Analysis Tools for Accelerated Development of Composite Materials

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Abstract: *Composite materials continue to rapidly improve in terms of structural performance. These materials offer the promise of significant weight reduction in many products—particularly aerospace structures, where weight minimization is critical to both cost and overall performance. Despite this potential, however, several challenges prevent composite materials from being used as widely and pervasively as traditional materials. Preliminary design concept evaluation of a structure with a novel material is difficult without a lengthy, expensive test program to provide the requisite material properties, but manufacturers are justifiably reluctant to invest this time and money without confidence that the material under consideration merits such expense. The stochastic nature of most composite materials means that a large number of samples may need to be tested, and conservative knockdown factors be used in developing strength allowables. A unified set of analysis tools has been developed leveraging the Abaqus-Python API to address these challenges with two material architectures in mind:, fiber-reinforced laminates and woven-fiber composites. Through the use of this tool, a tremendous savings in time and cost can be realized when developing and utilizing new composite material systems.*

Keywords: *Carbon, Composites, Damage, Delamination, Failure, Postprocessing, Reliability, Sensitivity, Statistics, Strength.*

1. Introduction

1.1 Background

One of the primary challenges of designing products that use composite materials is that the failure behavior of composite materials is extremely complex and the failure mechanisms are often poorly understood. This complexity is due to the heterogeneous composition and the orthotropic mechanical properties, and the inherently probabilistic material behavior. There are many possible failure modes, such as matrix cracking, fiber breakage, fiber debonding, and delamination. The failure mode is highly dependent on many variables, including fiber orientation, stacking sequence, manufacturing process variables (fiber and void volume ratio, fiber misalignment, and ply thickness), variability in elastic constants and strength parameters, and so on. To further complicate things, multiple failure modes can manifest in a single structure.

In the World Wide Failure Exercise (WWFE), conducted by Hinton, et al. (Soden, Hinton, & Kaddour, 1998; Hinton, Kaddour, & Soden, 2002; Hinton, Kaddour, & Soden, 2004), the current state of knowledge on this subject was assessed by comparing the predictive capabilities of many of the leading composite failure theories. It was concluded that no single theory was able to accurately predict all of the quantitative and qualitative aspects of failure for even simple test cases. The failure theories predicted significantly different final failure strengths (with differences of up to 970 percent), often with different failure modes.

The current methodology used for designing composite structures is the "building-block approach" (Whitehead & Deo, 1983). This is an empirically based deterministic method. This process involves the experimental determination of allowable strength parameters for the critical failure modes at one structural scale and then proceeds to increasingly detailed structural scales under the assumption that the same damage/failure mode is manifested throughout. This assumption is verified through testing at every level of detail until the full component design is obtained.

Characterization of individual ply properties forms the base of this building-block approach. There are five typical failure modes that are tested for a unidirectional ply: (1) longitudinal tension, (2) longitudinal compression, (3) transverse tension, (4) transverse compression, and (5) in-plane shear. As the design process continues to more detailed structural scales, component-level testing is required. If assumptions made at lower structural scales cannot be validated, then the entire process must restart at the appropriate lower level. Carrying the design process to a satisfactory completion may require extremely time-consuming and expensive testing programs.

The properties of laminated composites are dependent upon a multitude of variables that are statistical in nature, and cannot be adequately quantified deterministically. The observed variability in composite strength is accompanied by, and is often a result of, variability in the possible damage progression paths and failure modes that can occur in laminates with the same nominal configuration and materials (S.R. Hallett, 2009). The use of traditional deterministic methods in the design of composite structures may lead to either overconservative or underconservative designs. This can offset the potential benefits of composite laminates and often results in the use of large strength knockdown factors, and a substantial weight increase without a quantifiable increase in structural reliability (Long & Narciso, 1999). Thus there is a need for damage progression and failure models that can account for the probabilistic behavior of composites.

The foregoing discussion highlights the fact that designing and analyzing structures that use composite materials is fraught with difficulty. These problems are exacerbated when developing novel composite materials, which are often not well characterized.. On one hand, engineers need a complete set of orthotropic material properties to perform finite element simulations. Ideally these properties would be characterized statistically so that a probabilistic assessment of the material's performance in a structural application can be made. On the other hand, fully characterizing a material in such a fashion can require a significant investment of both time and money, and product developers are understandably reluctant to commit the resources without some assurance that the material under consideration shows some promise. New analysis frameworks are required to remedy this "chicken and egg" problem.

To accelerate the design and development of new composite materials, three domains are considered to reduce the time and money required to test, characterize, and simulate composite materials. The first domain is in preliminary analysis, when analysts would like to know in an order-of-magnitude sense whether a particular candidate material is suitable for a given application. At this stage, a fiber and matrix may be selected for fabrication into a lamina, or a commercially available prepreg lamina may be selected. In either case, a full set of material properties necessary for finite element analysis (FEA) are typically unavailable.

The second domain is in understanding the failure mode of a given laminate and the properties upon which the failure is most sensitive. A small change in some properties will result in a large change in failure strength, while other properties can change significantly with very little effect on the failure strength. Understanding these relationships is important to guide a preliminary material characterization test program. Focusing on the most meaningful tests early on in the design process can provide the most “bang for the buck” in terms of time and money invested into a test program.

The third domain is in virtually simulating a test program, including the stochastic variability of material properties. This requires finite element models that sufficiently capture the failure behavior of a laminate. Such simulations can provide the statistical properties to define A- and B-basis allowables.

A common theme in each of these three domains is that state-of-the-art finite element methods are used pervasively for composite material design and analysis. Abaqus is an industry standard FEA platform that provides advanced composite modeling techniques and enables implementation of more sophisticated models to study different failure mechanisms. Abaqus was selected as the platform for integration of the technology presented in this paper.

1.2 Rapid Composite Material Characterization and Development with Abaqus

A framework has been developed for integration of diverse technologies to accomplish the accelerated development of novel materials. This framework, known as COMPAS, has been developed by ATA Engineering and is implemented in an add-on to Abaqus/CAE. The Abaqus-Python API has been leveraged to provide the platform for the graphical user interface (GUI) development.

The COMPAS framework facilitates the analysis by providing a GUI that guides the user through the analysis of a new composite material. The required Abaqus capabilities are accessed through COMPAS and organized in a sequence designed for the material characterization process. The software package interacts with other numerical methods for property prediction, sensitivity analysis and Monte Carlo simulations. COMPAS provides recommendations for modeling techniques and parameter selection based on extensive research validated by material testing.

2. Methodology

As stated earlier, the objective of this research topic is to develop analytical tools to reduce testing costs associated with characterization of new material systems and to enable the design of composite structures with improved weight and strength performance. The COMPAS framework uses an approach that provides: (1) progressive-failure analysis with inter-ply cohesive elements to capture inter- and intra-laminar damage growth, (2) stochastic Monte Carlo simulation for “virtual testing” to reduce the required physical testing, (3) sensitivity analysis to target the most influential material properties for test, and (4) micromechanics and machine learning tools to predict missing properties from an incomplete material dataset. These capabilities are provided through a comprehensive set of computational methods.

2.1 Technology, Algorithms and Numerical Methods

Abaqus has several analytical capabilities for modeling laminated composites. The most basic capabilities are based on classical laminated plate theory (CLPT). The CLPT approach defines in-plane failure modes. Relatively crude approximations are made to evaluate delamination-type failures. CLPT approaches are unable to account for the damage progression of composite failure, which begins with damage initiation at some location, followed by an progressive failure process to ultimate failure (Pal & Ray, 2002). CLPT methods typically only provide information about the first-ply failure observed and ignore often significant residual strength beyond the first ply failure. As a result, CLPT methods tend to be overconservative with respect to ultimate strength.

In addition to CLPT approaches, Abaqus also has the capability to model progressive failure. Progressive failure analysis is a computational damage progression method aimed at predicting the multiple failure mechanisms in composite structures by supplementing finite element structural analysis with additional failure theories and material property/stiffness degradation methods. However, these progressive failure approaches are deterministic and unable to capture the stochastic damage progression and ultimate strength properties of composites.

To account for the probabilistic nature of strength and failure in composite structures, a variety of probabilistic analysis methods have been implemented. The Monte Carlo simulation technique has been shown to be the most flexible, robust, accurate, and widely used (McManus, 1993; Jeong & Shenoi, 2000). The Monte Carlo simulation operates by performing numerous deterministic analyses in which the input parameters are randomly selected from their probabilistic distributions. Through this process, it is possible to generate statistical distributions of laminate response. Two limitations of Monte Carlo methods are the lack of spatial variability in properties and the computational expense associated with a large number of statistical variables.

Sensitivity analysis is used to evaluate the relative importance of different parameters to the failure strength prediction. Understanding the importance of various parameters can guide what ply-level physical tests a designer will need to perform for a new material system. This helps minimize the amount of ply-level testing required by focusing only on the tests that have the most influence on the laminate-level properties. Three approaches to quantifying the parameter sensitivities were considered within the COMPAS framework: a variance-based full-factorial or fractional-factorial sensitivity analysis, a Morris "elementary effects" global screening method, and a local sensitivity one-factor-at-a-time (OAT) approach (Bolado-Lavin & Badea, 2008).

Machine learning techniques are used to predict material properties at both the constituent level and the single-ply level, even if several constituent properties are unknown, as is often the case with novel materials with limited experimental characterization. This approach accelerates the design and analysis if one has already performed some amount of testing to partially characterize ply-level properties. To provide an initial data set, COMPAS includes a database of material properties for 11 fiber materials, 5 polymer matrix epoxies, and 11 fiber-matrix combinations with unidirectional plies.

Another fundamental feature of the analysis tool is the capability to obtain ply-level properties from the underlying constituent materials. Several micromechanics methods have been implemented in the current framework. The methods used can be divided into two types: rule of mixture types and fully analytical types. The first type consists of simple algebraic property homogenization, mainly based on the Voigt (Voight, 1889) and Reuss (Reuss, 1929) model. Additional enhancements were made by Chamis (Chamis, 1989), Hashin and Rosen (Hashin & Rosen, 1964), and Halpin and Tsai (Halpin & Kardon, 1976) based on empirical observations. Because of the empirical component, some of these models are only appropriate for certain types of materials, namely carbon fiber and epoxy matrix composites. The other type utilizes of the Micromechanics Analysis Code with Generalized Method of Cells (MAC/GMC) developed by the NASA Glenn Research Center (Aboudi, Arnold, & Bednarcyk, 2012).

2.2 Implementation of COMPAS in Abaqus/CAE

The COMPAS framework is implemented as a plugin for the Abaqus/CAE environment. The framework architecture is shown schematically in Figure 2-1. The GUI was developed with the Abaqus-Python application programming interface..

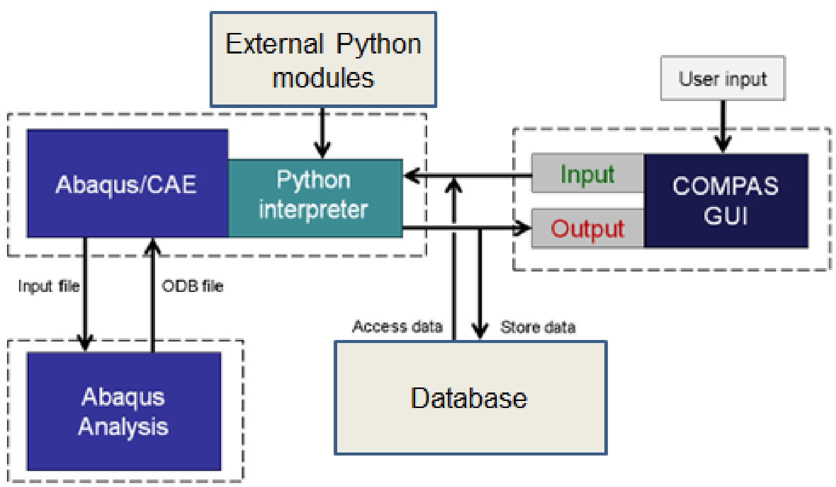

Figure 2-1. Preliminary development of GUI architecture.

Many different Python packages are utilized by COMPAS. A list of the major packages includes: “numpy” (van der Walt, 2011), “scipy” (Oliphant, 2007), “matplotlib” (Hunter, 2007), “Pandas” (McKinney, 2010), “Theano” (Bergstra, et al., 2010), “Lasagne”, “emcee” (Foreman-Mackey, Daniel, Hogg, Lang, & Goodman, 2013), and “Scikit-learn” (Pedregosa, Varoquaux, Gramfort, & Thirion, 2011).

COMPAS is divided into different modules that are accessible within different workflows. These modules are described in the context of the workflows in the next section.

A screenshot of one of the COMPAS modules is shown below in Figure 2-2. Because COMPAS is implemented as an Abaqus plugin, the syle of the dialog box will appear familiar to longtime Abaqus users.

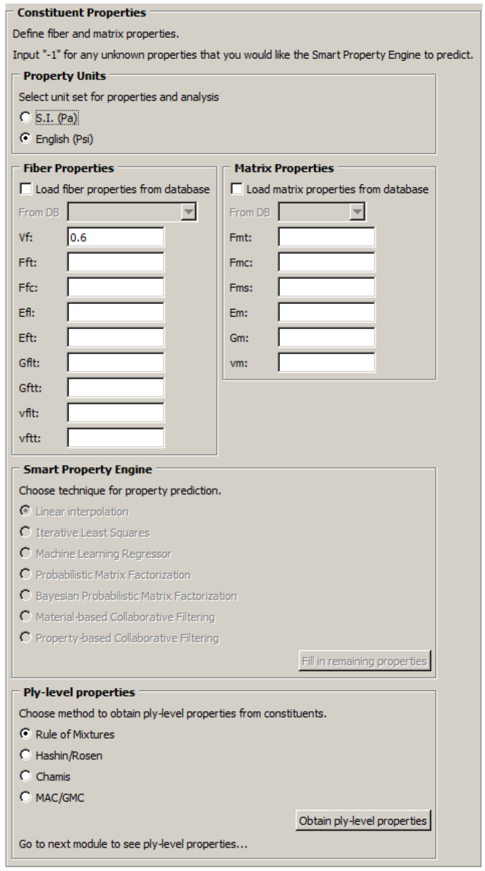

Figure 2-2. Property prediction module dialog box in the Abaqus/CAE environment.

3. Framework

The framework is designed to allow for three separate workflows that can be performed independently or in conjunction with one another for more complex tasks. The three workflows are property prediction, test reduction through sensitivity analysis, and virtual testing. The results produced by these workflows will be discussed in Section 4. Although each workflow is self-contained, they are ultimately integrated to provide full material characterization. The integration of these workflows is described generally in the flow chart shown in Figure 3-1. The details of the workflows are described in the following sections.

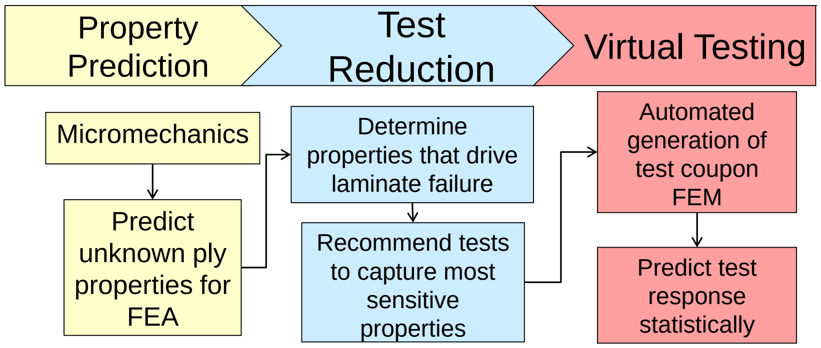

Figure 3-1. The three workflows enabled by the analysis tool.

3.1 Property Prediction

A detailed flow chart for the property prediction workflow is shown in Figure 3-2. Applicable at both the constituent level, with an uncharacterized combination of fiber and matrix, and at the ply level, with some properties available for a given lamina, the algorithms described in Section 2 predict the unknown material parameters. Starting at the constituent level, the micromechanical analysis methods described in Section 2 are used to determine ply properties on the basis of constituent properties. This function is available in both the "Constituents Module" and the "Ply-level Properties Module", where properties can be obtained at two different scales.

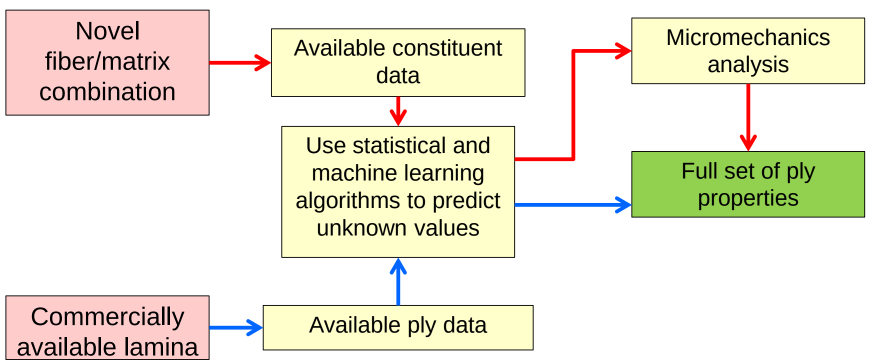

Figure 3-2. Detailed flow chart for the property prediction workflow.

3.2 Test Reduction Through Sensitivity Analysis

The sensitivity and test reduction workflow predicts the most meaningful standard tests (e.g., ASTM, SACMA, etc.) that provide the most "bang for the buck" in terms of allocating physical testing resources. A general flow chart is shown in Figure 3-3. Certain properties will highly influence the predicted failure response of a given laminate, while others will be much less influential. The aim of this workflow is to identify these relationships, and recommend tests that provide the influential properties. A smaller number of samples can be tested for the less influential properties. Some properties may have minimal influence and do not need to be determined via test at all, assumptions or analytical estimates suffice.

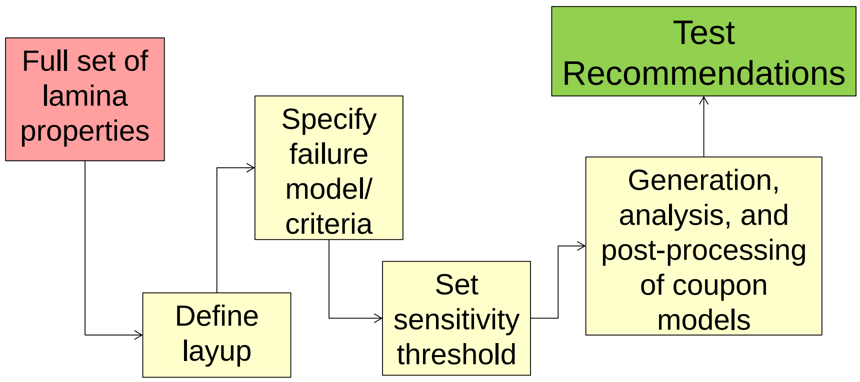

Figure 3-3. Detailed flow chart for the sensitivity and test reduction work flow.

3.3 Virtual Testing

Once a candidate laminate and the desired tests have been identified, the virtual testing workflow, shown below in Figure 3-4, a physical test program can be simulated, capturing stochastic variation in material properties. Results provided to the user include histograms and scatter plots to demonstrate the performance of the batch of test samples, as well as the means and standard deviations to define the corresponding A-basis and B-basis allowables.

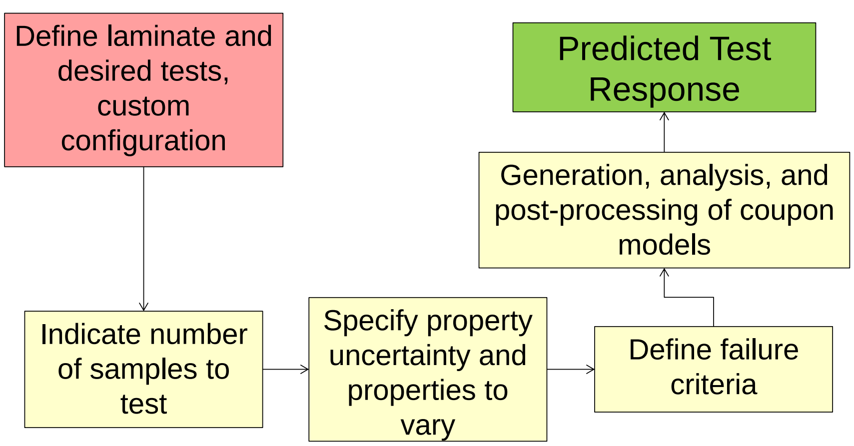

Figure 3-4. Detailed flow chart for virtual testing workflow.

4. Results

Demonstrative results for the three workflows of the analysis tool will be presented in this section. The format will mirror that used to describe the workflows in Section 3.

4.1 Property Prediction Results

As discussed in Section 3.1, there are two potential paths within the property prediction workflow. In one path, the user begins at the constituent level to predict lamina level properties and then use these lamina properties to define ply properties. In the other path, the starting point is from properties defined at the lamina level, with the goal to estimate any remaining unknown ply properties.

4.1.1 Ply Property Predictions from Constituent Data

Sample results for predicting ply-level properties using constituent-level properties are shown in Figure 4-1 for the four micromechanical analysis methods available in the framework, described in Section 2.1. The values have been normalized such that the true value, as indicated in the open literature, for any individual property is equal to one. As can be seen, there exists a range of accuracy in the predictions from method to method and also among the various properties. The property prediction accuracy is highly dependent on the material under consideration and the number of unknown properties.

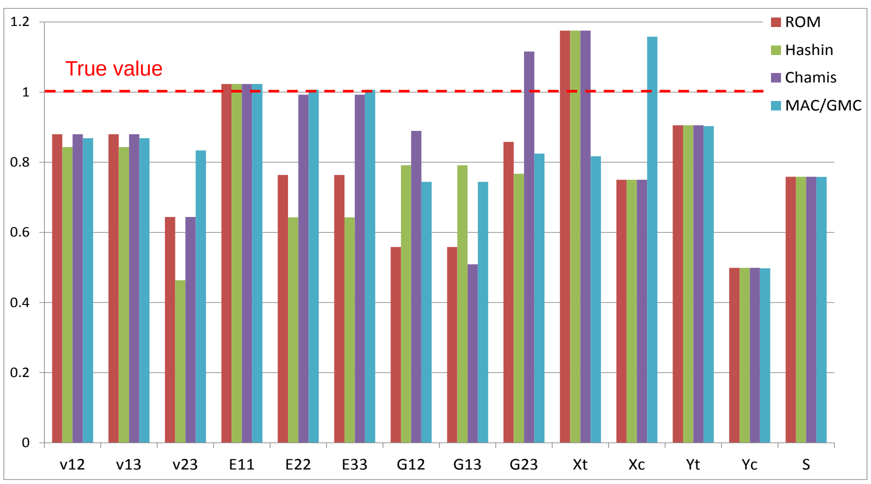

Figure 4-1. Predictions of properties at the ply level on the basis of constituent-level properties..

4.1.2 Unknown Ply Property Prediction

Sample results for predicting unknown ply-level properties using only a subset of all ply-level properties is shown in Figure 4-2 for six machine learning algorithms available in the analysis tool, described in Section 2.1. For the sake of brevity, the names of the algorithms have been abbreviated in the legend as follows: "Linear" refers to linear interpolation; "ALS" refers to alternating least squares; "ML" refers to the machine learning regressor; "Matl CF" refers to material-based collaborative filtering; "Prop CF" refers to property-based collaborative filtering; and "PMF" refers to probabilistic matrix factorization. In this example, a material for which all properties were well defined with test data was used so that the predictions could be compared to the measured values. To exercise the predictive algorithms, it was assumed that only *E1*, *XT*, *G12*, and *S* were known to the analyst. The other properties (listed on the horizontal axis in the figure) were not provided to the tool. The values on Figure 4-2 have been normalized such that the measured value for any individual property value is equal to one. We observe good correlation to measured values for many of the methods.

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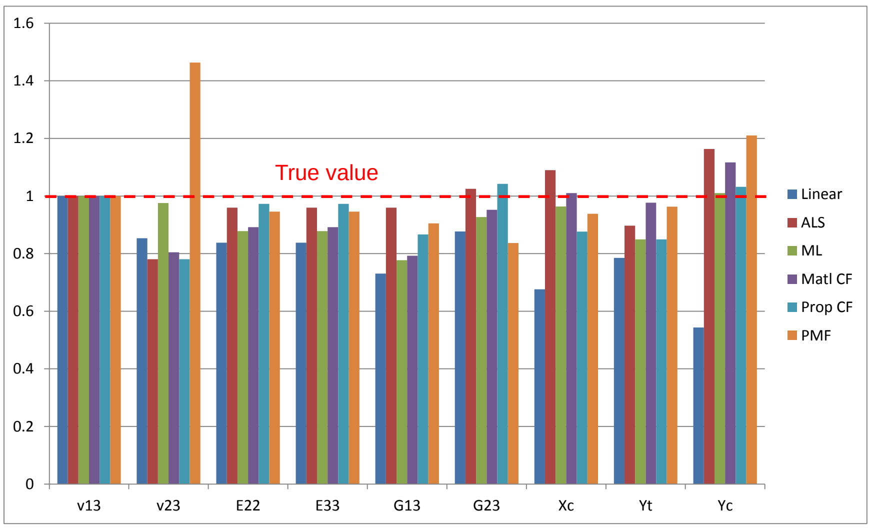


Figure 4-2. Predictions of properties at the ply level using a subset of the ply-level properties for an example material using six machine learning algorithms.

4.2 Test Reduction Results

As an example of the test reduction output, sample results for the one-at-a-time sensitivity method are shown in Figure 4-3(a). The various material properties are shown on the horizontal axis. The vertical axis shows the percent change from the nominal ultimate strength of the material due to a change in a particular property of one standard deviation. The tests recommended by the analysis tool on the basis of these sensitivity results are shown in Figure 4-3(b). The left portion of the figure indicates that the sensitive parameters are *E1*, *XT* (by far the most influential), *XC*, and *YT*. The right portion of the figure indicates the recommended tests based on a user defined threshold for parameter sensitivity.

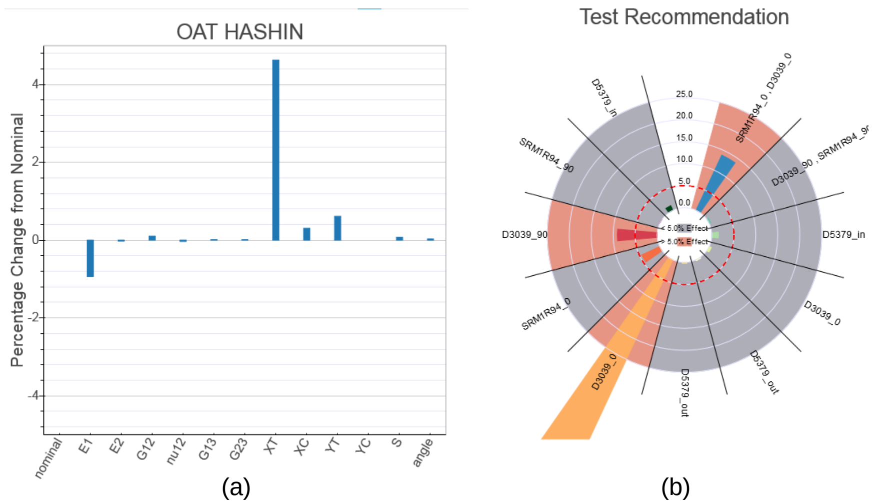
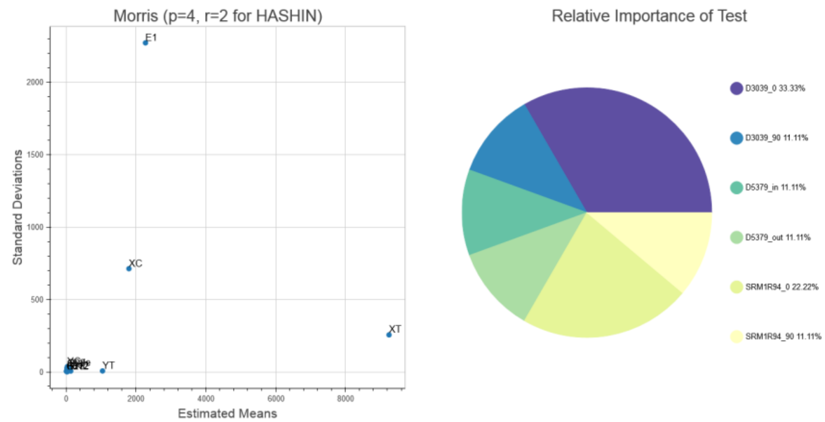


Figure 4-3. Sensitivity results and test recommendations for the one-at-a-time sensitivity method using the Hashin progressive failure approach.

Sample results for the Morris screening method are shown in Figure 4-4(a). In this figure, material properties are represented by the points on the scatter plot. The horizontal axis indicates the sensitivity of a property by itself. The vertical axis indicates the degree to which a property has interactive effects with in other properties. The terms “mean” and “standard deviation” used in the labels of the axes refer to nomenclature commonly used with the Morris screening method. The tests recommended by the Morris screening approach using the Hashin progressive failure approach are shown as a pie chart in Figure 4-4(b).



(a) (b)

Figure 4-4. Sensitivity results and test recommendations for the Morris sensitivity method.

An example using this approach to select ASTM standard tests showed a reduction of 52% in the number of test coupons required to characterize a material system.

One might naturally wonder what accuracy can be expected from finite element simulations where only some of the properties are characterized. To demonstrate the accuracy of this approach, we perform a set of stochastic Monte Carlo simulations in which all material properties vary according to their experimentally measured standard deviations to define a benchmark. This was compared to results from a separate set of simulations in which only the high-sensitivity properties vary and the moderate- and low-sensitivity properties were replaced with assumed or estimated properties that correspond to the significantly reduced test recommendations. The moderate- and low-sensitivity properties are held fixed (no variation) while only the high-sensitivity properties are randomly varied according to their defined distribution. The results of this comparison, shown in Table 4-1, demonstrate a high degree of stochastic accuracy is obtained using statistical property data for only the high-sensitivity properties and rough assumptions for other properties. Note that to allow for easier comparison, the values have been normalized such that the results for the full set of properties are equal to 1.

Table 4-1. Comparison of predicted mean strength and COV from virtual test with full set of properties varied and only a subset of properties varied.

Property	Full Set of Properties	Reduced Set of Properties
Mean Strength (ksi)	1	0.995
COV (%)	1	0.94

4.3 Virtual Testing Results

Traditionally, large knockdowns are applied to A- and B-basis strength allowables due to a limited number of test coupons. The COMPAS framework provides a method that uses a correlated model to reduce these knockdowns and obtain more-accurate strength values. The toolset provides a catalog of correlated test coupon models representative of typical strength and modulus coupon tests and provides a functional virtual testing resource.

Increasing the number of tested samples will necessarily increase the A- and B-basis strength allowables. However, it is not known a priori what this relationship is, i.e., what is the payoff in terms of increased allowables given the expense of additional testing. Consider the scenario in which an engineer is developing a test plan and deciding how many samples to test. The virtual testing capability of this analysis tool can be used to generated A- and B-basis allowables for an arbitrary number of test samples, thereby providing insight into how many samples should ideally be tested and what resulting allowables can be expected. Table 4-2 presents actual output from a virtual test performed with our analysis tool for 6, 20, and 80 test samples. In moving from 6 samples to 20 samples, the A-basis allowable increases by 26%. In increasing from 20 to 80 samples, the A-basis allowable only increases by 3%. Although it is unlikely that a test program would actually include 80 samples for a given test, or even 20, the numbers were chosen to illustrate that the analysis tool can be used to identify the point of diminishing returns as the number of tested samples increases. This information can help weigh the benefit of additional statistical characterization against the cost of additional testing.

Table 4-2. Summary of A- and B-Basis strength allowables for an example virtual test program.

No. of Samples	A-Basis Strength Allowable (ksi)	B-Basis Strength Allowable (ksi)
6	65.4	79.4
20	82.4	89.1
80	85.1	90.5

The results in the table above are presented graphically below in Figure 4-5, which shows the charts generated by the analysis tool.

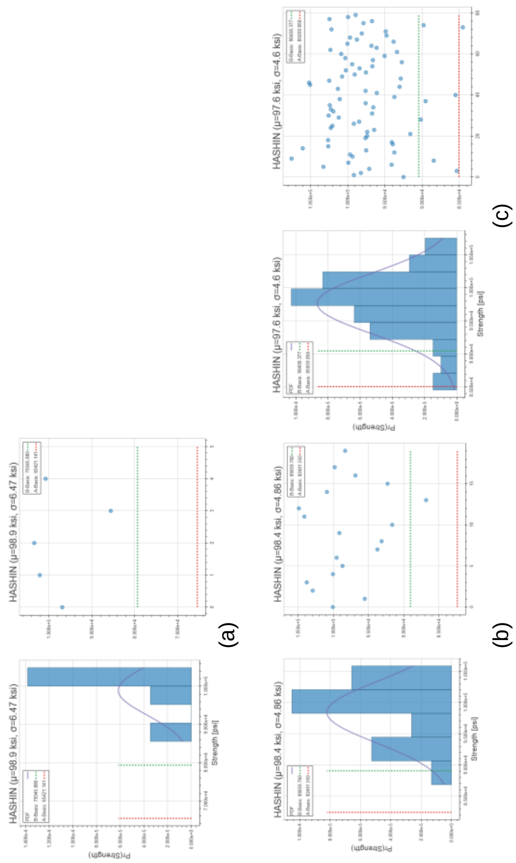


Figure 4-5. Stochastic simulation results for three different scenarios: (a) 6 samples, (b) 20 samples, and (c) 80 samples, showing histograms and scatter plots of coupon strength. Dotted lines represent A-basis (red) and B-basis (green) allowables.

5. Conclusion

A unified set of analysis tools have been packaged into COMPAS, an Abaqus/CAE plugin. that the tools seek to address some of the challenges of developing and implementing new material systems. COMPAS enables preliminary finite element and sensitivity analysis to guide the development of a more cost-effective material test program. Also, the study of material variance and its impact on strength allowables is improved with correlated models that are able to capture damage, progression, and failure with high fidelity.

There are still challenges associated with the development and implementation of the COMPAS framework. One of them is managing the different Python versions required for the Abaqus API and for the packages used. Integrating the broad array of technologies into a single framework has also been challenging and the best way of doing it is still not clear. Another challenge many researchers have faced when modeling progressive damage with composites is the sensitivity of damage evolution to certain parameters, such as fracture energy release rate. Our approach was to find these parameters through optimization, but more research into this topic is recommended.

COMPAS combines the advanced modeling techniques available in Abaqus with external Python algorithms for statistical analysis and property prediction to help overcome some of the challenges related to introducing new materials into the market. COMPAS contributes in three domains: the prediction of unknown properties for preliminary analysis, the determination of high-sensitivity properties for test reduction, and the stochastic simulation of correlated models for strength allowables estimation. Use of the framework's tools can deliver significant savings in time and money and lead to smarter decisions in working with novel composite materials.

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