. Furthermore, if the composite material bonded to the aluminum were to hypothetically have in-plane CTE's much closer to the aluminum, it is reasonable to expect that the Sobol indices would be more evenly distributed amongst the aluminum and composite in-plane thermal properties.

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5. UNCERTAINTY QUANTIFICATION METHODS SURVEY

Following the results of a sensitivity study, an uncertainty quantification (UQ) study is used to formulate finite element predictions, which encompass the most important sources of physical variability. Although a sensitivity study is not strictly required for an uncertainty quantification study, as mentioned previously, it reduces the material characterization effort through the elimination of parameters which do not contribute significantly to the quantity of interest's variability. This, in turn, reduces the parameter space to be explored during the uncertainty quantification and fewer samples will be required to understand the expected variability.

The purpose of the uncertainty quantification methods survey was twofold. First, to determine the expected mean and standard deviation associated with the center span deflection of the bi-material strip, and second, to determine the most efficient UQ methodology providing converged means and standard deviations. A similar set of sampling and surrogate methods were selected for considering during the uncertainty quantification survey, as were selected for the sensitivity study survey. Particularly, four of DAKOTA's UQ methods were examined and include both Monte Carlo and Latin Hypercube sampling, and two surrogate methods, a polynomial chaos expansion and a Gaussian process.

As stated in the previous section, the survey of sensitivity study methods identified a total of twelve critical parameters through the application of an ANOVA: E_{11}, E_{22}, ν_{12}, $\alpha_{11,G}$, $\alpha_{11,R}$, $\alpha_{22,G}$, $\alpha_{22,R}$, T_g, T_{sf}, E_{Al}, ν_{Al}, and α_{Al}. An additional eight parameters can be eliminated based on the Sobol indices in table 4.3, which indicate that four parameters ($\alpha_{11,G}$, T_g, T_{sf}, and α_{Al}) account for 99.8% of the observed variability. Characterization was completed for each of these twelve critical model inputs in order to provide distributions defining the variability for each parameter, as shown in table 5.1. All the composite's parameters and the aluminum's mechanical material properties were assumed to follow normal distributions. Alternatively, a uniform distribution was used to define the variability of α_{Al}, as the values found literature defining this parameter were limited to averages over different temperature ranges (table 5.2).

Table 5.1: Model parameter normal distributions for the uncertainty quantification

	Parameter	Mean	Standard Deviation
Composite Properties[1]	E_{11} (GPa)	63.86	2.40
	E_{22} (GPa)	62.74	2.36
	ν_{12}	0.048	0.0065
	T_g (ºC)	125.14	7.19
	T_{sf} (ºC)	128.8	4.30
	CTE_{11} (1/ºC, rubbery)	9.5e-7	1.6e-7
	CTE_{22} (1/ºC, rubbery)	2.18e-6	1.0e-8
	CTE_{11} (1/ºC, glassy)	3.15e-6	1.0e-7
	CTE_{22} (1/ºC, glassy)	3.62e-6	9.0e-8
Aluminum Properties[2]	E (GPa)	68.9	0.7
	ν	0.33	0.003

[1] Values taken from [24].
[2] Values taken from [25].

Table 5.2: Model parameter uniform distributions for the uncertainty quantification

	Parameter	Minimum	Maximum
Aluminum Properties	CTE (1/ºC)	2.18e-5[1]	2.45e-5[2]

[1]Average CTE for the temperature range -50°C to 20°C [25].
[2]Average CTE for the temperature range 20°C to 200°C [25].

Considering the material data provided in the above two tables, the two variations of reduced parameter spaces, found through the ANOVA and the Sobol indices, were sampled using the four specified DAKOTA uncertainty quantification methods. Upon completion of the survey, the primary metric that was used to compare the methods was the minimum number of samples necessary to provide a converged mean and standard deviation for the center span deflection of the bi-material strip.

5.1. Uncertainty Quantification Methods

Four of the methods used for the sensitivity study survey were also considered for the uncertainty quantification survey to determine the most efficient approach for the residual stress driven, out-of-plane displacement of the bi-material strip. The examined methods include Monte Carlo and Latin Hypercube sampling and the two surrogate methods: polynomial chaos expansion and Gaussian process. Neither the centered parameter study nor the Box-Behnken design of computer experiments were considered, as these methods do not effectively sample the entire parameter space.

5.1.1. Monte Carlo (MC)

The Monte Carlo method of sampling is purely random and was included as a baseline for the survey. While MC methods may not be the most efficient, given a large enough number of samples, MC will converge to the true result.

To generate a Monte Carlo based uncertainty quantification study for the bi-material strip model, the critical parameters were defined to have the distributions given in tables 5.1 and 5.2. Initially, the number of samples was set to $n + 1$ (13 and 5 for the sensitivity study results based on ANOVA or the Sobol indices, respectively), and then, the number of samples was systematically doubled until a converged mean and standard deviation were found.

5.1.2. Latin Hypercube Sampling (LHS)

As discussed in section 4.1.3.2, Latin Hypercube sampling is a more intelligent way to sample a parameter space compared to Monte Carlo, as it guarantees full coverage of the parameter space for sample sizes greater than the number of parameters. Like Monte Carlo sampling, given a large enough sample size, LHS will converge to the true result.

To generate a LHS based uncertainty quantification study, all parameters were given the distributions detailed in tables 5.1 and 5.2 and the initial sample size was set to $n + 1$. The

sample size was then systematically doubled until a converged mean and standard deviation were found.

5.1.3. Polynomial Chaos Expansion (PCE)

The details of a polynomial chaos expansion (PCE) surrogate are given in section 4.1.4.1. In order to generate the PCE-based uncertainty quantification study, all parameters were given the distributions detailed in tables 5.1 and 5.2 and $n + 1$ LHS samples were used to create the surrogate. Like the sensitivity study, polynomial orders of one to five were fit to the response, and the LHS sample size used to generate the surrogate model was systematically doubled until a converged mean and standard deviation were found.

5.1.4. Gaussian Process (GP)

The details of a Gaussian process (GP) surrogate are given in section 4.1.4.2. In order to generate the GP-based uncertainty quantification study, all parameters were given the distributions detailed in tables 5.1 and 5.2 and the initial sample size used to create the surrogate was set to $n + 1$. Both MC and LHS sampling were applied to generate the sample set used to create the surrogate, and the sample size was systematically doubled until a converged mean and standard deviation were found.

5.2. Uncertainty Quantification Results and Discussion

Uncertainty quantification studies were completed considering the prediction of residual stresses in a bi-material composite strip. Particularly, the mean and standard deviation of the maximum out-of-plane displacement of the strip were estimated with four of DAKOTA's UQ methods. As discussed, the sample size of each method was increased until converged, or near converged, means and standard deviations were found. Furthermore, each of the four methods discussed in the preceding section was applied to investigate the twelve critical parameters found through the ANOVA and three of the UQ methods were applied to the four critical parameters identified with the Sobol indices. Specifically, Monte Carlo sampling and the Monte Carlo based Gaussian process surrogate were omitted from investigation of the Sobol index parameter space for efficiency. Tables 5.3 and 5.4 summarize the results for the ANOVA and Sobol index based parameter spaces and figures 5.1 and 5.2 show the convergence trends for the means and standard deviations.

Table 5.3: Summary of the uncertainty quantification methods survey based on the ANOVA critical parameters

	Samples	Mean (mm)	Standard Deviation (mm)
MC	13	25.577	1.255
	26	25.478	1.135
	52	25.410	1.291
	104	25.392	1.282
	208	25.270	1.331
LHS	13	25.231	1.409
	26	25.195	1.352
	52	25.205	1.356
	104	25.201	1.353
	208	25.200	1.346
	416	25.200	1.336
PCE	13	25.194	1.319
	26	25.203	1.307
	52	25.198	1.322
	104	25.197	1.322
GP (LHS)	13	25.223	1.260
	26	25.194	1.288
	52	25.201	1.321
	104	25.200	1.323
GP (MC)	13	25.231	1.187
	26	25.206	1.245
	52	25.200	1.324
	104	25.199	1.323

Table 5.4: Summary of the uncertainty quantification methods survey based on the Sobol indices critical parameters

	Samples	Mean (mm)	Standard Deviation (mm)
LHS	5	25.503	1.081
	10	25.249	1.190
	20	25.214	1.294
	40	25.208	1.319
	80	25.197	1.368
PCE	5	24.092	2.169
	10	25.205	1.292
	20	25.203	1.324
	40	25.199	1.320
GP (LHS)	5	25.227	1.194
	10	25.206	1.308
	20	25.198	1.324
	40	25.199	1.324

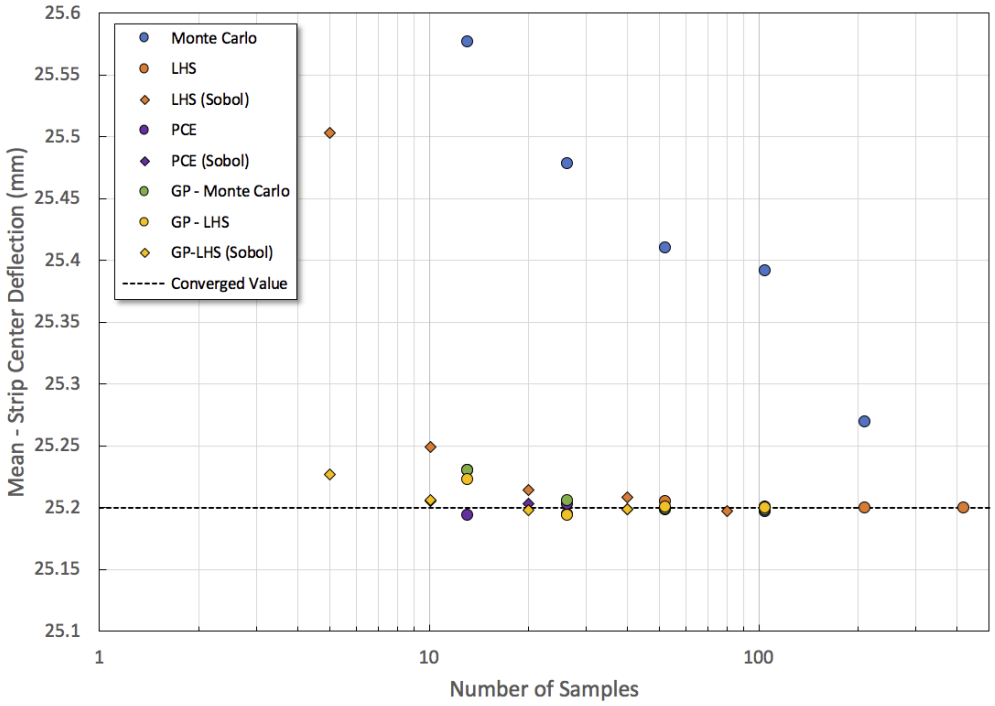

Figure 5.1: Center deflection mean with respect to the sample size

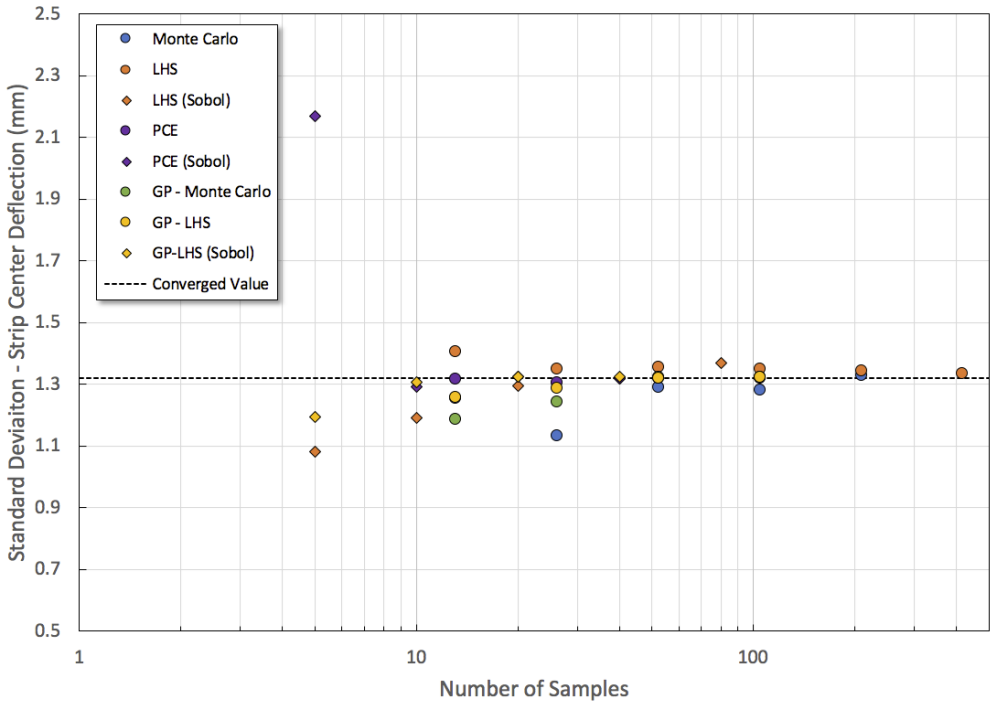

Figure 5.2: Center deflection standard deviation with respect to the sample size

As shown by the above figures and tables, all of the methods converge to the same mean and standard deviation for the center deflection of the bi-material strip: 25.2 mm and 1.32 mm, respectively. This compares well with the experimental measurements discussed in Section 2.2 (26.44mm ± 0.21mm). Specifically, the predictions are within one standard deviation of the physical observation. While all methods were successful, several observations can be made regarding performance and efficiency:

- The Monte Carlo sampling method was the least efficient, as expected, and was not fully converged at 16($n + 1$), or 208, samples. Furthermore, a smooth convergence trend was not shown by the Monte Carlo method and, without the results from the other methods, convergence would be difficult to identify. This would most likely lead to running an excessive number of simulations.
- The LHS method gave a mean value that was nearly converged at $n + 1$, or 13, samples and fully converged at 4($n + 1$), or 52 samples. However, even at 32($n + 1$), or 416, samples the standard deviation was not fully converged.
- The polynomial chaos expansion surrogate method provided a converged mean and standard deviation at n + 1 samples, although the standard deviation wasn't fully settled until 4($n + 1$) samples.
- The Gaussian process surrogate method performed similarly when applying either Monte Carlo sampling or LHS to generate the sample set used to create the surrogate. The means were nearly converged at $n + 1$ samples, which would be expected for the GP (LHS) method, but less so of the GP (MC) method. By 4($n + 1$) samples, the standard deviations for both methods were converged.
- Using a surrogate method based on 4($n + 1$) samples appears to give a converged expected normal distribution of the center deflection of the bi-material strip. For the critical parameters identified by ANOVA, this results in 52 samples; however, for the critical parameters defined by the Sobol indices, this would be only 20 samples.

The survey using the critical parameters based on the Sobol indices performed similarly to the initial survey using critical parameters identified by ANOVA. Particularly, the means converged quickly with both sampling and surrogate methods, but only the surrogate methods provided fully converged standard deviations. Comparing the two surveys allows for the following observation:

- The rule-of-thumb, which indicates that a surrogate based upon 4($n + 1$) samples will provide a converged mean and standard deviation, appears to hold true with a reduced parameter space.
- The polynomial chaos expansion surrogate performed very well at $n + 1$ samples for the ANOVA based survey, but $n + 1$, or 5, samples for the Sobol index based survey did not provide a reasonable result for the mean or standard deviation. This leads to the conclusion that there will be a minimum number of samples needed to provide quality results, which will be problem dependent and potentially in excess of 4($n + 1$).

6. SUMMARY AND CONCLUSIONS

Process-induced residual stresses must be considered when designing composite components for structural applications. Furthermore, as an alternative to the experimental quantification of these stresses, finite element modeling methods can be employed to simulate a composite's curing process. However, accurate simulations of a composite structure's post-fabrication residual stress state requires the definition of many model input parameters and, given realistic time and cost constraints, not all of these parameters can be rigorously characterized. Alternatively, verification and validation methods, such as sensitivity analyses and uncertainty quantification studies, can be employed to better understand which of a model's required input parameters are most critical to the simulated response and how uncertainty in those critical parameters can affect the simulated predictions. Many different sensitivity analysis and uncertainty quantification methods exist, each offering potential benefits and trade-offs related to computational complexity and cost. Therefore, detailed surveys were undertaken considering the sensitivity and uncertainty quantification tools available within DAKOTA. The examined methods included both simple techniques, such Monte Carlo sampling, as well more sophisticated approaches, such as a polynomial chaos expansion. The survey outcomes strongly indicate that, when computational cost is the metric for comparison, the surrogate approaches provide the best performance. Specifically, the investigated surrogate methods required 4x to16x less computational resources than the more commonly used sampling approaches, which offered the worst performances.

While the surrogate methods demonstrated the best efficiency, several conclusions and recommendations can be made regarding the ideal methodology to be employed when considering parameter sensitivity or uncertainty. First, provided the data summarized in table 4.2, four observations can be made concerning the ideal sensitivity analysis approach, bearing in mind both computational complexity and cost:

- The surrogate methods (PCE/GP) require the fewest samples for a converged list of critical parameters. While PCE and GP demonstrated the same computational cost, a Gaussian process may be preferred, as it requires less user interaction.
- The sampling methods (MC/LHS) are the least efficient approaches, as they require the most samples for a converged list of critical parameters. However, these methods are computationally the simplest and merit consideration when lacking access to an iterative analysis toolkit, such as DAKOTA.
- A centered parameter study (CPS) provides a reasonable list of critical parameters at a low number of samples, but seems to omit some of the less influential critical parameters. Therefore, a CPS should be considered when a measure of sensitivity is required, but only a handful of samples are computationally affordable.
- The design of experiments approach (BBD) was shown to be much more efficient than the sampling methods, but twice as expensive as the surrogate approaches. Although BBD was shown to be more expensive than either PCE or GP, it is much less technically complex and could be implemented without an iterative analysis toolkit, like DAKOTA. Therefore, according to a user's computational resource limitations and technical expertise, a design of experiment approach could be appropriate.

Next, considering the data presented in section 5 of this report, several observations can be made regarding the ideal uncertainty quantification methodology to be employed following a parameter sensitivity study:

- The surrogate methods (PCE/GP) require the fewest samples for converged means and standard deviations. PCE and GP performed similarly, therefore GP may be preferred, as it requires less user interaction.
- The sampling methods were much less efficient than the surrogate approaches, requiring greater than eight times as many samples as the surrogate approaches to find converged standard deviations. However, as with the sensitivity analysis survey, these methods are computationally the simplest and merit consideration when lacking access to an iterative analysis toolkit, such as DAKOTA
- A surrogate methods based upon $4(n+1)$ samples appears sufficient for converged predictions of the mean and standard deviation values.

Provided these observations and conclusions regarding the surveys of DAKOTA's various sensitivity analysis and uncertainty quantification tools, an idealized validation procedure can be recommended for the future residual stress analysis of composite structures, as well as other potential loading scenarios. Particularly, if a parameter sensitivity survey will precede the uncertainty quantification, a surrogate model should be built, based upon either a polynomial chaos expansion or a Gaussian process, and sampled. However, if a measure of parameter sensitivity is desired and the finite element model is too expensive to permit a sufficient number of samples to develop a converged surrogate, then a centered parameter study (CPS) should be utilized. Next, if uncertainty quantification is to be completed, either a Gaussian process or a polynomial chaos expansion should be employed. These methods demonstrated a converged mean and standard deviation with a response function set size of only $4(n+1)$ LHS samples.

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